DEPENDENCE OF THE BARIC COEFFICIENT OF A QUANTUM POINT ON ITS DIMENSIONS

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In the framework of the deformation potential model, the baric coefficient of a quantum point (QP) of spherical symmetry has been calculated as a function of the QP dimensions and the energy of the transition into the ground state. The baric coefficient of the material of the InAs QP with a radius of about 40 Åhas been determined to be smaller than that of the bulk InAs by 19%.

1. Introduction

Today, semiconductor nanoheterostructures are among the key objects of experimental [1, 2] and theoretical [3, 4] physical researches. The studies of physical processes in zero-dimensional heterostructures occupy a particular position, because the unique fundamental properties which are not inherent to massive crystals can be observed in such systems. Nanostructures were successfully used in opto- and microelectronics during last years. Thus, the interest to semiconductor nanoheterostructures is connected not only with the opportunity to study new fundamental physical phenomena, but also with wide perspectives of their practical application.

Modern technological methods allow the perfect ordered arrays of QPs of complex forms to be grown. However, the further progress in the physics of quantum zero-dimensional nanostructures is connected not only with the improvement of a fabrication technology, but also with the perfection of analytical models of heterosystems with QPs. Nowadays, the theory is being developed intensively, because a lot of problems which demand the adequate understanding of physical processes in nanosystems with QPs remain unsolved.

One of the problems lies in the fact that the basic physical characteristics of nanoobjects (the baric coefficient, Young's modulus, Poisson's ratio, and effective masses of current carriers) are accepted in the majority of theoretical models to coincide with the corresponding characteristics obtained from macroscopical experiments. However, if the described structures contain a few nuclear layers, the physical characteristics of nanostructures appreciably differ from the corresponding characteristics of bulk crystals [5]. In particular, a discrepancy between the values of the baric coefficient of the InAs QPs in an InAs/GaAs heterostructure and in a bulk InAs crystal is observed. The results of experimental researches, dealing with the dependence of the energy shift of the InAs-QP luminescence lines on hydrostatic pressure at various energies of the transition into the ground state (1.13, 1.15, 1.8, 1.96, 1.28, and 1.40 eV) and the dependence of the QP baric coefficient on the energy of the transition into the ground state, show that the value of the InAs-QP baric coefficient differs from that of the bulk InAs crystal ($K_\infty = 12$ meV/kbar) by about 30—40%.

The aim of this article is therefore to calculate the dependence of the QP baric coefficient on its dimensions in the framework of the deformation potential model.

2. Model of the InAs/GaAs Heterosystem with Coherently Stressed InAs QPs of Spherical Symmetry

An InAs/GaAs heterosystem with coherently stressed InAs QPs of spherical symmetry is examined. The

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model of this heterosystem constructed with regard for deformation effects is displayed in Fig. 1. In order to reduce the problem with a plenty of QPs to a problem with a single QP, we replace the elastic interaction energy of QP pairs by the interaction energies of each QP with the averaged field of elastic deformation $\sigma\,(N-1)$ of all other QPs.

The formation of QPs in the InAs/GaAs system according to the method of molecular-beam epitaxy is carried out in two stages. At the first stage, the growth of the pseudomorphic stressed InAs layer takes place. When this layer will reach the critical thickness (1.5—1.7 times the monolayer thickness), the second stage, which comprises a spontaneous decomposition of the pseudomorphic layer into both a set of crystal islets, i.e. QPs, and a wetting InAs layer of about one monolayer in thickness, begins. Such a decomposition is caused by the relaxation of elastic stresses which arise in the heteroepitaxial system due to a mismatch of lattice constants, the different factors of thermal expansion in the GaAs substrate and InAs epitaxial layer, and the gain in the free energy of the system.

Since the lattice constant of InAs ($a^{(1)} = 6.08$ Å) exceeds that of the GaAs matrix ($a^{(2)} = 5.65$ Å), InAs and GaAs undergo, respectively, squeezing and stretching upon the heteroepitaxial buildup of InAs onto a GaAs layer within the scope of the pseudomorphic growth.

A spherical QP of radius R_0 can be therefore represented (see Fig. 1) as an elastic dilatational spherical microinclusion (the dash-dotted line) inserted into a spherical cavity, which exists in the GaAs matrix (the dashed line) and whose volume is smaller by ΔV than the volume of the microinclusion.

For such a spherical microinclusion to find room in the cavity, it must be squeezed, whereas the GaAs matrix should be stretched in radial directions. The result of simultaneous actions of those deformations is shown in Fig. 1 by a solid line.

3. Potential Energies of Electrons and Holes in the InAs/GaAs Heterosystem with InAs QPs

The electronic structure of a QP, due to the dimensional quantization, consists of a set of discrete levels and is similar, in this sense, to that of an individual atom. The depth and the character of a quantizing potential are determined by the profiles of the bottom of the conduction band and the top of the valence band of the heterostructure. These profiles are regarded as a

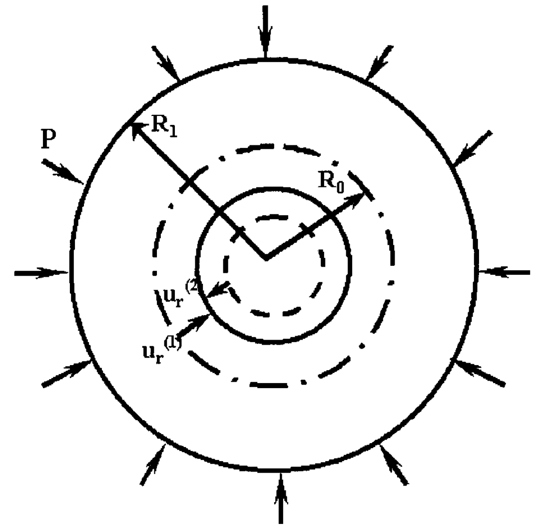

Fig. 1. Spherical model of a quantum point

potential energy which defines the energy spectrum and the electron (hole) quantum states.

In the case of coherently stressed QPs under the presence of the fields of elastic non-uniform stresses in their vicinity, the depth and the form of the quantizing potential are determined not only by the energy gap difference between the QP and matrix substances, but also by the character of a non-uniform deformation of the matrix and a QP. In particular, the mismatch of the lattice constants in the InAs/GaAs heterosystem [plane (001)] and the InAs QP constitutes $f = 7\%$. Since the difference between the lattice constants in InAs and GaAs is big, the stresses that arise in the heterosystem containing QPs essentially affect the structure of the allowed energy bands and the gap between them. Thus, the energy shifts of the conduction and valence bands under an action of elastic deformations are, respectively,

$$\Delta E_c^{(i)}\left(\varepsilon^{(i)}\right) = a_c^{(i)}\varepsilon^{(i)}, \quad \Delta E_v^{(i)}\left(\varepsilon^{(i)}\right) = a_v^{(i)}\varepsilon^{(i)}, \tag{1}$$

where $\varepsilon^{(i)} = \mathrm{Tr}\,\hat{\varepsilon}^{(i)}$ is the sum of diagonal elements of the strain tensor; $a_c^{(i)}$ and $a_v^{(i)}$ are the constants of the hydrostatic deformation potential of the conduction and valence bands, respectively, and the subscript i equals hereafter 1 for InAs and 2 for GaAs.

To find the components of the strain tensor, it is necessary to determine explicitly the expressions for atom displacements $u_r^{(1)}$ and $u_r^{(2)}$ in InAs and GaAs, respectively. For this purpose, let us write down the balance equation [6]

$$\vec{\nabla}\operatorname{div}\vec{u} = 0 \tag{2}$$

with the following boundary conditions for a spherical QP:

$$\left\{\begin{array}{l} 4\pi R_0^2 \left(u_r^{(2)}\Big|_{r=R_0} - u_r^{(1)}\Big|_{r=R_0} \right) = \Delta V, \\ \Delta V = 4\pi R_0^3 f; \\ \sigma_{rr}^{(1)}\Big|_{r=R_0} = \sigma_{rr}^{(2)}\Big|_{r=R_0} + P_{\mathrm{L}}, \\ P_{\mathrm{L}} = \frac{2\alpha}{R_0}; \\ \sigma_{rr}^{(2)}\Big|_{r=R_1} = -P - \sigma_{\mathrm{eff}} (N-1), \\ P \gg \sigma_{\mathrm{eff}} (N-1), \end{array}\right. \tag{3}$$

where R_0 is the radius of the InAs QP, $R_1 - R_0$ is equal to the thickness of the GaAs-matrix plate, P is the uniform pressure, P_{L} is the Laplace pressure, and α is the surface energy of the InAs QP [7].

The parameter f is represented by the sum

$$f = f_1 + f_2. \tag{4}$$

Here, $f_1 = \left(\alpha_T^{(2)} - \alpha_T^{(1)}\right)(T_k - T_0)$ is the parameter of the deformation mismatch induced by the different thermal coefficients of the QP and the matrix ($\alpha_T^{(1)} = 4.52 \times 10^{-6}$ K^{-1} and $\alpha_T^{(2)} = 5.73 \times 10^{-6}$ K^{-1}, respectively), and $f_2 = \left(a^{(1)} - a^{(2)}\right)/a^{(1)} \approx 7\%$ is the mismatch parameter of the QP and matrix lattice constants, $a^{(1)}$ and $a^{(2)}$, respectively. The quantity ΔV in the first equation of system (3) is equal to the geometrical difference of the microinclusion volume and that of the cavity in the GaAs matrix, represented in Fig. 1.

As a result of symmetry, the displacement field which is defined by a solution of Eq. (2), contains only the radial component both inside the QP,

$$u_r^{(1)} = C_1 r + \frac{C_2}{r^2}, \quad 0 \le r \le R_0, \tag{5}$$

and beyond it, i.e. in the GaAs matrix,

$$u_r^{(2)} = C_3 r + \frac{C_4}{r^2}, \quad R_0 \le r \le R_1. \tag{6}$$

Since the solution must be finite at $r = 0$, we have to put $C_2 = 0$ in formula (5).

The displacement field determines the following components of the strain tensor:

$$\varepsilon_{rr}^{(1)} = C_1, \tag{7}$$

$$\varepsilon_{rr}^{(2)} = C_3 - \frac{2C_4}{r^3}, \tag{8}$$

$$\varepsilon_{\varphi\varphi}^{(1)} = \varepsilon_{\Theta\Theta}^{(1)} = C_1, \tag{9}$$

$$\varepsilon_{\varphi\varphi}^{(2)} = \varepsilon_{\Theta\Theta}^{(2)} = C_3 + \frac{C_4}{r^3}. \tag{10}$$

Mechanical stresses in InAs and GaAs are

$$\sigma_{rr}^{(1)} = \frac{E_1}{(1+\nu_1)(1-2\nu_1)} \times \left[(1+\nu_1)\,\varepsilon_{rr}^{(1)} + \nu_1 \left(\varepsilon_{\varphi\varphi}^{(1)} + \varepsilon_{zz}^{(1)}\right)\right], \tag{11}$$

and

$$\sigma_{rr}^{(2)} = \frac{E_2}{(1+\nu_2)(1-2\nu_2)} \times \left[(1+\nu_2)\,\varepsilon_{rr}^{(2)} + \nu_2 \left(\varepsilon_{\varphi\varphi}^{(2)} + \varepsilon_{zz}^{(2)}\right)\right], \tag{12}$$

respectively, where $\nu_{1,2}$ and $\mathrm{E}_{1,2}$ are Poisson's ratios and Young's moduli, respectively, in the QP and the surrounding matrix. They are expressed in a certain way [8] through the elastic constants C_{11} and C_{12} of those materials.

The coefficients C_1, C_3, and C_4 are obtained by solving system (3) and taking into account Eqs. (5)–(12).

Thus, knowing the components of the strain tensor which depend on the QP radius R_0, the QP form, and the uniform pressure P, it is possible to find the potential energy of electrons and holes in a stressed heterostructure with QPs

$$U_e = \left\{\begin{array}{l} -\left(|\Delta V_c(0)| - |a_c^{(1)}\varepsilon^{(1)}| - |a_c^{(2)}\varepsilon^{(2)}|\right), \\ \quad 0 \le r \le R_0, \\ 0, \quad R_0 \le r \le R_1; \end{array}\right. \tag{13}$$

$$U_h = \left\{\begin{array}{l} -\left(|\Delta V_h(0)| - |a_v^{(1)}\varepsilon^{(1)}| - |a_v^{(2)}\varepsilon^{(2)}|\right), \\ \quad 0 \le r \le R_0, \\ 0, \quad R_0 \le r \le R_1. \end{array}\right. \tag{14}$$

Here, $\Delta V_c(0)$ and $\Delta V_h(0)$ are the depths of the potential wells of holes and electrons, respectively, in the QP in a nondeformed heterostructure.

The geometry of the InAs/GaAs heterosystem with InAs QPs and the dependences of the potential energies of electrons and holes on the radius r without (short-dashed curves) and with regard (solid curves) for the effect of uniform deformation are schematically shown in Fig. 2. The dotted lines mark the energy levels $E_{e,h}^{(1)}$ of electrons and holes in the ground state in the potential wells U_e and U_h, respectively.

The energy of the transition into the ground state is determined as follows:

$$E_0^{(1)} = E_e^{(1)} + E_h^{(1)} + E_g^{(1)}, \tag{15}$$

where $E_g^{(1)}$ is the energy gap in the InAs QP.

4. Calculation of the Baric Coefficient of InAs QPs in the InAs/GaAs Heterosystem Depending on Their Dimensions

The baric coefficient of InAs QPs in the InAs/GaAs heterosystem is determined by the sum of three components, namely, two components caused by the shifts of the electron and hole levels under the action of hydrostatic pressure and the baric coefficient of the energy gap width:

$$K = \frac{\partial E_0^{(1)}}{\partial P} = \frac{\partial E_e^{(1)}}{\partial P} + \frac{\partial E_h^{(1)}}{\partial P} + \frac{\partial E_g^{(1)}}{\partial P} =$$

$$= \frac{\partial \varepsilon^{(1)}}{\partial P} \frac{1}{\frac{\partial \varepsilon^{(1)}}{\partial R_0}} \left[\frac{\partial E_e^{(1)}}{\partial R_0} + \frac{\partial E_h^{(1)}}{\partial R_0} + \frac{\partial E_g^{(1)}}{\partial R_0} \right]. \quad (16)$$

To find the baric coefficient K of InAs QPs, the electron and hole energy spectra in the InAs/GaAs heterosystem with InAs QPs are to be obtained first. (Since the calculations of the electron and hole energy spectra will be carried out in the effective mass approximation, a physical condition must be satisfied that the geometrical dimensions of the QPs and the distance between two neighboring QPs should considerably exceed the lattice constants of the QP crystals and the matrix, i.e. $R_0 \gg a^{(1)}, a^{(2)}$ for a spherical QP.) For this purpose, the Schrödinger equations

$$H_{e,h} \Psi_{e,h} (\vec{r}) = E_{e,h} \Psi_{e,h} (\vec{r}) \quad (17)$$

with the Hamiltonians

$$H_{e,h} = -\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{m_{e,h}^* (\vec{r})} \vec{\nabla} + U_{e,h} (r, R_0, P) . \quad (18)$$

are to be solved. The electron ($m_{1,2_e}^*$) and hole ($m_{1,2_h}^*$) effective masses in a QP and the surrounding matrix are supposed to be known and equal to those in corresponding bulk crystals.

A solution of the Schrödinger equation (17) in a spherical coordinate system is sought in the form

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

Here, $Y_{lm}(\Theta, \varphi)$ is the spherical harmonics. The radial functions $R_{nl}(r)$ are expressed through the spherical Bessel functions as follows:

$$R_{1_{nl}} (r) = A j_l (k_{e,h} r) + B n_l (k_{e,h} r) , \quad 0 \le r \le R_0, \quad (20)$$

$$R_{2_{nl}} (r) = C h_l^{(1)} (i \chi_{e,h} r) + D h_l^{(2)} (i \chi_{e,h} r) ,$$

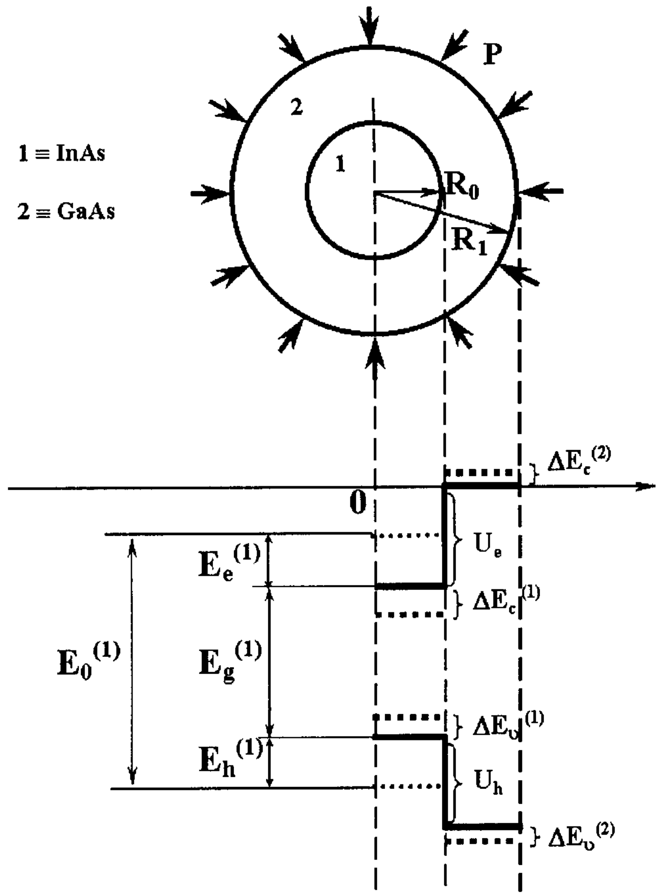

Fig. 2. Dependences of the electron and hole potential energies on the radius r in a InAs/GaAs heterosystem with InAs QPs

$$R_0 \le r \le R_1 \quad (21)$$

where

$$k_{e,h}^2 = \frac{2 m_{1e,h}^*}{\hbar^2} \left(|U_{e,h}| - |E_{nl}^{e,h}| \right) , \quad (22)$$

and

$$\chi_{e,h}^2 = \frac{2 m_{2e,h}^*}{\hbar^2} |E_{nl}^{e,h}| , \quad (23)$$

and the potential energies $U_{e,h}$ of electrons and holes are determined by formulae (13) and (14).

The continuity conditions for the wave functions and the probability flow density at the QP—matrix interface,

$$\begin{cases} R_1 (r)_{|r=R_0} = R_2 (r)_{|r=R_0} , \\ \frac{1}{m_{1e,h}^*} \frac{d R_1 (r)}{dr}_{|r=R_0} = \frac{1}{m_{2e,h}^*} \frac{d R_2 (r)}{dr}_{|r=R_0} , \end{cases} \quad (24)$$

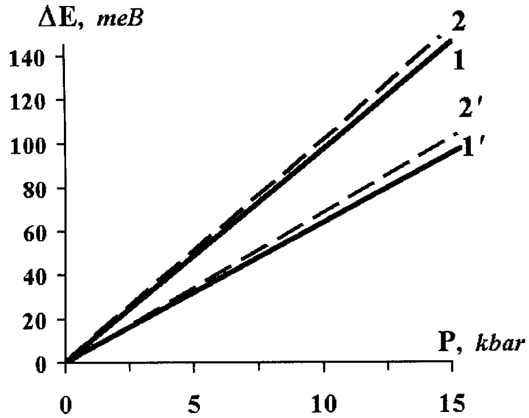

Fig. 3. Dependences of the energy shift of the InAs-QP luminescence lines on hydrostatic pressure at various energies of the transition into the ground state ($R_1 = 500$ Å): $E = 1.13$ eV at $R_0 = 42$ Å(*1* and *1′*) and $E = 1.15$ eV at $R_0 = 39$ Å(*2* and *2′*); theory (*1* and *2*), experiment (*1′* and *2′*)

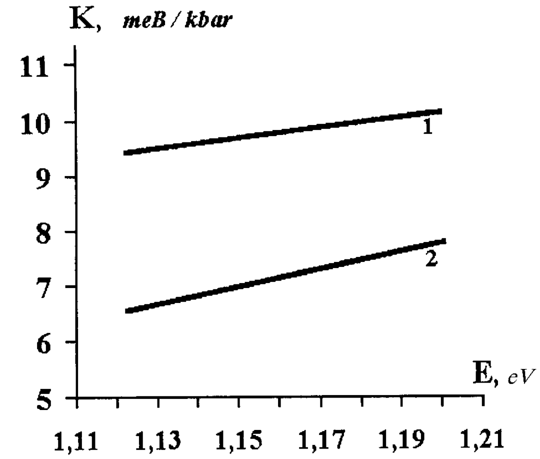

Fig. 4. Dependences of the QP baric coefficient on the energy of the transition into the ground state: theory (*1*), experiment (*2*)

the regularity conditions for the functions $R_{nl}(r)$ at $r \to 0$ and $r \to R_1$, and the normalization define the spectrum E_{nl} and the wave functions of electrons and holes in the InAs/GaAs heterosystem with InAs QPs.

The energies of the ground states of an electron and a hole in the QP are therefore the roots of the following transcendental equation:

$$\frac{m^*_{2e,h}}{m^*_{1e,h}}[1 - k_{e,h}R_0 \mathrm{ctg}\,(k_{e,h}R_0)] =$$

$$= \frac{1 + \chi_{e,h}R_0 + e^{2\chi_{e,h}(R_0-R_1)} \cdot (\chi_{e,h}R_0 - 1)}{1 - e^{2\chi_{e,h}(R_0-R_1)}},$$

$$n = 1, 3, 5, \ldots \tag{25}$$

From (25) and making use of (16), one can calculate the dependence of the QP baric coefficient on its dimensions, taking into account that

$$\frac{\partial E_e}{\partial R_0} = -\left(\frac{\partial f}{\partial R_0}\right) / \left(\frac{\partial f}{\partial E_e}\right),$$

$$\frac{\partial E_h}{\partial R_0} = -\left(\frac{\partial \varphi}{\partial R_0}\right) / \left(\frac{\partial \varphi}{\partial E_h}\right),$$

where

$$f = k_e \mathrm{tg}\left(k_e R_0 - n\frac{\pi}{2}\right) -$$

$$-\frac{\chi_e(m^*_{1_e}/m^*_{2_e})\left(1 + e^{2\chi_e(R_0-R_1)}\right)}{1 - e^{2\chi_e(R_0-R_1)}}$$

and

$$\varphi = k_h \mathrm{tg}\left(k_h R_0 - n\frac{\pi}{2}\right) -$$

$$-\frac{\chi_h(m^*_{1_h})/(m^*_{2_h})\left(1 + e^{2\chi_h(R_0-R_1)}\right)}{1 - e^{2\chi_h(R_0-R_1)}}.$$

5. Numerical Calculations and Discussion of Results

Numerical calculations of the QP baric coefficient as a function of its dimensions were carried out for the InAs/GaAs heterosystem with InAs QPs, which is widely used by experimenters. Its parameters are presented in the table.

With the help of the formulae given in the previous section, the energy shift of the QP-luminescence lines of the examined stressed heterosystem with QPs was calculated. The results of calculations are shown in Fig. 3. As is seen from it, the increase of the hydrostatic pressure in the interval 0—15 kbar results in the growth of the shift concerned. This result is clear, because the increase of the external pressure stimulates the enhancement of optical transitions in the QPs.

The increase of QP dimensions does not change qualitatively the character of the obtained dependence, but reduces the shift of the InAs-QP-luminescence lines. In particular, the increase of the QP radius R_0 from

Parameters of InAs and GaAs crystals [7—9]

Crystal	a, Å	C_{11}, Mbar	C_{12}, Mbar	a_c, eV	a_v, eV	E_g, eV	$\frac{m_e^*}{m_0}$	$\frac{m_h^*}{m_0}$	α, N/m
InAs	6.08	0.833	0.453	–5.08	1	0.36	0.057	0.41	0.657
GaAs	5.65	1.223	0.571	–7.17	1.16	1.452	0.065	0.45	

39 to 42 Åunder the action of the external hydrostatic pressure $P = 5$ kbar results in a reduction of the shift by about 1 meV. As is seen from Fig. 3, the obtained theoretical results agree well with experimental ones.

The InAs-QP baric coefficient in the stressed InAs/GaAs heterosystem with InAs QPs was calculated in the framework of the above-described model with the help of the dependences displayed in Fig. 3 and formula (16). The value of the baric coefficient for the spherical QP of the radius $R_0 = 45$ Åequals 9.45 meV/kbar provided the plate thickness of the surrounding matrix $R_1 = 500$ Å. This means that the value of the InAs-QP baric coefficient is smaller than that of the bulk InAs crystal by 21%.

The value of the QP baric coefficient is sensitive to variations in the geometrical parameters of heterosystems including QPs. In Figs. 4 and 5, the dependences of the InAs-QP baric coefficient on the energy of the transition into the ground state and on the QP dimensions are presented. As is seen, an increase of the energy of the transition into the ground state results in a linear growth of the baric coefficient K. Such a behavior of the baric coefficient can be explained by different characters of variations of its components: the components caused by the shifts of the electron and hole levels under the action of hydrostatic pressure decrease, when the QP radius enlarges, more quickly than the baric coefficient of the energy gap width grows. The increase of the QP radius stimulates the opposite effect (Fig. 5): the baric coefficient diminishes. This is connected to the fact that the increase of the QP radius results in a deepening of the electron and hole potential wells in the QPs, which lowers their energy levels. Accordingly, the energy gap of the QP material undergoes the reduction as well. This means that the increase of the QP dimensions narrows its optical gap.

After the quantitative analysis of the results obtained, it should be noted that, as the energy of the transition into the ground state decreases from 1.15 to 1.13 eV, which corresponds to an increase of the QP radius R_0 by 3 Å, the baric coefficient accordingly diminishes by 0.1 meV/kbar.

As is seen from Fig. 4, the results of experimental researches qualitatively coincide with theoretical ones. Some discrepancy between the values of the QP baric coefficient obtained theoretically and experimentally can be explained by the fact that QPs were investigated theoretically only as spheres. In practice, QPs possess different dimensions and are of different forms, i.e. there is a dispersion of dimensions and forms among them.

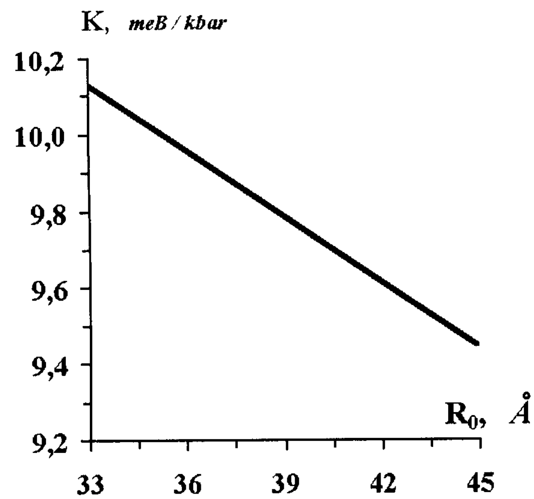

Fig. 5. Dependence of the QP baric coefficient on the QP radius

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БАРИЧНИЙ КОЕФІЦІЄНТ КВАНТОВОЇ ТОЧКИ В ЗАЛЕЖНОСТІ ВІД ЇЇ РОЗМІРІВ

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Р е з ю м е

В рамках моделі деформаційного потенціалу розраховано баричний коефіцієнт квантової точки (КТ) сферичної симетрії в залежності від її розмірів та енергії переходу в основний стан. Встановлено, що значення баричного коефіцієнта матеріалу КТ InAs (радіусом близько 40 Å) є меншим за значення баричного коефіцієнта об'ємного матеріалу InAs на 19%.