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

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

LIGHT ABSORPTION of SMALL *CdS* QUANTUM DOTS

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Abstract. The energy of interface states was obtained which is caused by the polarization charges at the interfaces. This energy was compared with the energy of electron internal states for CdS quantum dot sizes 1,2–2 nm. The interlevel absorption coefficient versus an electromagnetic wave frequency was defined.
Keywords: polarization trap, quantum dot, surface states

ПОГЛИНАННЯ СВІТЛА МАЛИМИ КВАНТОВИМИ ТОЧКАМИ *CdS*

В. І. Бойчук, Р. Я. Лешко, Д. С. Карпин

Анотація. Визначено енергію поверхневих станів, що зумовлені поляризаційними зарядами, які виникають на гетеромежах. Проведено порівняння отриманих енергій з енергіями внутрішніх

станів електрона для квантової точки *CdS* розмірами 1,2-2 нм. Обчислено коефіцієнт поглинання світла, що зумовлений міжрівневими переходами для різних частот електромагнітної хвилі.

Ключові слова: поляризаційна пастка, квантова точка, поверхневі стани

ПОГЛОЩНИЕ СВЕТА МАЛЫМИ КВАНТОВЫМИ ТОЧКАМИ *CdS*

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Аннотация. Определено энергию поверхностных состояний, обусловленных поляризационными зарядами, которые возникают на гетерограницах Проведено сравнение полученных энергий с энергиями внутренних состояний электрона для квантовой точки *CdS* размерами 1,2-2 нм. Вычислено коэффициент поглощения света, обусловленный межуровневыми переходами для различных частот электромагнитной волны.

Ключевые слова: поляризационная ловушка, квантовая точка, поверхностные состояния

INTRODUCTION

Already several decades physics of quasizerodimension semiconductor clusters (nanocrystals, quantum dots) caused evident interest of researches [1-2]. Low dimension of the system evokes a number of interesting changes of physical characteristics of crystals. Among their number properties one can obtain discrete structure of the electron, hole and exciton energy spectrum. The main condition must be true – nanocrystal size is smaller then radius of Wannier-Mott exciton in volume crystals [2-5]. During investigation quasiparticle energy levels, spectroscopy methods play the important role. Modern detail researches confirm existence in nanocrystals the strength quantum restriction particle regime.

In this study significant place had led by heterostructures with *CdS* quantum dots (QDs). Such QDs will be able become by the substitute of organic substance in the biologic sensors and other optical electronic devices. Therefore the last years many researchers had paid attention to elaborate of the new technology of production higth-quality and stable *CdS* QD in the solid state and polymer matrix.

Many works [4-14] had devoted to investigation of *CdS* nanocrystal's photoluminescence properties. It was shown, that *CdS* QDs in polymer matrix contain own defects of two types. It caused of red and green region luminescence. It was determined that defects Cd_iV_{cd}-V_s are reason of the existence mentioned optic strips as in bulk *CdS* crystals. The analyses of experimental data shows, that physical nature of the matrix do not influence to type of radiation centers in DQ [15,16]. But it was shown, that matrix plays significant role in the proses of luminescence stimulating. Specifically, the gelatin presence much increase intensity of the red luminescence.

The heretosystem interfaces play important role for optic properties of QD's system. The size diminishing QD accompany increasing role of the surfaces for absorption and luminescence spectra. In majority physical situation, red part of the radiation spectrum is not caused by the interband transition, but caused by electrons transition with surface traps participation [14].

In majority works for QD luminescence phenomenon had indicated various causes of the surface states rize. Among their number it was considered broken the electronic couplings and presence of an absorbed atoms in the systems [11-12]. Other reason surface states rise is the interaction charged particles and coupling surface charges on the heterostructure interfaces [17-18]. The physical condition of the display this states are studied less.

In present paper we study CdS/SiO_2 heterostructure with spherical QDs. Interface states energy was calculated. Models of abrupt and fluent coordinate changes of a dielectric permittivity

near surface of QD was considered. The role of interface states on interlevel absorption coefficient was studied.

I. POTENTIAL ENERGY OF THE CHARGED PARTICLE IN QD/MATRIX HETEROSYSTEM

Let us consider heterosystem which is consisting dielectric or semiconductor matrix witch contains spherical QDs. Every charged particle is characterized by own effective mass in each medium (   ). The mediums are described by own dielectric permittivity (   ).

Modern technology enables to obtain sufficient quality of semiconductor and dielectric nanoheterostructures. In reality, it is difficult to create a heterogeneous system with sharp variable of all physical parameters at the interface, where particle's coordinate $r = a$, (a is QD radius). There is always a transitional layer in with a particular physical parameter (particle's effective mass, dielectric constant) varies from its value in some crystal to the corresponding value in other crystal.

1. Heterosystem with sharp variable of the dielectric permittivity at the interface

We simplify model by assuming that in the point r=a dielectric permittivity is abruptly varied. That is

$$\varepsilon(r) = \varepsilon_1 \theta(a-r) + \varepsilon_2 \theta(r-a), \; r \geq a, \quad (1)$$

where $\theta(x)$ is Heaviside function. It can be found potential in the system QD/matrix if one solves Poisson and Laplace equations as in [15]:

$$\Phi(\vec{r}, \vec{r}_0) = \begin{cases} \Phi_1(\vec{r}, \vec{r}_0), \; r < a, \\ \Phi_2(\vec{r}, \vec{r}_0), \; r > a, \end{cases} \quad (2)$$

where   are the radius-vectors of an arbitrary point in the space and the particle, respectively. We know that bonded charges arise at the interfaces of the nonhomogeneous environment. A surface density of this charges we can obtain after use of the polarization boundary condition:

$$\sigma = P_{1n} - P_{2n} = \frac{1}{4\pi}\left(\frac{\partial \Phi_1(\vec{r}, \vec{r}_0)}{\partial r} - \frac{\partial \Phi_2(\vec{r}, \vec{r}_0)}{\partial r} \right)\Bigg|_{r=a}. \quad (3)$$

The potential energy of $q=1$ charge with interact with surface bound charges arising from the existence of the same charge is determined by the formula [15]:

$$V_p(r) = \begin{cases} \frac{1}{2a\varepsilon_1}\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}\left[\frac{a^2}{a^2 - r^2} + \frac{\varepsilon_1}{\varepsilon_2}F\left(1, \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2}; \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2} + 1; \left(\frac{r}{a}\right)^2 \right)\right], \; r < a, \\ \frac{1}{2a\varepsilon_2}\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}\left[\frac{a^2}{a^2 - r^2} + \left(\frac{a}{r}\right)^2 F\left(1, \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2}; \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2} + 1; \left(\frac{a}{r}\right)^2 \right)\right], \; r < a, \end{cases} \quad (4)$$

where F – hypergeometric function. Analysis of (4) shows that for the small particle distance to the interface the first term is foundation in both situation: if $r<a$ or $r>a$. In addition the function $V_p(r)$ includes a nonphysical discontinuity in the point $r=a$. If inequality $\epsilon_1 > \epsilon_2$ is true, then potential $V_p(r)$ represents by the function as in fig1. Otherwise, a coordinate dependence of the potential changes. It will be characterize by the opposite sign.

2. Heterosystem with smooth variable of the dielectric permittivity at the interface

Let at the interface exist the transitional layer where dielectric permittivity changes from its significance in the QD to corresponding matrix value. In this case one may respect the calculation of [16] and obtain the potential energy of interaction the charge particle and polarization charges as follows:

$$V_p(r) = \frac{\gamma}{4\varepsilon(r)}\int_0^\infty dr_0 \frac{\operatorname{th}\left(\frac{r_0 - a}{L}\right) + \frac{r_0}{L}\operatorname{sech}^2\left(\frac{r_0 - a}{L}\right)}{r_0^2 - r}, \quad (5)$$

$$\varepsilon(r) = \frac{\varepsilon_1 + \varepsilon_2}{2}\left[1 - \gamma\operatorname{th}\left(\frac{r - a}{L}\right)\right], \quad (6)$$

$$\gamma = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}. \quad (7)$$

L is not transition layer width. L is a parameter which defining transition layer width. Based on the formula (5) the analysis shows that the width of the transitional layer is near crystal constant a_0, when $L\sim a_0/4$. In fig 1, 2 the potential $V_p(r)$ based on the expression (4) and (5) are shown as function of coordinate r. Potential (4) has discontinuity at the interface, that is why we used only potential (5).
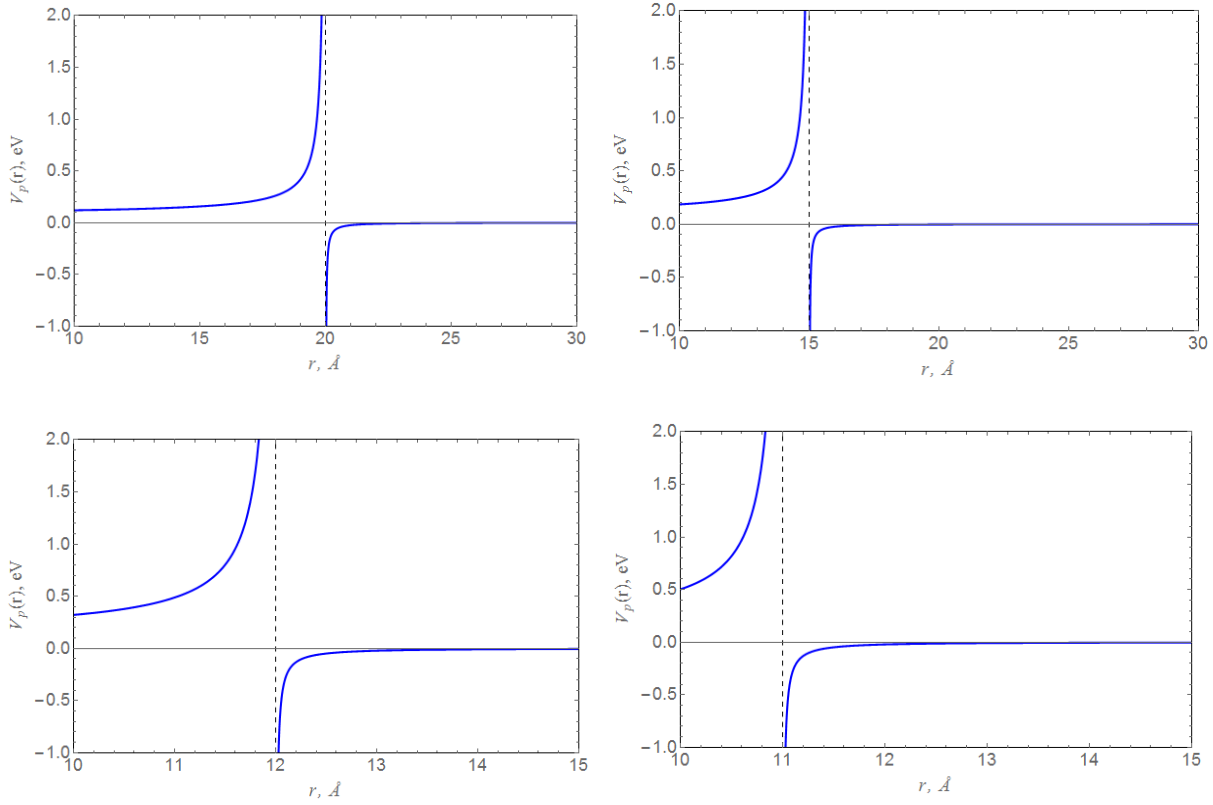
Fig.1. Potential (4) for different QD radii.

II. Schrödinger equation of the charged particle (electron) in the heterosystem

We consider the electron of *CdS* spherical QD in the matrix *SiO₂*. We use the same parameters as in [15] (Table 1). We write the Hamiltonian of the system using Hartree units ($m_0 = 1$, $\hbar = 1$, $e = 1$):

$$\hat{\mathbf{H}} = -\frac{1}{2}\nabla \frac{1}{m(r)}\nabla + U(r) + V_p(r), \qquad (8)$$

where confinement potential is

$$U(r) = \begin{cases} 0, & r \le a, \\ U_0, & r > a, \end{cases} \qquad (9)$$

and the potential energy $V_p(r)$ expressed by (5). Taking into account the view of total potential energy $(U(r)+V_p(r))$ as the function of the coordinate r it can be assumed that the charge can be localized both in the middle and outside of the QD.

Table 1.

Crystals parameters

	m^*/m_0	ε	U_0, eV
CdS	0.2	5.5	0
SiO₂	0.42	2.1	2.7

It is opportunity to do analysis of the SE for the model with potentials (5). We take into account that in this problem potential (5) is the small perturbation. In zero approximation the solution of the SE can be write [16] as

$$\psi_{e;n,l,m}(\vec{r}_e) = R_{e;n,l}(r_e)Y_{l,m}(\Omega_e) =$$

$$= \begin{cases} A_{n,l}\, \mathrm{j}_l(k_{n,l}r_e/a), & r_e \le a \\ B_{n,l}\, \mathrm{k}_l(x_{n,l}r_e/a), & r_e > a \end{cases} \times Y_{l,m}(\Omega_e), \qquad (10)$$

where

$$k_{n,l} = a\sqrt{2m_{e1}^* E_{e;n,l}}, \quad x_{n,l} = a\sqrt{2m_{e2}^*\left(U_0 - E_{e;n,l}\right)},$$

and $j_l(x)$, $k_l(x)$ are spherical Bessel functions. The electron energy we found from the boundary conditions (non discontinuity of the wave functions and probability density flux on the QD surface). In this approach the electron even in ground state with a certain probability can penetrable from QD into the matrix because the wave function "tail" is not equal zero in the matrix space due to finite particle confinement. Electron energy we found after the perturbation theory:

$$E_{n,l} = E_{e;n,l} + \langle n,l|V_p|n,l\rangle . \qquad (11)$$

First of all, we have been calculated all possible energies levels in the QD without taking into account (5). We find out, that in the range of QD radius $a \in (12\,\text{Å}, 21\,\text{Å})$, there are two s-states. That is why we assume, that 3s-state may be in the polarization trap. If it exists, then we can say, that it is caused only by the surface. Also there are other states (beside s-states) in the QD for QD radius $a \in (12\,\text{Å}, 21\,\text{Å})$.

Therefore, if the electron is outside of the QD (in polarization trap) it also solved variational problem. In this case trial function s-type we chose in the form

$$\psi_{e;300}^{out}(\vec{r}_e) = D\left(1 - A_1 r_e\right)\left(1 - A_2 r_e^2\right)\exp\left[-\beta\left(\frac{r_e}{a} - 1\right)^2\right]. \qquad (12)$$
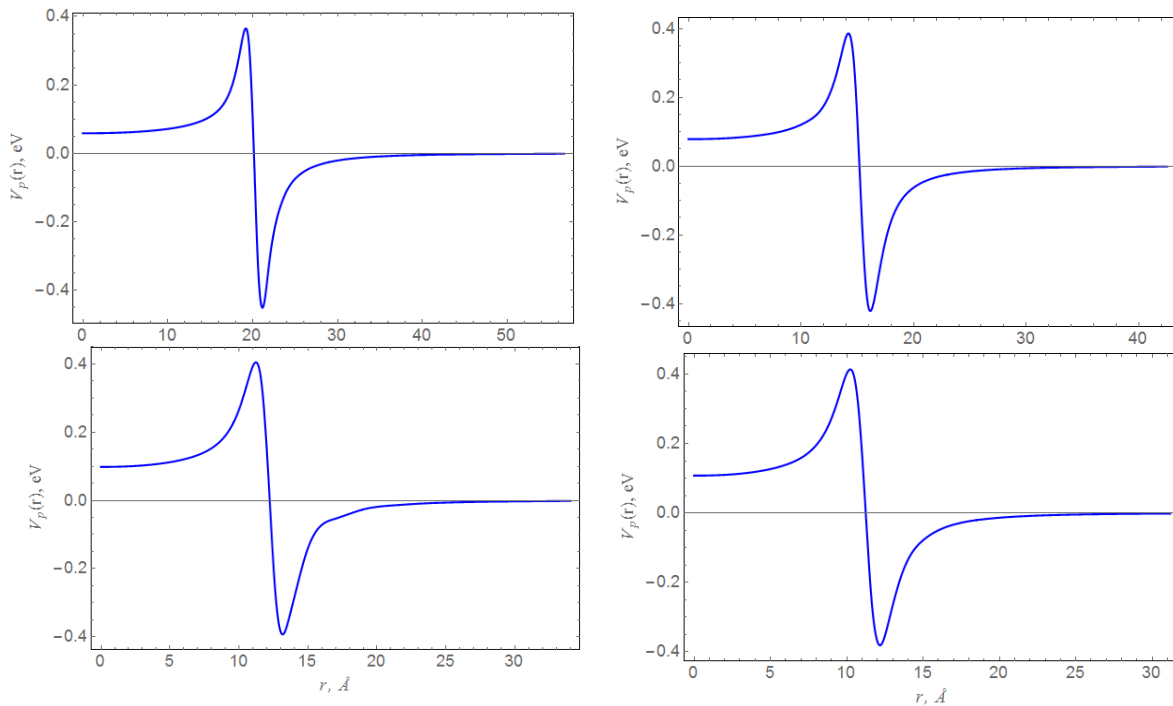

Fig.2. Potential (5) for different QD radii.

Choosing the wave function in the form (12) provides the wave function decreasing versus distance from a boundary of the QD in both on direction (a bound interface state of the electron). Constants A_1, A_2, D can be found from orthogonal conditions and normalization condition:

$$\langle\psi_{e;300}^{out}(\vec{r}_e)|\psi_{e;100}(\vec{r}_e)\rangle = 0, \qquad \langle\psi_{e;300}^{out}(\vec{r}_e)|\psi_{e;200}(\vec{r}_e)\rangle = 0,$$
$$\qquad (13)$$
$$\langle\psi_{e;300}^{out}(\vec{r}_e)|\psi_{e;300}^{out}(\vec{r}_e)\rangle = 1.$$

Minimizing a corresponding functional we got electron energy and wave function of the bound interface 3s-state. Since we calculated s-state, (12) will be orthogonal to other types states such as p-, d-, and so on.

We perform calculation in the QD range $(12\,\text{Å} - 21\,\text{Å})$. Smaller QD radii we do not consider, because the effective mass approximation in this range cannot be used. Bigger QD radii require to modify (12), because there appears 3s-state (not associated with polarization trap).

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Therefore, in the QD range (12 Å – 21 Å) we have only two (1s-, 2s-) states, with associated with QD well (9). Higher energy, which was calculated by the use (12) associated with polarization trap only. Also we consider two parameters L ($a_0/4$, $a_0/2$).

In fig.3 it can see the dependence of the electron energy as a function of the radius QD for the inside and outside problems. As seen in fig.3, energy of interface state depends on QD radius very weak. If QD radius reduce, this energy lever grows up due to reducing well depth (5). The reason of grows up 1s-, 2s- and 1p-states is quantum localization of the electron.
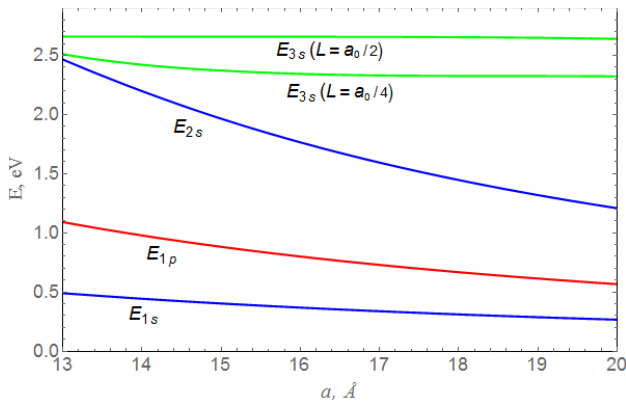

Fig. 3. Electron energy in the QD. Energies E_{3s} (interface energy) were calculated by using (12) with two different parameters L.

To estimate obtained results we also approximate $U(r) + V_p(r)$ by the rectangular quantum wells and barriers as shown in the fig.4. In every region we got exact solution of Schrodinger equation, like in [20] with account different energies regions in potential wells and barriers. Using the parameters from table 1 and fig.4, we perform calculation s-states. We found, that E_{1s}=0.32218 eV, E_{2s}=1.31293 eV, E_{3s}= 2.69797 eV. Also we plotted probability density for electron in the 3s-state with account our variational function (12) and exact solution of rectangular well and barriers (fig.5). The graphics show, that both wave functions provides localization of the particle in the polarization trap in the 3s-state.
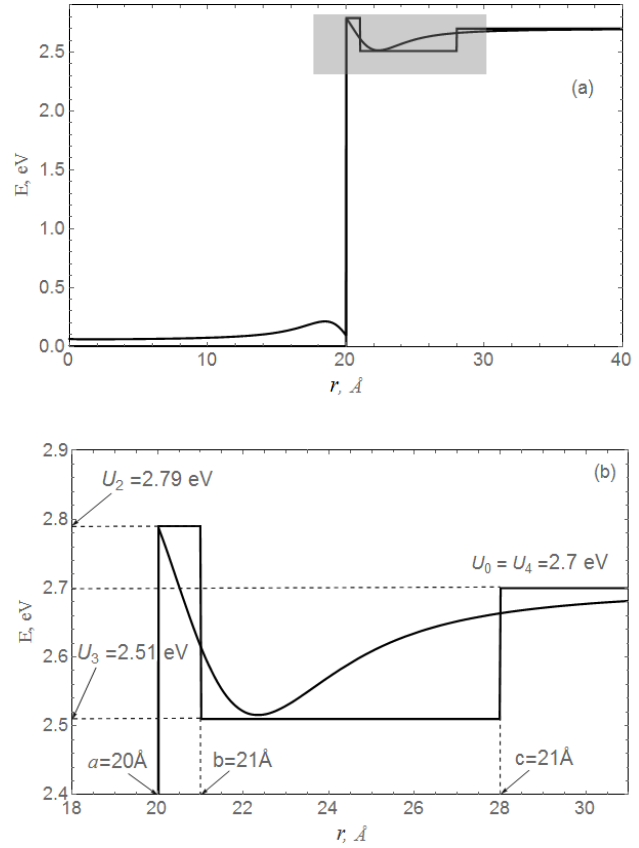

Fig. 4. Total potential energy and approximate potential energy (rectangular potential wells and barriers).
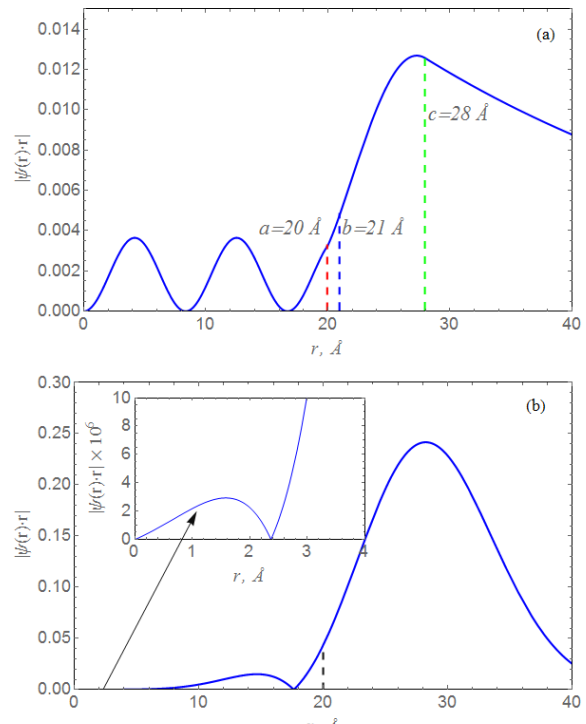

Fig. 5. Probability density of electron it the QD heterosystem. (a) – by the use approximation of rectangular wells and barriers; (b) – by the use (12).

III. INTERLEVEL TRANSITION AND LIGHT ABSORPTION OF THE HETERO-SYSTEM

Let the heterosystem is irradiated by the linearly polarized light along z direction. Then in the dipole approximation the interlevel transitions are possible between states where $\Delta l = \pm 1$ and $\Delta m = 0$. For the QD radius 20 Å (exciton radius CdS is equal 16,9 Å) we calculate the energy levels and show the all possible transitions in the fig 6. In this case it is possible 3 transitions which can caused the absorption of the electromagnetic light. Therefore, the density matrix and iterative procedure were applied to derive the absorption coefficient [19]. In this approach the linear absorption coefficient can be expressed as

$$\alpha_{m,n}(\omega) = \omega\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}\frac{N|d_{mn}|^2\hbar\Gamma}{(E_n - E_m - \hbar\omega)^2 + (\hbar\Gamma)^2}, \quad (14)$$

where ε_0 is electric constant, μ_0 is magnetic constant, $\hbar\Gamma$ is the scattering rate caused by the electron-phonon interaction and some other factors of scattering. If T≈4 K and $\hbar\Gamma$ limits to zero, one can obtain:

$$\alpha_{m,n}(\omega) = \lim_{\hbar\Gamma\to 0}\left(\omega\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}\frac{N|d_{mn}|^2\hbar\Gamma}{(E_n - E_m - \hbar\omega)^2 + (\hbar\Gamma)^2}\right) =$$

$$= \omega\pi\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}N|d_{mn}|^2\delta(E_n - E_m - \hbar\omega). \quad (15)$$

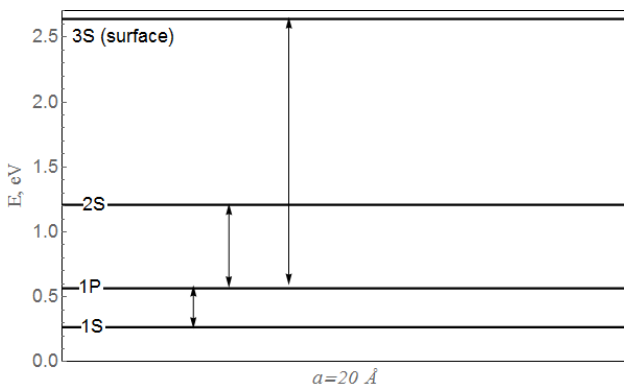$N \approx 3\cdot10^{16}$ cm^{-3} is carrier concentration.

Fig.6. Quantum transitions in the heterosystem. Average radius of the QD is 20 Å.

In practice, the QDs sets are obtained which are located in crystal and polymer matrix. Whatever method of cultivation is not used, the set of QDs are always characterized by the size dispersion. Let the QD size distribution is approximated by the Gauss function:

$$g(s,\bar{a},a) = \frac{1}{s\sqrt{2\pi}}\exp\left(-\frac{(a-\bar{a})^2}{2s^2}\right), \quad (16)$$

where a is the QD radius (variable), s is half-width of the distribution (16), which is expressed by the average radius $\bar{a}$ and the value σ which is considered as the variance in the QD sizes expressed in the percent: $s = \bar{a}\sigma/100$. By regarding of the QD dispersion (16) the absorption coefficient had been obtained for the QDs set

$$\alpha_{m,n;system}(\omega) = \omega\pi\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}N\int g(s,\bar{a},a)|d_{mn}|^2\delta(E_n(a) -$$

$$- E_m(a) - \hbar\omega)da. \quad (17)$$

After using delta-function properties it has been obtained:

$$\alpha_{m,n;system}(\omega) = \omega\pi\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}N\int g(s,\bar{a},a)|d_{mn}|^2\sum_i \times$$

$$\times \frac{\delta(a - a_{0i})}{\left|\frac{d}{da}(E_n(a) - E_m(a) - \hbar\omega)\right|_{a=a_{0i}}}da,$$

where a_{oi} are simple zeros of the function $F(a) = (E_n(a) - E_m(a) - \hbar\omega)$. Therefore,

$$\alpha_{m,n;system}(\omega) = \omega\pi\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}}N\sum_i \frac{g(s,\bar{a},a_{0i})|d_{mn}(a_{0i})|^2}{\left|\frac{d}{da}(E_n(a) - E_m(a) - \hbar\omega)\right|_{a=a_{0i}}}. \quad (18)$$

The dependence of the absorption coefficient on the energy quant of light for the QD average radius and dispersion σ=3% was plotted by the use expression (18) and $L=a_0/2$. Fig.7 shows coefficients of light absorption for all possible transition cases (Fig.6). The graphics shows thin absorption bands. Also we indicate, that absorption band from 1p-state to 3s-state (surface state) is smaller than other possible. It caused by the large transition energy and small dipole momentum. Also we can signify that this transition will effect on the pho-

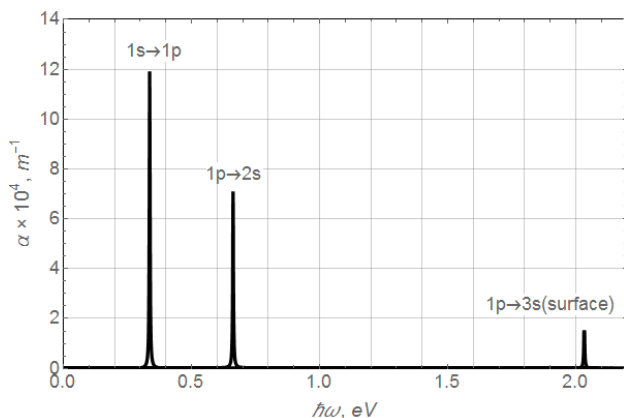toluminescence spectra which will be studied in our next works.

Fig.7. Light absorption coefficient of the heterosystem. Average radius of the QD is 20 Å, σ=3%.

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LIGHT ABSORPTION of SMALL *CdS* QUANTUM DOTS

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Summary

The aim of article is to analyze the conditions of the interface states arise which caused by the polarization trap, and determine the impact of these conditions on the light absorption. Therefore, it was determined the energy of interface states caused by polarization charges arising on heteroboundaries. For calculations we took into account two models: the transition layer on the interface and his absence. In both cases, we shown that polarization traps exist, which can capture the electrons in the case of the small size of quantum dots.

The energy spectrum of surface states was calculated by the Ritz variational method. A comparison of these energy states with energy internal states was made. The internal states are defined accurately using the effective masses approximation and the model of rectangular potential wells and barriers. This made it possible to conclude that for the real quantum dot size, the ground state of an electron is always in the internal states of quantum dot. Excited state is not affected. The dependence of the surface states energy on the quantum dot size was obtained. The corresponding energy of these states increases with decreasing of the quantum dot size. This is due to the polarization dependence of the depth of the trap sizes.

We calculated matrix elements of the dipole moment of interlrvel transitions into surface states. The light absorption coefficient caused by the interlrvel transitions was defined as a function of the electromagnetic wave frequency. In the final formula of absorption coefficient, we take into account the quantum dots size distribution. It is shown that absorption bands which corresponds to electron transitions into surface states is much smaller than the absorption bands caused by transitions between inner states.

Keywords: polarization trap, quantum dot, surface states

ПОГЛИНАННЯ СВІТЛА МАЛИМИ КВАНТОВИМИ ТОЧКАМИ CdS

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Реферат

Метою роботи було проаналізувати умови виникнення поверхневих станів, що зумовлені поляризаційною пасткою, і визначити вплив цих станів на поглинання світла. Саме тому було визначено енергію поверхневих станів, що зумовлені поляризаційними зарядами, які виникають на гетеромежах. Для обчислень взято до уваги дві моделі: з урахуванням поверхневого перехідного шару і з його відсутністю. В обох випадках доведено існування поляризаційної пастки, куди можуть потрапляти електрони у випадку малих розмірів квантових точок.

Обчислено енергетичний спектр поверхневих станів варіаційним методом Рітца. Проведено порівняння енергії цих станів із енергією внутрішніх станів, які визначено точно з використання методу ефективної маси в рамках моделі прямокутних потенціальних ям і бар'єрів. Це дало змогу зробити висновок, що для реальних розмірів квантових точок основний стан електрона є завжди у внутрішніх станах КТ (у поверхневі стани не переходить). Збуджених станів це не стосується. Встановлено залежність енергії поверхневих станів від розмірів квантової точки. Відповідна енергія цих станів збільшується при зменшенні розмірів квантової точки. Це зумовлено залежністю глибини поляризаційної пастки від розмірів.

Обчислено матричні елементи дипольного моменту міжрівневих переходів у поверхневі стани. Обчислено коефіцієнт поглинання світла, що зумовлений міжрівневими переходами, як функцію частоти електромагнітної хвилі. У кінцевій формулі коефіцієнта поглинання враховано розподіл квантових точок за розмірами. Показано, що смуги поглинання, які зумовлені переходами електрона у поверхневі стани є набагато меншими, ніж смуги поглинання, що зумовлені переходами між внутрішніми станами.

Ключові слова: поляризаційна пастка, квантова точка, поверхневі стани