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EXCITON SPECTRA IN MULTI-SHELL OPEN SEMICONDUCTOR NANOTUBE

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Abstract. The spectral parameters (resonance energies and resonance widths) of electron, hole and exciton in multi-shell open cylindrical semiconductor nanotube are theoretically studied within the models of effective mass and rectangular potentials using the function of distribution over the energy for the probability of quasi-particle location in nanosystem.

These parameters as functions of nanotube thickness are analyzed for the nanostructure composed of $GaAs$ and $Al_xGa_{1-x}As$ semiconductors.

Keywords: nanotube, exciton, resonance energy, resonance width

ЕКСИТОННІ СПЕКТРИ У БАГАТОШАРОВІЙ ВІДКРИТІЙ НАПІВПРОВІДНИКОВІЙ НАНОТРУБЦІ

О. М. Маханець, А. І. Кучак, О. М. Войцехівська, В. І. Гуцул

Анотація. У моделі ефективних мас та прямокутних потенціалів, з використанням функції розподілу за енергією ймовірності знаходження квазічастинки у наносистемі теоретично досліджено спектральні параметри (резонансні енергії та резонансні ширини) електрона, дірки та екситона у багатошаровій “відкритій” циліндричній напівпровідниковій нанотрубці.

На прикладі наносистеми на основі напівпровідників $GaAs$ та $Al_xGa_{1-x}As$ проаналізовано залежності резонансних енергій і резонансних ширин квазічастинок від товщини нанотрубки.

Ключові слова: нанотрубка, екситон, резонансна енергія, резонансна ширина

ЭКСИТОННЫЕ СПЕКТРЫ В МНОГОСЛОЙНОЙ ОТКРЫТОЙ ПОЛУПРОВОДНИКОВОЙ НАНОТРУБКЕ

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Аннотация. В модели эффективных масс и прямоугольных потенциалов, с использованием функции распределения по энергии вероятности нахождения квазичастицы в наносистеме теоретически исследованы спектральные параметры (резонансные энергии и резонансные ширины) электрона, дырки и экситона в многослойной открытой цилиндрической полупроводниковой нанотрубке.

На примере наносистемы созданой из полупроводников $GaAs$ и $Al_xGa_{1-x}As$ проанализированы зависимости резонансных энергий и резонансных ширин квазичастиц от толщины нанотрубки.

Ключевые слова: нанотрубка, экситон, резонансная энергия, резонансная ширина

1. Introduction

The multi-shell semiconductor nanotubes have been recently studied both theoretically and experimentally [1-7]. The unique properties of quasi-particles (electrons, excitons and so on) in such nanostructures allow using them as basic elements for the devices of modern nanoelectronics [8-12]: nanosensors, tunnel nanodiodes, wavelength-controlled nanolasers, effective solar energy conversion devices [8-12].

The authors of ref. [3] have been grown the arrays of semiconductor nanotubes consisting of the sequence of $GaAs$ and $Al_x Ga_{1-x} As$ nanoshells using the method of molecular beam epitaxy. This nanostructure was covered by rather thick shell of $GaAs$ in order to avoid $Al_x Ga_{1-x} As$ oxidizing.

The multi-shell nanotube under study is considered as an open one because the potential energy of electron and in $GaAs$ is smaller than that in $Al_x Ga_{1-x} As$. In open systems, on the contrary to the closed ones, the quasi-particles can tunnel through the potential barrier into the outer medium, creating an additional channel of energy relaxation for the quasi-particles excited in the quantum well. It is clear that in such systems the energy spectra of quasi-particles are the quasi-stationary ones, characterized by the resonance energies and resonance widths.

The theory of exciton and phonon stationary spectra together with the theory of electron- and exciton-phonon interaction well correlating to the experimental data and general physical considerations is already developed for the closed cylindrical and hexagonal nanotubes [5-7]. The quasi-stationary spectra of electrons, holes and excitons were theoretically studied for the spherically-symmetric quantum dots and single cylindrical quantum wires [13-17].

In this paper, we present the theoretical study of electron, hole and exciton quasi-stationary spectrum in multi-shell open cylindrical semiconductor nanotube. The dependences of resonance energies and resonance widths on nanotube thickness are obtained and analyzed for the nanostructure composed of $GaAs$ and $Al_x Ga_{1-x} As$ semiconductors.

2. The theory of electron and exciton energy spectra in multi-shell open cylindrical semiconductor nanotube

The multi-shell open cylindrical semiconductor nanotube consisting of inner wire with radius ρ_0 („0” – $GaAs$), barrier-shell with thickness Δ_1 („1” – $Al_x Ga_{1-x} As$), nanotube with thickness d („2” – $GaAs$) and one more barrier-shell with thickness Δ_2 („3” – $Al_x Ga_{1-x} As$) embedded into the outer structure („4” – $GaAs$) is studied. The cross-section and energy scheme of this nanostructure is presented in fig.1. The potential energy of electron and hole in outer medium is smaller than that in barrier-shells, thus the system is an open one and the electron, hole and exciton energy spectra is quasi-stationary.

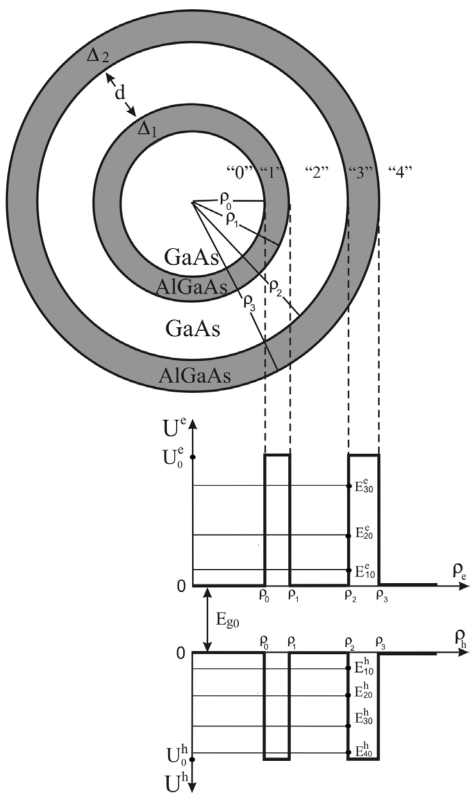

Figure 1. Cross-section and energy scheme of multi-shell nanotube.

At first, we are going to study the quantum states of uncoupling electron and hole in order to analyze further the exciton spectrum. The geometrical sizes of nano-system elements are chosen in such a way that the approximation of effective mass for the electron (hole) is valid and interaction between them is determined by the Coulomb potential with dielectric constants of the respective bulk crystals.

Considering the symmetry of the system, all further calculations are performed in cylindrical coordinate system (ρ, φ, z) with Oz axis directed along the axial axis of nanotube. Thus, the dielectric constants, effective masses and potential energies of electron (hole) are fixed as

$$\varepsilon(\rho)=\begin{cases}\varepsilon_0\\ \varepsilon_1\end{cases}, \qquad \mu^{e(h)}(\rho)=\begin{cases}\mu_0^{e(h)}\\ \mu_1^{e(h)}\end{cases}, \tag{1}$$

$$U^{e(h)}(\rho)=\begin{cases}0, & 0\le\rho\le\rho_0, \quad \rho_1\le\rho\le\rho_2, \quad \rho>\rho_3,\\ U_0^{e(h)}, & \rho_0<\rho<\rho_1, \quad \rho_2<\rho\le\rho_3\ .\end{cases}$$

As far as for the system under study the theory of quasi-stationary spectrum is equal both for the electron and the hole, let us further observe the electron, temporarily dropping index “e”. In order to obtain its energy spectrum and wave functions we solve the stationary Schrodinger equation

$$\widehat{H}(\rho,\varphi,z)\Psi(\rho,\varphi,z)=E\,\Psi(\rho,\varphi,z) \tag{2}$$

with Hamiltonian

$$\widehat{H}(\rho,\varphi,z)=-\frac{\hbar^2}{2\rho}\left[\frac{\partial}{\partial\rho}\left(\frac{\rho}{\mu(\rho)}\frac{\partial}{\partial\rho}\right)+\frac{1}{\mu(\rho)}\frac{1}{\rho}\frac{\partial^2}{\partial\varphi^2}\right]- -\frac{\hbar^2}{2\mu(\rho)}\frac{\partial^2}{\partial z^2}+U(\rho). \tag{3}$$

Considering the symmetry, the wave function ($\Psi(\rho,\varphi,z)$) is written as

$$\psi_{mq}(\boldsymbol{r})=\frac{1}{\sqrt{2\pi L}}\,R_{mq}(\rho)\,e^{iqz}\,e^{im\varphi}. \tag{4}$$

Here $q-$ the axial quasi-momentum; $m=0,\pm1,\pm2,..-$ magnetic quantum number; $L-$ the effective length of electron movement along the axial axis of nanotube.

Substituting (4) and (3) into equation (2), the variables (ρ, φ, z) are separated and the equation for the radial wave functions ($R_{mq}(\rho)$) is obtained

$$\left\{-\frac{\hbar^2}{2}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\frac{\rho}{\mu(\rho)}\frac{\partial}{\partial\rho}\right)-\frac{m^2}{\rho^2\mu(\rho)}-\frac{q^2}{\mu(\rho)}\right]+ +U(\rho)-E\right\}R_{mq}(\rho)=0\,. \tag{5}$$

This equation is exactly solved for each part of nanostructure. The solutions are written as

$$R_{mq}(k\rho)=\begin{cases} R_{mq}^{(0)}(k\rho)=A_m^{(0)}[H_m^-(k\rho)+H_m^+(k\rho)], & \rho<\rho_0 \\ R_{mq}^{(1)}(k\rho)=A_m^{(1)}H_m^-(i\chi\rho)+B_m^{(1)}H_m^+(i\chi\rho), & \rho_0\le\rho\le\rho_1 \\ R_{mq}^{(2)}(k\rho)=A_m^{(2)}H_m^-(k\rho)+B_m^{(2)}H_m^+(k\rho), & \rho_1<\rho\le\rho_2 \\ R_{mq}^{(3)}(k\rho)=A_m^{(3)}H_m^-(i\chi\rho)+B_m^{(3)}H_m^+(i\chi\rho), & \rho_2<\rho\le\rho_3 \\ R_{mq}^{(4)}(k\rho)=A_m^{(4)}H_m^-(k\rho)+B_m^{(4)}H_m^+(k\rho), & \rho>\rho_3 \end{cases},\qquad (6)$$

where

$$k=\sqrt{\frac{2\mu_0}{\hbar^2}E-q^2}\,,\qquad \chi=\sqrt{\frac{2\mu_1}{\hbar^2}U_0-\frac{\mu_1}{\mu_0}k^2+(1-\frac{\mu_1}{\mu_0})q^2}\,,\qquad (7)$$

H_m^-, H_m^+ – the Hankel functions of the whole order.

Using the condition of wave function and its density of current continuity at all nanotube interfaces

$$\begin{cases} R_{mq}^{(p)}(\rho_p)=R_{mq}^{(p+1)}(\rho_p) \\ \left.\dfrac{1}{\mu_p}\dfrac{\partial R_{mq}^{(p)}(\rho)}{\partial\rho}\right|_{\rho=\rho_p}=\left.\dfrac{1}{\mu_{p+1}}\dfrac{\partial R_{mq}^{(p+1)}(\rho)}{\partial\rho}\right|_{\rho=\rho_p} \end{cases}\quad (p=0,1,2,3),\qquad (8)$$

together with the normality condition

$$\int_0^\infty R_{mq}^*(k\rho)\,R_{mq}(k'\rho)\rho\,d\rho=\delta(k-k')\qquad (9)$$

the coefficients $A_m^{(i)}$, $B_m^{(i)}$, in expr. (6), are definitely obtained and, thus, the radial wave functions of electron are fixed too. The explicit expressions for these coefficients are not presented due to their sophisticated form.

Further, we introduce the distribution function $W_m(E)$ (over the energy E) of the probability of electron location in the space of four inner shells of nanotube

$$W_{mq}(E)=\frac{1}{\rho_3}\int_0^{\rho_3}\left|R_{mq}(k(E)\rho)\right|^2\rho\,\mathrm{d}\rho\,.\qquad (10)$$

In refs. [13, 16] it was shown that dependence of such function on energy at fixed m looks like a set of peaks with quasi-Lorentz shape. The radial quantum number n_ρ is introduced in order to number them. The position of maximum of each peak in energy scale fixes the electron resonance energy ($E_{n_\rho m}^{(e)}(q)$). The energy interval, defined by the distance (in energy scale) between the abscissa of cross-points of the line parallel to the energy axis (E) and crosses the peak $W_{n_\rho m\,q}^{(e)}(E)$ at the half of the height, fixes the resonance width $\Gamma_{n_\rho m}^{(e)}(q)$ of electron energy level. The resonance energies ($E_{n_\rho m}^{(h)}(q)$) and widths ($\Gamma_{n_\rho m}^{(h)}(q)$) of hole energy states are obtained in analogy.

In order to study the exciton quasi-stationary states in open nanotube we solve the stationary Schrodinger equation with Hamiltonian

$$\hat{H}_{ex}=E_g+\hat{H}^{(e)}(\boldsymbol{r}_e)+\hat{H}^{(h)}(\boldsymbol{r}_h)-\frac{e^2}{\varepsilon(\boldsymbol{r}_e,\boldsymbol{r}_h)\left|\boldsymbol{r}_e-\boldsymbol{r}_h\right|}\,.\qquad (11)$$

Here E_g – the energy gap for the components “0”, “2”, “4”; $H^{(e)}(\boldsymbol{r}_e)$, $H^{(h)}(\boldsymbol{r}_h)$ – the Hamiltonians of uncoupling electron and hole, expr. (3); ε – dielectric constant of nanotube which, in general case, strongly depends on spatial location of electron and hole in nanosystem.

The Schrodinger equation with Hamiltonian (11) can’t be solved exactly analytically. Thus, we use the approximated method. At the condition that the sum of resonance energies of uncoupling electron and hole in the respective exciton quasi-stationary states is much bigger than the energy of their interaction in these states, we assume that the distribution function over the energy of probability of exciton location in nanotube is written as

$$W_{p_e}^{p_h}(E^{(e)},E^{(h)})=W_{p_e}^{(e)}(E^{(e)})W_{p_h}^{(h)}(E^{(h)}),\quad (p=n_\rho mq).\qquad (12)$$

It defines the resonance energies and widths of exciton quasi-stationary states.

The Coulomb potential energy of electron-hole interaction does not create the additional potential barrier for the quasi-particles exit of multi-shell nanotube, thus, it is assumed that in the first approximation it only renormalizes the energy of exciton resonance quasi-stationary states, not changing their widths. Therefore, the resonance energies ($E_{n_\rho^h m^h}^{n_\rho^e m^e}$) and widths ($\Gamma_{n_\rho^h m^h}^{n_\rho^e m^e}$) of exciton states in the center-mass system

$$Z=\frac{\mu_0^e z_e+\mu_0^h z_h}{\mu_0^e+\mu_0^h}, \qquad z=z_e-z_h \tag{13}$$

are written as

$$\Gamma_{n_\rho^h m^h}^{n_\rho^e m^e}=\Gamma_{n_\rho^e m^e}^{(e)}+\Gamma_{n_\rho^h m^h}^{(h)}, \tag{14}$$

$$E_{n_\rho^h m^h}^{n_\rho^e m^e}(P)=E_g+\frac{P^2}{2M}+E_{n_\rho^e m^e}^{(e)}+ \\ +E_{n_\rho^h m^h}^{(h)}+\Delta E_{n_\rho^h m^h}^{n_\rho^e m^e}. \tag{15}$$

Here $E_{n_\rho^e m^e}^{(e)}=E_{n_\rho^e m^e}^{(e)}(q=0)$ ($E_{n_\rho^h m^h}^{(h)}=E_{n_\rho^h m^h}^{(h)}(q=0)$) – the resonance energies of electron (hole) transversal movement, P – quasi-momentum, corresponding to the free movement of exciton with the mass $M=\mu_0^{(e)}+\mu_0^{(h)}$ along the Oz axis.

The energy of electron-hole interaction $\Delta E_{n_\rho^h m^h}^{n_\rho^e m^e}$ is approximately obtained using the modified Bethe variational method, presented in details in ref. [7]. According to it, the binding energy is obtained from the minimum of functional [7]

$$\Delta E_{n_\rho^h m^h}^{n_\rho^e m^e}(n_z,\beta)=E_{n_z}(\beta)+\frac{e^2}{\bar{\varepsilon}_0}\langle n_z|\left(\frac{1}{\beta+|z|}-V_{n_\rho^e m^e}^{n_\rho^h m^h}(z)\right)|n_z\rangle. \tag{16}$$

Here β - variational parameter;

$$\langle n_z|=\Psi_{n_z}(z)=A\exp(-\chi(z+\beta))\,U(-\frac{\nu}{2\chi};0;2\chi(z+\beta)), \tag{17}$$

$$\nu=\frac{2\mu}{\hbar^2}\frac{e^2}{\bar{\varepsilon}}, \quad \chi^2=\frac{2\mu}{\hbar^2}E_{n_z}, \quad \bar{\varepsilon}=(\varepsilon_0+\varepsilon_1)/2, \\ \mu=\frac{\mu_0^e\mu_0^h}{\mu_0^e+\mu_0^h}, \tag{18}$$

$$V_{n_\rho^h m^h}^{n_\rho^e m^e}(z)=\frac{e^2}{\bar{\varepsilon}}\int d\boldsymbol{\rho}_e d\boldsymbol{\rho}_h\frac{\left|\varphi_{n_\rho^e m^e}^{(p)}(\boldsymbol{\rho}_e)\,\varphi_{n_\rho^h m^h}^{(p)}(\boldsymbol{\rho}_h)\right|^2}{\sqrt{(\boldsymbol{\rho}_e-\boldsymbol{\rho}_h)^2+z^2}} \tag{19}$$

$p=0,1,2,3,4$

- the effective potential of electron-hole interaction, calculated using the wave functions $\varphi_{n_\rho^e m^e}^{(p)}(\boldsymbol{\rho}_e)$ ($\varphi_{n_\rho^h m^h}^{(p)}(\boldsymbol{\rho}_h)$) of electron (hole) in closed ($\Delta_2\to\infty$) nabnotube; $E_{n_z}(\beta)$ - the energy of bound state (E_{n_z}) along Oz axis, obtained from the equations [7]

$$\begin{cases}\left.\dfrac{\partial\Psi_{n_z}(z)}{\partial z}\right|_{z=0}=0, & \Psi_{n_z}(z)-\text{even}\\ \Psi_{n_z}(0)=0, & \Psi_{n_z}(z)-\text{odd}\end{cases} \tag{20}$$

U - confluent hyper-geometrical function.

As a result, the resonance energies ($E_{n_\rho^h m^h}^{n_\rho^e m^e}$) and widths ($\Gamma_{n_\rho^h m^h}^{n_\rho^e m^e}$) of exciton states and the energies of electron-hole interaction $\Delta E_{n_\rho^h m^h}^{n_\rho^e m^e}$ are obtained.

3. Analysis of the results

The numeric calculation of electron, hole and exciton spectra is performed for the multi-shell open nanotube composed of $GaAs/Al_xGa_{1-x}As$ semiconductors with the parameters: $\mu_0^e=0.063m_0$, $\mu_0^h=0.51m_0$, $\mu_1^e=(0.063+0.083x)m_0$, $\mu_1^h=(0.51+0.25x)m_0$ (m_0 – mass of pure electron in vacuum), $U_0^e=0.57(1.155x+0.37x^2)$ eV, $U_0^h=0.43(1.155x+0.37x^2)$ eV, $E_g=1{,}52$ eV and lattice constant $a_{GaAs}=5.65\,\mathrm{\mathring{A}}$.

In fig.2 we present the shape of distribution function $W_{10}^{10}(E^{(e)},E^{(h)})$ in energy scale (a), the coordinate plane crossing the peak $W_{10}^{10}(E^{(e)},E^{(h)})$ at the half of the height (b) and, as an example, the terms of resonance energies ($E_{10}^{(e)}$, $E_{10}^{(h)}$) and widths ($\Gamma_{10}^{(e)}$, $\Gamma_{10}^{(h)}$) of exciton ground quasi-stationary state obtained at the fixed values of inner wire radius ($\rho_0=10a_{GaAs}$), nanotube thickness ($d=15a_{GaAs}$) and potential barriers thicknesses ($\Delta_1=\Delta_2=4a_{GaAs}$).

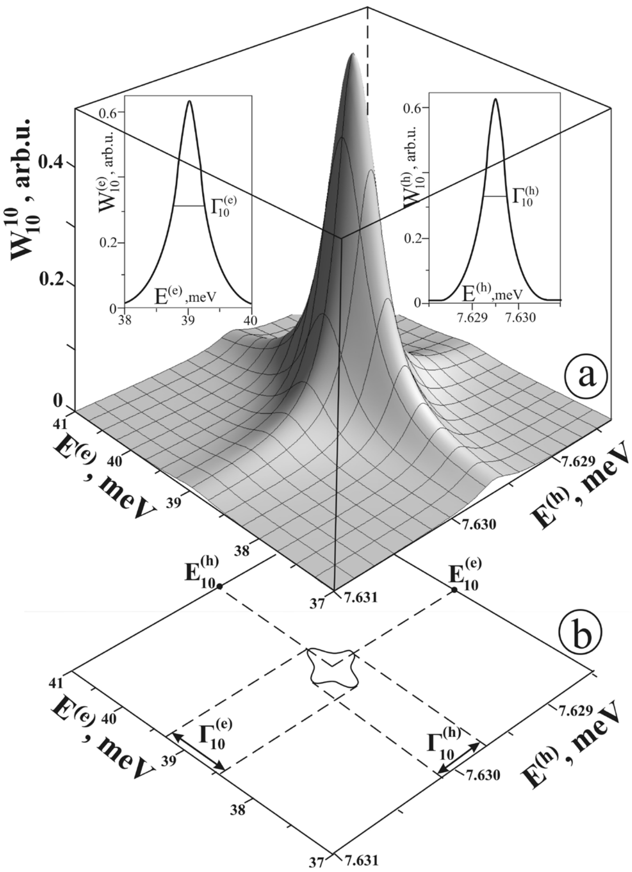

Figure 2. The shape of distribution function $W_{10}^{10}(E^{(e)},E^{(h)})$ in energy scale (a), the coordinate plane crossing the peak $W_{10}^{10}(E^{(e)},E^{(h)})$ at the half of the height (b) at $x=0.4$ and fixed values of inner wire radius $\rho_0=10a_{GaAs}$ and potential barriers thicknesses $\Delta_1=\Delta_2=4a_{GaAs}$.

In fig.3 the electron resonance energies $E_{n_\rho 0}^{(e)}$ (a) and widths $\Gamma_{n_\rho 0}^{(e)}$ (b) and hole ones $E_{n_\rho 0}^{(h)}$ (c) and $\Gamma_{n_\rho 0}^{(h)}$ (d) are presented as functions of nanotube thickness (d) at fixed radius of inner wire $\rho_0=10a_{GaAs}$ and thicknesses of potential barriers $\Delta_1=\Delta_2=4a_{GaAs}$. Fig. 3 a, b proves that both the resonance energies and widths of electron states non monotonously depend on nanotube thickness. Herein, the resonance energies as functions of d are the sequence of horizontal and decaying plots, while at the functions of resonance widths the brightly visible maxima are observed for the small Γ. Horizontal plots in fig. 3a correspond to the states where the electron is located in inner wire with bigger probability. In the states corresponding to the decaying plots the electron is, mainly, located in nanotube. Its increasing thickness causes the decreases of resonance energy.

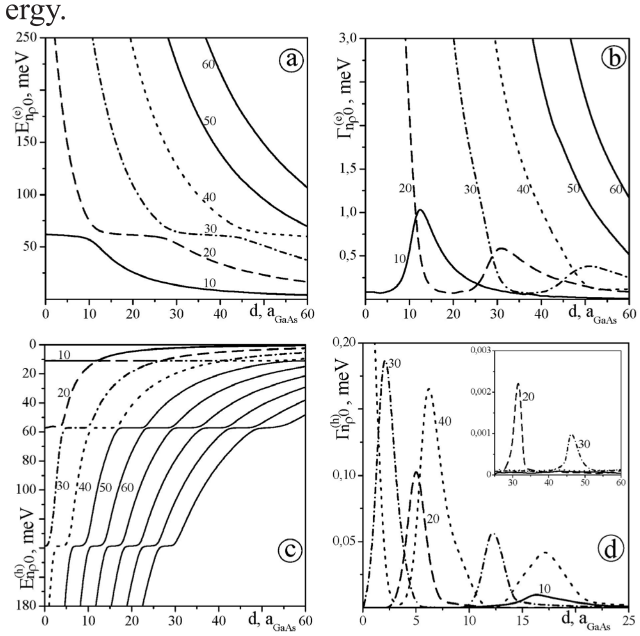

Figure 3. The electron resonance energies $E_{n_\rho 0}^{(e)}$ (a) and widths $\Gamma_{n_\rho 0}^{(e)}$ (b) and hole ones $E_{n_\rho 0}^{(h)}$ (c) and $\Gamma_{n_\rho 0}^{(h)}$ (d) as functions of nanotube thickness (d) at $x=0.4$ and fixed radius of inner wire $\rho_0=10a_{GaAs}$ and thicknesses of potential barriers $\Delta_1=\Delta_2=4a_{GaAs}$.

The dependences of resonance widths on d (fig.3b) are explained in the following way. Let us observe, for example, the ground electron state ($n_\rho=1$, $m=0$): at $d=0$ the nanotube is absent and the electron is localized in inner wire, in order to transit into the outer medium it has to tunnel through the rather strong potential barrier with the thickness $\Delta_1+\Delta_2$. Thus, the resonance width ($\Gamma_{10}^{(e)}$) of energy level is small. The electron penetrates into nanotube more and more when d increases. Now, it has to tunnel through the only one barrier-shell with thickness Δ_2 in order to transit into the outer medium. Consequently, the resonance width of energy level increases, approaching its maximum. Further, it only decays because the resonance energy becomes smaller and the height of the potential barrier effectively increases, respectively.

The function $\Gamma_{20}^{(e)}$ does not look the same as $\Gamma_{10}^{(e)}$ (fig. 3b). One can see that for the small d the electron energy of second quasi-stationary state rapidly decreases when d increases (fig. 3a). The electron is localized in nanotube and its resonance width is rather big but rapidly decays due to the bigger effective height of the potential barrier (fig.3b). It approaches the minimal magnitude at nanotube thickness from $d \approx 15a_{GaAs}$ till $d \approx 25a_{GaAs}$, when the electron is located in inner wire and its energy almost does not depends on d (fig. 3a). The electron energy ($E_{20}^{(e)}$) decays while d increases further. The quasi-particle is localized in nanotube and function $E_{20}^{(e)}$ is similar to $\Gamma_{10}^{(e)}$: at first it increases and then decreases only.

The non monotonous behavior of resonance widths of other energy states is also explained by the different location of electron in the space of multi-shell nanostructure.

We must note that on the contrary to the single open quantum wires, where the higher energy level (over n_ρ quantum number) at fixed m has bigger resonance width [15], in the case of nanotube under study one can see that, for example, when its thickness varies from $d \approx 12a_{GaAs}$ till $d \approx 26a_{GaAs}$, $E_{20}^{(e)} > E_{10}^{(e)}$, however $\Gamma_{20}^{(e)} < \Gamma_{10}^{(e)}$. Such peculiarity of spectral parameters gives opportunity to produce multi-shell nanotubes with the inverse occupied levels, which can be used as active elements of semiconductor lasers.

The effective mass of the hole is an order bigger than that of the electron, thus, the quantum wire with $\rho_0 = 10a_{GaAs}$ contains three energy levels of the hole. Since, in the hole resonance energies as functions of d (fig.3b) one can see three regions of anti-crossings: $E_{n_\rho 0}^{(h)} \approx 10\,meV$, $E_{n_\rho 0}^{(h)} \approx 60\,meV$ and $E_{n_\rho 0}^{(h)} \approx 140\,meV$. Herein, the resonance widths $\Gamma_{n_\rho 0}^{(h)}$ as functions of d , for all quasi-stationary states except the ground one, have more than one maximum (рис.3d). In general case, as it is clear from figures 3a,b,c,d, the number of maxima for $\Gamma_{n_\rho 0}^{(e)}$ ($\Gamma_{n_\rho 0}^{(h)}$) is equal to the number of horizontal plots at the curves $E_{n_\rho 0}^{(e)}$ ($E_{n_\rho 0}^{(h)}$).

In fig. 4a,b the resonance energies $E_{n_\rho^h 0}^{n_\rho^e 0}$ (a) and widths $\Gamma_{n_\rho^h 0}^{n_\rho^e 0}$ (b) of four lowest exciton states are presented as functions of nanotube thickness (d) at $P = 0$, fixed values of inner wire radius $\rho_0 = 10a_{GaAs}$ and potential barriers thicknesses $\Delta_1 = \Delta_2 = 4a_{GaAs}$. At the inset in fig.4a the binding energy of exciton in the ground state is shown as function of d . It is clear that binding energy non monotonously depends on nanotube thickness and its absolute magnitude is not bigger than $20\,meV$. Such situation is quite caused by the complicated character of probability distribution of exciton's electron and hole location in the space of multi-shell nanotube, described in details in ref. [7].

The sum of size-quantized resonance energies of electron and hole are two orders bigger than the absolute magnitude of binding energy. Thus, the dependences of resonance energies of exciton states $E_{n_\rho^h 0}^{n_\rho^e 0}$ on d in low-energy region of the spectrum, fig.4a, are mainly caused by the peculiarities of electron and hole energies behavior. In particular, in these functions one can see the exciton anti-crossing, being the display of the electron and hole ones.

For the observed exciton states the resonance widths $\Gamma_{n_\rho 0}^{(e)} > \Gamma_{n_\rho 0}^{(h)}$ almost in the whole range of d (fig. 3b,d), thus, the resonance widths $\Gamma_{n_\rho^h 0}^{n_\rho^e 0}$ are mainly formed by electron ones. Just therefore, as it is clear from fig.4b, $\Gamma_{10}^{20} \approx \Gamma_{20}^{20}$, and $\Gamma_{10}^{10} \approx \Gamma_{20}^{10}$ everywhere, except the small vicinity $d \approx 5\,a_{GaAs}$.

Finally we should note that the evaluation of electron, hole and exciton life times ($\tau = \hbar / \Gamma$) gives opportunity to assert that all studied states are the typical resonance quasi-stationary states of Breit-Wigner type. They are well localized in the space of multi-shell nanotube and can be observed experimentally.

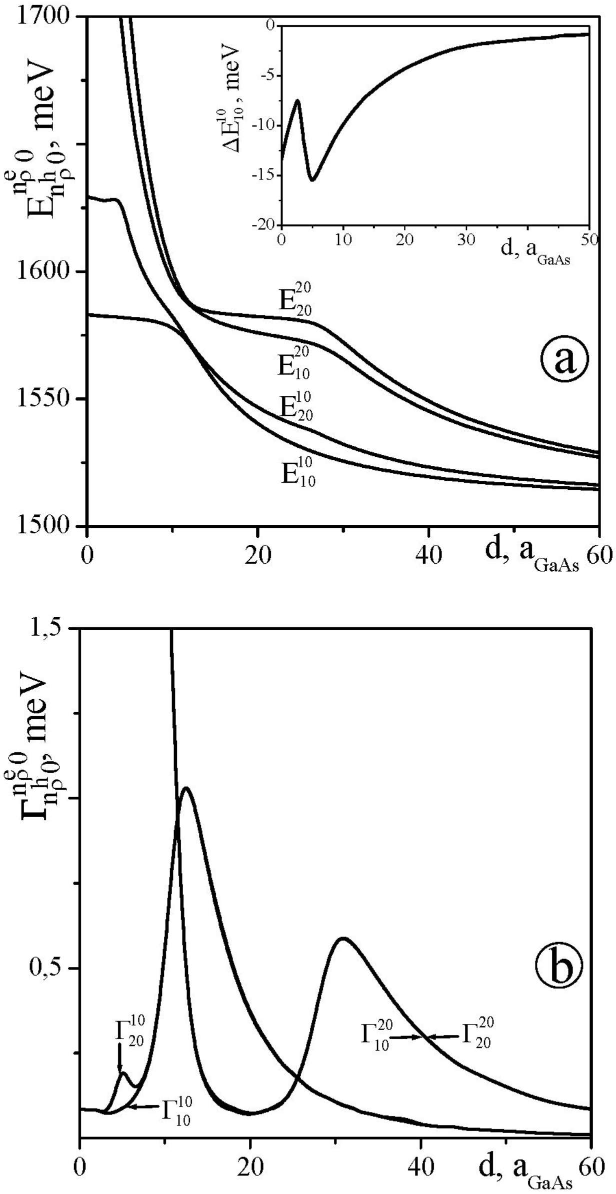

Figure 4. The exciton resonance energies $E^{n^e_\rho 0}_{n^h_\rho 0}$ (a) and widths $\Gamma^{n^e_\rho 0}_{n^h_\rho 0}$ (b) as functions of nanotube thickness (d) at $P = 0$, $x = 0.4$ and fixed values of inner wire radius $\rho_0 = 10a_{GaAs}$ and potential barriers thicknesses $\Delta_1 = \Delta_2 = 4a_{GaAs}$.

3. Conclusions

Within the model of effective mass and rectangular potentials and using the distribution function over the energy for the probability of quasi-particle location in nanosystem, we investigated the spectral parameters of electron, hole and exciton in multi-shell open cylindrical nanotube composed of $GaAs / Al_xGa_{1-x}As$ semiconductors.

Both the resonance energies and widths of quasi-stationary states of all quasi-particleas non-monotonously depend on nanotube thickness. Herein, at the functions of resonance energies one can see the sequence of horizontal and decaying plots, while at the functions of resonance widths the brightly visible maxima and minima are observed. Such behavior of electron, hole and exciton spectral parameters is quite caused by the complicated character of probability distribution of quasi-particles location in the space of multi-shell nanotube.

The resonance widths of electron states are much bigger than that of the hole and the exciton binding energy is two orders smaller than the sum of size-quantized electron and hole resonance energies. Just therefore the dependences of resonance energies of exciton states on nanotube thickness in low-energy region of the spectrum are mainly caused by the peculiarities of electron and hole energy states and the exciton resonance widths almost coincide with electron ones.

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EXCITON SPECTRA IN MULTI-SHELL OPEN SEMICONDUCTOR NANOTUBE

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Summary

The purpose of this paper is the theoretical investigation of electron, hole and exciton spectral parameters in multi-shell open cylindrical semiconductor nanotube composed of the semiconductors $GaAs$ and $Al_xGa_{1-x}As$.

All analytical calculations are performed using the models of effective mass and rectangular potential barriers. Resonance energies and widths of electron (hole) quasi-stationary states are obtained within the exact solution of stationary Schrodinger equation and distribution function of the probability of quasi-particle location in the space of four inner shells of nanotube. The exciton Schrodinger equation is approximately solved using the modified Bethe variational method.

The dependences of resonance energies and resonance widths on nanotube thickness are obtained and analyzed in the paper. Both the resonance energies and widths of quasi-stationary states of all quasi-particleas non-monotonously depend on nanotube thickness. Herein, at the functions of resonance energies one can see the sequence of horizontal and decaying plots, while at the functions of resonance widths the brightly visible maxima and minima are observed. Such behavior of electron, hole and exciton spectral parameters is quite caused by the complicated character of probability distribution of quasi-particles location in the space of multi-shell nanotube.

The resonance widths of electron states are much bigger than that of the hole and the exciton binding energy is two orders smaller than the sum of size-quantized electron and hole resonance energies. Just therefore the dependences of resonance energies of exciton states on nanotube thickness in low-energy region of the spectrum are mainly caused by the peculiarities of electron and hole energy states and the exciton resonance widths almost coincide with electron ones.

Keywords: nanotube, exciton, resonance energy, resonance width

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ЕКСИТОННІ СПЕКТРИ У БАГАТОШАРОВІЙ ВІДКРИТІЙ НАПІВПРОВІДНИКОВІЙ НАНОТРУБЦІ

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Реферат

Метою даної роботи є теоретичне дослідження спектральних параметрів електрона, дірки та екситона у багатошаровій “відкритій” циліндричній напівпровідниковій нанотрубці на основі напівпровідників $GaAs$ та $Al_xGa_{1-x}As$.

Усі аналітичні розрахунки виконано в моделі ефективних мас та прямокутних потенціалів. Резонансні енергії та ширини квазістаціонарного спектра електрона (дірки) знаходяться шляхом точного розв’язку стаціонарного рівняння Шредінгера з використанням граничних умов неперервності хвильових функцій та потоків густин ймовірностей на всіх межах поділу складної нанотрубки та функції розподілу за енергією ймовірності знаходження квазічастинки у наносистемі. Екситонне рівняння Шредінгера розв’язується наближено з використанням модифікованого варіаційного методу Бете та хвильових функцій електрона (дірки) відповідної закритої нанотрубки.

У роботі проаналізовано залежності резонансних енергій і резонансних ширин квазічастинок від товщини нанотрубки.

Показано, що як резонансні енергії, так і ширини квазістаціонарних станів усіх квазічастинок немонотонно залежать від товщини нанотрубки. При чому, якщо у залежностях резонансних енергій ця немонотонність проявляється, як чергування горизонтальних та спадних ділянок, то у залежностях резонансних ширин спостерігаються яскраво виражені максимуми та мінімуми. Така поведінка спектральних параметрів електрона, дірки й екситона цілком зумовлена складним характером розподілу густини ймовірності знаходження квазічастинки у просторі складної нанотрубки.

Встановлено, що резонансні ширини електронних станів набагато більші за ширини діркових, а енергія зв’язку екситона на два порядки менша від суми розмірно-квантованих резонансних енергій електрона і дірки. Саме тому залежності резонансних енергій екситонних станів у низькоенергетичній області спектра від товщини нанотрубки в основному зумовлюються особливостями поведінки енергетичних станів електрона і дірки, а екситонні резонансні ширини практично співпадають із електронними.

Ключові слова: нанотрубка, екситон, резонансна енергія, резонансна ширина