# ФІЗИЧНІ, ХІМІЧНІ ТА ІНШІ ЯВИЩА, НА ОСНОВІ ЯКИХ МОЖУТЬ БУТИ СТВОРЕНІ СЕНСОРИ

# PHYSICAL, CHEMICAL AND OTHER PHENOMENA, AS THE BASES OF SENSORS

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## INFLUENCE OF THE QUANTUM DOT MATERIAL DEFORMATION ON TAMM SURFACE LEVELS

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## INFLUENCE OF THE QUANTUM DOT MATERIAL DEFORMATION ON TAMM SURFACE LEVELS

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**Abstract.** Influence of the quantum dot material deformation on Tamm surface levels in the strained InAs/GaAs nanosystem has been studied. The research has been provided in the framework of deformation potential. The dependence of the Tamm surface energy on the quantum dot size in the strained InAs/GaAs nanosystems has been obtained.

**Keywords:** electron-deformation interaction, quantum dot, surface states, strained nanoheterosystem.

## ВПЛИВ ДЕФОРМАЦІЇ МАТЕРІАЛУ КВАНТОВОЇ ТОЧКИ НА ПОВЕРХНЕВІ РІВНІ ТАММА

*Р. М. Пелещак, Р. Я. Лешко, Д. С. Карпин*

**Анотація.** Досліджено вплив деформації матеріалу квантової точки на поверхневі рівні Тамма у напруженій наногетеросистемі InAs/GaAs. Дослідження проведено у рамках деформаційного потенціалу. Отримано залежність енергії поверхневих рівнів Тамма від розмірів квантової точки у напруженій гетеросистемі InAs/GaAs.

**Ключові слова:** електрон-деформаційна взаємодія, квантова точка, поверхневі стани, напружена наногетеросистема.

## ВЛИЯНИЕ ДЕФОРМАЦИИ МАТЕРИАЛА КВАНТОВОЙ ТОЧКИ НА ПОВЕРХНОСТНЫЕ УРОВНИ ТАММА

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**Аннотация.** Исследовано влияние деформации материала квантовой точки на поверхностные уровни Тамма в напряженной наногетеросистеме InAs/GaAs. Исследование проведено в рамках деформационного потенциала. Получена зависимость энергии поверхностных уровней Тамма от размеров квантовой точки в напряженной гетеросистеме InAs/GaAs.

**Ключевые слова:** электрон-деформационная взаимодействие, квантовая точка, поверхностные состояния, напряженная наногетеросистемах.

### I. INTRODUCTION

Modern technologies for the fabrication of quasi-dimensional systems (for example, the Stransky-Krastanov method) make it possible to obtain stressed QDs on a substrate of a given semiconductor [1]. The reason of appearance of strained QDs is the InAs/GaAs heterosystem is the mismatch of the constant lattices of these materials.

The theory, which describing the effect of deformation on the spectra of quasiparticles in stressed QDs is well developed for today [2–5]. In these works, the equation of elasticity is solved taking into account the Laplace pressure, external pressure, growth temperature, mismatch of lattice parameter, presence of impurity and self-consistent elastic interaction between QDs. It has been shown that, due to these effects, the depth of the potential well for quasiparticles (electrons and holes) decreases, so their energy decreases. This leads to change the effective band gap (optical gap), which influence on absorption and luminescence spectra.

Experimental works (devoted to the photoluminescence) shows that in addition to the main sharp peaks (caused by excitons), a longwave wide peak [6–8] is observed, which is associated with impurity and surface states. Theoretical work [9] clearly shows that the contribution to this longwave luminescence "tail" is given by impurity acceptor states. However, the full explanation of this dependence is not exhaustive. The reasons for the existence of a "tail" of luminescence, which consist in the presence of surface states, are assumed. Therefore, it is logical to determine the influence of the surface. It can be the next step of constructing a clear and consistent theory of QD surface states.

As shown in [10, 11], there is a specific type of surface states, which are caused by the presence of a polarization trap near the QD surface. Moreover, the trap depth is determined by the difference in the dielectric constant of the materials of the QD and the matrix. In addition to these types of surface states, there are also other surface states, in particular Tamm surface states [12], which are modified due to the confinement potential. These states also are changed due to the electron-deformation interaction, which is essential in strained heterosystems with QDs [5]. That is why the aim of this work is to determine the effect of electron-deformation interaction on the formation of Tamm surface states in nanosystems as the next step in the construction of the theory of surface states in nanoheterosystems with QDs

### II. THE NANOSYSTEM ENERGY TAKING INTO ACCOUNT ELASTIC DEFORMATIONS

Let us to consider an InAs/GaAs heterosystem with a coherently stressed spherical QDs InAs with the radius $a \geq a_0$ , where $a_0$ is the lattice constant of the QD material. The following approxi-

mations have been used to reduce the problem with a large number of QDs to a single QD task: the energy of pair-wise elastic interaction between QDs is replaced by the energy of interaction of every QD with the average field of elastic deformation of all other QDs $\sigma_{eff}(N-1)$ (self-consistent elastic interaction between QDs) [3–5]. Due to the mismatch of the lattices constant of the QD and the matrix, the QD can be considered as a dilation nanoinclusion in the GaAs matrix (the cavity volume is less than the inclusion volume on). The electrons are confined in a spherical rectangular well.

$$U_{conf}(r)=\begin{cases}0, & r\le a,\\ U_{conf} & r>a.\end{cases} \qquad (2.1)$$

We denote the change in the depth of the potential well for the electron (electron-deformation potential) due to deformations by

$$U_d(r)=\begin{cases}0, & r\le a,\\ -\left|D^{(1)}\varepsilon^{(1)}\right|-\left|D^{(2)}\varepsilon^{(2)}\right| & r>a,\end{cases} \qquad (2.2)$$

where $\varepsilon^{(i)}=\mathrm{Sp}\boldsymbol{\varepsilon}^{(i)}$, $\boldsymbol{\varepsilon}^{(i)}$ is deformation tensor in i-th environment, $D^{(i)}$ is hydrostatic deformation potential constants, $i=\begin{Bmatrix}1\equiv InAs\\ 2\equiv GaAs\end{Bmatrix}$.

Accordingly, the total potential energy of the electron has form

$$U(r)=U_{conf}(r)+U_d(r)=$$

$$=\begin{cases}0, & r\le R_0,\\ U_{conf}-\left(\left|D^{(1)}\varepsilon^{(1)}\right|+\left|D^{(2)}\varepsilon^{(2)}\right|\right) & r>R_0,\end{cases}=$$

$$=\begin{cases}0, & r\le a,\\ U_0 & r>a.\end{cases} \qquad (2.3)$$

For finding $\varepsilon^{(i)}=\mathrm{Sp}\boldsymbol{\varepsilon}^{(i)}$, the displacement of atoms were calculated, as in [3–5], and the corresponding boundary conditions were applied, taking into account the Laplace pressure and the mean field of elastic deformations. Schrodinger equation for electron with Hamiltonian which account $U_d(r)$

$$\hat{\mathbf{H}}_e=-\frac{\hbar^2}{2}\nabla\frac{1}{m_e}\nabla+U(r) \qquad (2.4)$$

has been solved exactly, where

$$m_e=\begin{cases}m_e^{(1)}, & r\le a,\\ m_e^{(2)}, & r>a\end{cases}$$

is the electron effective mass in each medium. Solutions for states where $E<U_0$, due to the spherical symmetry of the problem, is given by the product of an angular component (spherical harmonics) and a radial component, which is expressed by a Bessel first-order spherical function and a modified spherical Bessel function of the second kind:

$$\psi_e(r,\theta,\varphi)=\chi_e(r)Y_{l,m}(\theta,\varphi),$$

$$\chi_e(r)=\begin{cases}A_e^{(1)}\,\mathrm{j}(kr), & r\le a,\\ A_e^{(2)}\,\mathrm{k}(\eta r), & r>a,\end{cases} \qquad (2.5)$$

where $k=\sqrt{2m_e^{(1)}E/\hbar^2}$, $\eta=\sqrt{2m_e^{(2)}(U_0-E)/\hbar^2}$. With using the Ben-Daniel-Duke standard boundaries conditions and normalize conditions, the system energy and unknown coefficients has been determined.

After calculating, the energy of the ground $E_{1s}$ state and first excited state $E_{1p}$ have been determined, with and without electron-deformation interaction. The parameters of crystals and constants have been used as in [5]. The results of the calculations are presented in figure 1.

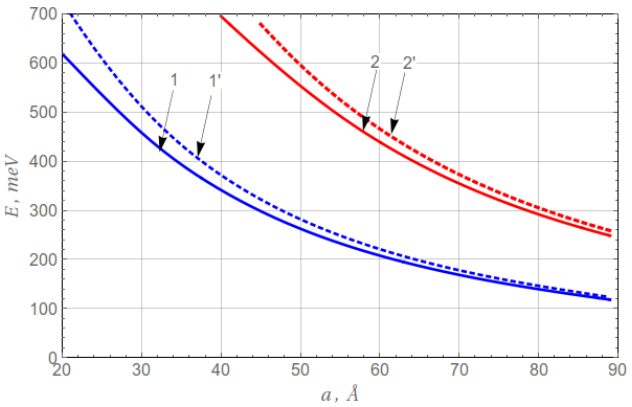


**Fig. 1. The energy of the ground (curves 1, 1') and first excited (curves 2, 2') states of the electron, taking into account the electron-deformation interaction (curves 1, 2) and without it (curves 1', 2'), as a function of the QD radius**

The figure 1 shows that taking into account the electron-deformation interaction leads to a decrease in the energy of the ground and excited states due to the reduction of the effective depth of the potential well due to deformation effects. Accordingly, the transition energy between these states will vary depending on the electron-deformation interaction (see figure 2).

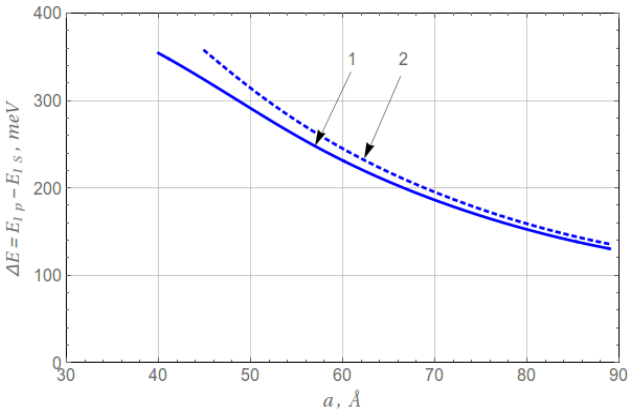


**Fig. 2. The transition energy with deformation effects (curve 1) and without deformation effects curve (2) as a function of the QD radius**

As can be seen from the figures 1, 2 , taking into account the deformation effects leads to a decrease in the transition energy compared to the case of their neglect. The results obtained will be used in the determination of surface Tamm states.

## III. SURFACE TAMM STATES IN THE STRAINED QD

We has been build the QD model ( $a \geq 5a_0$ ) as a crystal whose atoms are spaced apart at distance $a_0$. In the region near the atom, we suppose that there is a potential barrier for the electron with height $U_1$ and with width b (figure 3). On the surface, the QD is bounded by a matrix that separates the QD by the barrier $U_0$ (see (2.3)).

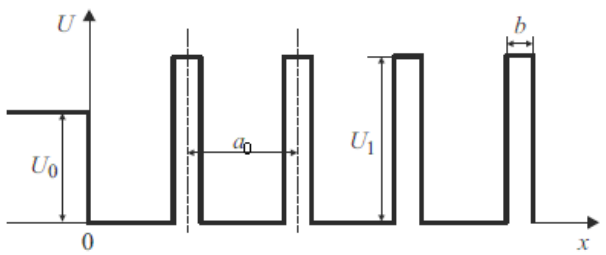


**Fig. 3. The crystal energy and surface within the Tamm-Kronig-Penney model**

The described model is well known as the Tamm-Kronig-Penney model. According to the basic Tamm model [13], the equation for determining surface energy has the form:

$$\xi \operatorname{ctg} \xi = \frac{q^2}{2p^2} - q\sqrt{1 - \frac{\xi^2}{q^2}}, \qquad (3.1)$$

where

$$\xi = a_0\sqrt{\frac{2m_0}{\hbar^2}E}, \quad q = a_0\sqrt{\frac{2m_0}{\hbar^2}U_0}, \quad p = a_0 b\frac{m_0 U_1}{\hbar^2},$$

$m_0$ is free-electron mass, $a_0$ is lattice constant.

According to the Kronig-Penny model, the system of equations for determining the allowed values of energies (in the notation [14]) has the form

$$\begin{cases} \left|\cos\left(ka_0 - \operatorname{arctg}\left(\dfrac{\Omega a_0}{ka_0}\right)\right)\right| \leq \dfrac{1}{\sqrt{1+\left(\dfrac{\Omega a_0}{ka_0}\right)^2}}, \\ E = \dfrac{\hbar^2}{2m_0 a_0^2}(ka_0)^2, \end{cases} \qquad (3.2)$$

where $\Omega a_0$ characterizes the dimensionless permeability of barriers. In the case of small energies $(\Omega a_0)/ka_0 \gg 1$ the (3.2) is reduced to

$$\begin{cases} \left|\sin(ka_0)\right| \leq \left(\dfrac{ka_0}{\Omega a_0}\right), \\ E = \dfrac{\hbar^2}{2m_0 a_0^2}(ka_0)^2. \end{cases} \qquad (3.3)$$

Let us to consider further that the energy is small and expand it into a series, and limit to the first two nonzero additives. We got

$$\begin{cases} \left|ka_0 - \dfrac{(ka_0)^3}{6}\right| \leq \left(\dfrac{ka_0}{\Omega a_0}\right), \\ E = \dfrac{\hbar^2}{2m_0 a_0^2}(ka_0)^2. \end{cases} \qquad (3.4)$$

Substitute the first two solution for the product $ka_0$ into the second expression (3.4) and find two energy values as functions of the barrier permeability $\Omega a_0$

$$E_1 = 0, \quad E_2 = \frac{\hbar^2}{2m_0 a_0^2} 6\left(1 - \frac{1}{\Omega a}\right)^2. \qquad (3.5)$$

The width of the first forbidden zone (first band gap) in the Kronig-Penney model is

$$E_{K-P}^{gap} = E_2 - E_1. \qquad (3.6)$$

Let us reconcile the Kronig-Penney and Tama models with the condition $\Omega a = p$ [13, 14] and express the parameter $p$ through the band gap $E_{K-P}^{gap}$

$$\frac{1}{\Omega a_0} \equiv \frac{1}{p} = 1 - a_0\sqrt{\frac{2m_0}{\hbar^2}\frac{E_{K-P}^{gap}}{6}}. \qquad (3.7)$$

In the deformed QD, the parameter of the crystal lattice on its surface are the function of the QD radius

$$a_0{}^{def}(a) = a_0\left(1 - \left|\varepsilon^{(1)}(a)\right|\right), \qquad (3.8)$$

$\varepsilon^{(1)} = \mathrm{Sp}\varepsilon^{(i)}$, $\varepsilon^{(i)}$ is deformation tensor in the QD. We consider the uniform deformation of compression of the QD. Therefore angles between edges of the crystal lattice are not changed. Therefore, in formulas (3.1) - (3.7) it is necessary to replace $a_0 \to a_0{}^{def}$ (3.8).

In the QD model, the first band gap in the potential well is the distance from the bottom of the potential well to the energy level $E_{1s}$ (electron-hole interaction is not accounted). Therefore, we will consider this distance as $E_{K-P}^{gap}$, that is $E_{K-P}^{gap} = E_{1s}$. Then the expression for parameter $p$ (3.7) is substituted into (3.1) and account that $E_{K-P}^{gap} = E_{1s}$. From here we find the energy of the surface Tamm level.

Figure 4 shows the results of numerical calculations of the energies of the ground (curves 1', 1) and the first excited (curves 2', 2) states of the electron and the surface energy of the Tamm level (curves 3', 3) in the stressed QD of the InAs/GaAs nanoheterosystem, parameters which is the same as in [5].

It can be seen from the graphical dependence of the energy, the decrease in the size of the QD leads to a monotonous increase of the energy of the ground and first excited states, both with and without electron-deformation interaction. In particular, at the QD radius $a = 30$ Å, the difference between the ground state energy levels with and without electron-deformation interaction is 50 meV.

As can be seen from figure 4, the energy of the surface state increases with decreasing the QD size. In particular, the energy of the surface Tamm level, taking into account the electron-deformation interaction, is greater than the corresponding energy without considering it. This is due to the compression of the QD material (3.8), which leads to an increase in the degree of overlap of the electronic wave functions of the individual atoms on the QD surface. As a result, the Coulomb repulsion energy $V_c \sim \frac{1}{\left|\vec{r}\right| - \left|\vec{u}^{(1)}\right|}$ increases. $\vec{u}$ is explicit forms of atom displacements. It can be defined from the equations of balance, like in [3-5].

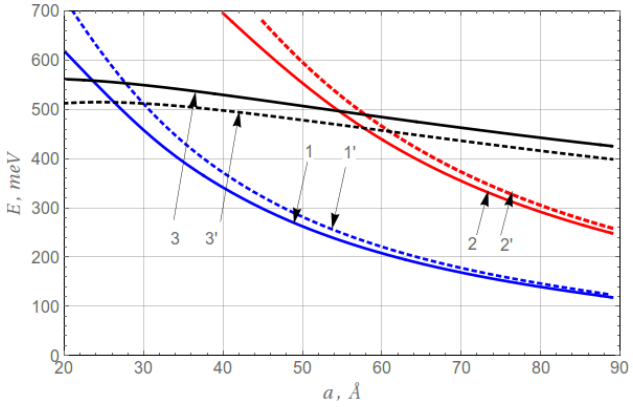


**Fig. 4. The energy of the ground (curves 1,1') and first excited (curves 2, 2') states of the electron, taking into account the electron-deformation interaction (curves 1, 2) and without it (curves 1', 2'), as a function of the QD radius. Curves 3, 3' denote the energy of the Tamm surface level with and without electron-deformation interaction, respectively**

$$\vec{\nabla} div\,\vec{u} = 0. \qquad (3.9)$$

In case of spherical QDs, the solution of (3.9) looks like

$$u_r = \begin{cases} u_r^{(1)}, & r \le a, \\ u_r^{(2)}, & a < r \le R_1 \end{cases} = \begin{cases} C_1 r, & r \le a, \\ C_2 r + \dfrac{C_3}{r}, & a < r \le R_1, \end{cases} \qquad (3.10)$$

where $R_1$ is the radius of the matrix. Coefficients $Ci$ were defined in [3-5] from the boundary condition for displacements and mechanical stresses.

Thus, for smaller QD sizes $a < 20$ Å, the main role in filling in the electronic levels belongs to surface states. Due to this, the photoluminescence curve has an additional peak appeared in the long arbitrary region of the visible optical spectrum [6].

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**Summary**

The change of Tamm surface states in the InAs quantum dots of the InAs/GaAs heterosystem due to the interaction of quasiparticles (electrons) with the elastic deformation of the crystal lattice on the surface of the quantum dot has been studied. The dependence of the energies of the electron Tamm levels is established both taking into account the deformation of the crystal lattice and without it. To do this, on the one hand, a model of the strained quantum dot as a semi-finite chain of atoms (Kronig-Penny-Tamm model) is constructed, taking into account the change in the lattice parameter due to deformation, which depends on the quantum dot size. On the other hand, the quantum dot is described in the framework of the effective mass theory, the model of the elastic medium and the model of the rectangular potential barrier, which defines the limiting potential for the electron. The models are matched by equating the energy distances between the first allowed levels in both models.

It is shown that due to the electron-deformation interaction, the electron energy of the Tamm surface levels increases for the quantum dot, while the electron energy decreases in the quantum dot volume. The reason for the increase in the energy of the Tamm surface levels for the InAs quantum dot of the InAs / GaAs heterosystem is the decrease in the distance between the atoms due to deformation. And the decrease in the energy of an electron in the volume of a quantum dot is explained by a change in the effective depth of potential wells due to the deformation of the quantum dot. It is established that the energy of the surface Tamm level, taking into account the deformation, increases with decreasing quantum dot size. This is consistent with the data of other works, which do not take into account the electron-deformation interaction.

**Keywords:** electron-deformation interaction, quantum dot, surface states, strained nanoheterosystem.

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# ВПЛИВ ДЕФОРМАЦІЇ МАТЕРІАЛУ КВАНТОВОЇ ТОЧКИ НА ПОВЕРХНЕВІ РІВНІ ТАММА

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**Реферат**

У роботі досліджено зміну поверхневих станів Тамма у квантових точках InAs гетеросистеми InAs/GaAs внаслідок взаємодії квазічастинок (електронів) з пружною деформацією кристалічної гратки на поверхні квантової точки. Встановлено залежність енергій рівнів Тамма для електрона як з урахуванням деформації кристалічної гратки, так і без неї. Для цього з одного боку побудовано модель напруженої квантової точки як напівскінченного ланцюжка атомів (модель Кроніга-Пені-Тамма) з урахуванням зміни параметра гратки внаслідок деформації, яка у свою чергу залежить від розміру квантової точки. З іншого боку квантову точку описано у рамках теорії ефективної маси, моделі пружного середовища та моделі прямокутного потенціального бар'єру, що задає потенціал обмеження для електрона. Моделі узгоджено шляхом прирівняння енергетичних відстаней між першими дозволеними рівнями в обох моделях.

Показано, що внаслідок електрон-деформаційної взаємодії енергія електрона поверхневих рівнів Тамма у квантовій точці зростає, тоді як у об'ємі квантової точки енергія електрона зменшується. Причиною зростання енергії поверхневих рівнів Тамма у квантовій точці InAs гетеросистеми InAs/GaAs є зменшення відстані між атомами внаслідок деформації. А зменшення енергії електрона в об'ємі квантовій точці зумовлено зміною ефективної глибини потенціальних ям внаслідок деформації квантової точки. Встановлено, що енергія поверхневого рівня Тамма з урахуванням деформації зростає при зменшення розмірів квантової точки. Це узгоджується з даними інших робіт, в яких не враховано електрон-деформаційну взаємодію.

**Ключові слова:** електрон-деформаційна взаємодія, квантова точка, поверхневі стани, напружена наногетеросистема.