Direct interband absorption of light in a strongly oblate truncated ellipsoidal quantum dot’s ensemble

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Abstract. Within the framework of adiabatic approximation the energy levels and direct interband absorption of light in a strongly oblate truncated ellipsoidal quantum dot’s ensemble are studied. Analytical expressions for the particle energy spectrum and absorption threshold frequencies in the regime of strong size quantization are obtained. Selection rules for quantum transitions are revealed. To facilitate the comparison of obtained results with the probable experimental data, size dispersion distribution of growing quantum dots by the minor semiaxe by two experimentally realizing distribution functions have been taken into account. Distribution functions of Lifshits-Slezov and Gaussian have been considered.

1. Introduction

Development of the novel growth techniques, such as the Stranski–Krastanov epitaxial method etc., makes possible to grow semiconductor quantum dots (QDs) of various shapes and sizes [1-3]. As it is known, the energy spectrum of charge carriers in QDs is completely quantized and resembles the energy spectrum of atoms (“artificial atoms”). A key factor to control the energy level structure of semiconductor QDs is the external geometrical shape. It is shown that even the small change in external shape of QD strongly influences the energy spectrum and other characteristics of such semiconductor structures ([4] and Ref. therein). From the theoretical point of view, spherical QDs are the easier to investigate taking into account their symmetry, which allows to obtain analytical solutions for the energy spectrum, coefficient of absorption, charge carriers mobility, etc. [8,9]. However, modern growth techniques make possible to obtain QDs of different geometrical shapes and sizes. Spherical, cylindrical, pyramidal, lens shaped, ellipsoidal QDs are considered in many works [10-15]. The confinement potential of QD can be approximated by a parabolic potential with a high accuracy in most cases. However, an effective parabolic potential may arise due to QD external shape [5,6].

Theoretical investigations of optical properties of QDs of various shapes are important task for modelling and constructions of new generation semiconductor devices [7]. Investigations of the optical absorption spectrum of various semiconductor structures are a powerful tool for determination

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of many characteristics of these systems: forbidden band gaps, effective masses of electrons and holes, their mobilities, dielectric permittivities, etc. There are many works devoted to the theoretical and experimental study of the optical absorption both in bulk semiconductors and in low-dimensional systems. The presence of size quantization (SQ) essentially influences the absorption mechanism. In fact, the formation of new energy levels of the SQ makes possible new interlevel transitions.

Special interest represents consideration of semiellipsoidal QDs, which two geometrical parameters (semiaxes) allows one to control energy spectrum inside QD.

In this paper the electronic states and direct interband absorption of light in a strongly oblate truncated ellipsoidal QD (SOTEQD) are discussed. Absorption edge and absorption coefficient are obtained in a strong SQ regime. To facilitate the comparison of obtained results with the probable experimental data size dispersion distribution of growing QDs by the minor semiaxe has been taken into account for two experimentally realizing distribution functions. Distribution function of Lifshits-Slezov has been considered in the first model and distribution function of Gauss has been considered in the second case.

2. Theory

Let us consider an opaque strongly oblate truncated ellipsoidal QD (fig. 1 a)). The potential energy of a particle (electron, hole, exciton) in the cylindrical coordinates can be presented in the form

\[
U(X,Y,Z) = \begin{cases} 
0, & \frac{X^2 + Y^2}{a_i^2} + \frac{Z^2}{c_i^2} \leq 1, |Z| \geq -b_i \\
\infty, & \frac{X^2 + Y^2}{a_i^2} + \frac{Z^2}{c_i^2} > 1, |Z| < -b_i 
\end{cases}, \quad c_i \ll a_i ,
\]

(1)

where \(c_i\) and \(a_i\) are the minor and major semiaxes of the SOTEQD, respectively.

![Figure 1. Strongly oblate truncated ellipsoidal QD. a) 3D picture, b) cross-section.](image)

In the regime of strong SQ the energy of the Coulomb interaction between an electron and hole is much less than the energy determined by the walls of the SOTEQD. In this approximation the Coulomb interaction can be neglected. Then the problem is reduced to the determination of the energy states of an electron and hole separately. From the geometrical form of a QD it follows that the particle motion along the Z-direction is faster than in the plane perpendicular to it. This allows one to use the adiabatic approximation [16]. The Hamiltonian of this system in the cylindrical coordinates has the form

\[
\hat{H} = -\frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right\} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial Z^2} + U .
\]

(2)
It can be represented as a sum of the “fast” ($\hat{H}_1$) and “slow” ($\hat{H}_2$) subsystems Hamiltonians in dimensionless quantities:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{U}(r, \varphi, z),$$

where

$$\hat{H}_1 = -\frac{\partial^2}{\partial z^2},$$

$$\hat{H}_2 = \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right].$$

Here $\hat{H} = \frac{\hat{\mathbf{H}}}{E_R}$, $r = \frac{\rho}{a_g}$, $z = \frac{Z}{a_g}$, $e$ and $\mu_r$ are the charge and effective mass of a particle (electron, hole, exciton), correspondingly, $E_R = \frac{\hbar^2}{2m'a_g}$ is the effective Rydberg energy, $a_g = \frac{\mu_r h^2}{m'e^2}$ is the effective Bohr radius of a particle, $\kappa$ is the dielectric permittivity. The wave function is sought in the form

$$\psi(r, \varphi, z) = e^{im\varphi} \chi(z; r) R(r).$$

At a fixed value of the coordinate $r$ of the slow subsystem the particle motion is localized in a one-dimensional potential well with the effective width (fig. 1 b))

$$z(r) = \begin{cases} 2c, & r \geq r_0 \\ \frac{2c}{\sqrt{1 - \frac{r^2}{a^2}, r < r_0}} \\ \frac{2c}{\sqrt{1 - \frac{r^2}{a^2} + b}}, & r < r_0 \end{cases},$$

where $a = \frac{a_1}{a_g}$, $c = \frac{c_1}{a_g}$, $b = \frac{b_1}{a_g}$ and $r_0 = a \sqrt{1 - \frac{b_1^2}{c_1^2}}$. Solving the Schrödinger equation for the first subsystem, we obtain for the energy spectrum of a particle

$$\varepsilon_n(r) = \frac{\pi^2 n^2}{c \sqrt{1 - \frac{r^2}{a^2} + b}}, \quad n = 1, 2, \ldots.$$  

Here $n$ is a quantum number (QN) of the “fast” subsystem. For the low levels of the spectrum a particle is localized mainly in the region $r \ll a$. Based on this one can expand $\varepsilon_n(r)$ into a series

$$\varepsilon_n(r) \approx \alpha_n + \beta_n r^2,$$

where $\alpha_n = \frac{\pi^2 n^2}{(b + c)^2}, \quad \beta_n = \frac{\pi n}{a} \sqrt{\frac{c}{(b + c)^3}}$. Expression (9) enters the Schrödinger equation of the slow subsystem as an effective potential. For the total energy and the wave functions of the system finally we get

$$\varepsilon = \alpha_n + 2\beta_n (N + 1), \quad N = 0, 1, 2, \ldots.$$
Here $N$ is oscillatory QN, $m$ is magnetic QN, $r_n$ is radial QN, $L$ is Laguerre polynomials.

3. Direct interband absorption of light

We proceed to the consideration of the direct interband absorption of light in a SOTEQD in the regime of strong SQ, when the Coulomb interaction between an electron and hole can be neglected. We consider the case of a heavy hole, when $m_e = m_h$. The absorption coefficient is defined by the expression

$$K = A \sum_{\nu, \nu', m} |\Psi_{\nu} \Psi_{\nu'}|^2 \delta \left( h\Omega - E_{\nu} - E_{\nu'} \right),$$

(12)

where $\nu$ and $\nu'$ are the sets of QNs corresponding to an electron and heavy hole, $E_{\nu}$ is the forbidden band width of a bulk semiconductor, $\Omega$ is the frequency of the incident light, $A$ is a quantity proportional to the square of the matrix element, taken over the Bloch functions [17]. Finally, in the regime of strong SQ, for the quantity $K$ and absorption edge (AE) we obtain

$$W_{100} = 1 + \frac{\pi^2 d^2}{\left( b_1 + c_1 \right)^2} + 2\pi d^2 \frac{c_i}{a_i \sqrt{\left( b_i + c_i \right)}}$$

(14)

where $W_{100} = \frac{h\Omega_{100}}{E_g}$ and $d = \frac{\hbar}{\sqrt{2\mu E_g}}$. Expression (14) characterizes the dependence of the effective forbidden band width on the semiaxes $a_i$ and $c_i$. The AE shifts to the short-wave region with decrease in the both semiaxes, but the dependence on the minor semiaxis is stronger. Consider now the selection rules for QNs. For the magnetic QN the transitions between the levels with $m = -m'$ are allowed, and for the QN of the first subsystem – the transitions with $n = n'$. For the oscillatory QN the transitions for the levels with $N = N'$ are allowed. Note that the analytic form of expression (13) is presented with allowance for the mentioned selection rules of QNs.

So far we have studied the absorption of a system consisting of semiconductor QDs having identical dimensions. For comparison of the obtained results with experimental data, one has to take into account the random character of SOTEQD dimensions (or semiaxis) obtained in the growth process. The absorption coefficient should be multiplied by concentration of QDs. Instead of distinct absorption lines, account of size dispersion will give a series of maximums. In the first model we use the Lifshits-Slezov distribution function [9]:

$$P(u) = \begin{cases} 3^4 \bar{c} u^2 \exp \left( -1/2u/3 \right) & u < 3/2 \\ 2^{3/2} (u + 3)^{3/2} (3/2 - u)^{1/2} & u = \frac{b + c}{b + c}, \\ 0, u > 3/2 \end{cases}$$

(15)

where $\bar{c}$ is some average value of the semiaxis. In the second model the Gaussian distribution function is used (see e.g. [18]):
\[ P(u) = C e^{-\frac{(u-u_0)^2}{\sigma^2}}. \]  

(16)

Two types of QDs ensembles with symmetric and asymmetric distributions can be formed using these two distribution functions specifying the growth process. Gaussian distribution describes the symmetric case and the Lifshits-Slezov distribution describes the asymmetric case. With a consideration of size distribution function the absorption coefficient is defined by the following expression

\[ K = A \sum_{u_0, u} \int \frac{1}{\sqrt{\lambda_1^2 + 4 \lambda_1 \lambda_2}} \left( \frac{2 \lambda_2}{\sqrt{\lambda_1^2 + 4 \lambda_1 \lambda_2 - \lambda_3}} \right)^2 P(u) dq \left( \frac{\hbar \Omega - E_g}{E_g} \right). \]  

(17)

In the strong SQ regime, with account of general size distribution function \( P(u) \), we obtain for the absorption coefficient corresponding formula:

\[ K = \frac{A}{E_g} \sum_{n,n',a} \lambda_1 \left( \frac{\hbar \Omega - E_g}{E_g} \right) \left( \frac{d}{b_1 + c_1} \right)^2 \left( \frac{\pi n d^2 (N + 1)}{a_i} \right) \frac{\sigma}{\sqrt{\left( \frac{b_1}{b_1 + c_1} \right)^4}}. \]  

(18)

4. Discussion

As it is seen from formula (10), the energy spectrum of CCs in a SOTEQD has equidistant character. These results is true only for the low levels of the spectrum (for small values of QNs), when the adiabatic approximation is applicable. Numerical calculations for the regime of strong SQ were carried out for a GaAs QD with the following parameters: \( m_e' = 0.067 m_e, \ m_h' = 0.12 m_e, \ \kappa = 13.8, \ E_g = 5.275 \text{meV}, \ a_i = 104 \text{Å} \) and \( a_h = 15 \text{Å} \) are the effective Bohr radii of an electron and hole, \( E_g = 1.43 \text{eV} \) is the forbidden band width of a bulk semiconductor. In the regime of strong SQ the frequency corresponding to the transition between the equidistant levels (for the value \( n = 0 \)), for fixed values \( a = 2a_e, \ c = 0.5a_e \) and \( b = 0.2a_e \) is \( \omega_{10} = 1.85 \times 10^4 \text{s}^{-1} \), which corresponds to the infrared region of the spectrum. At the same value of the QN but with \( a = 2a_e, \ c = 0.4a_e \) and

Figure 2. Dependences of the AE on the minor semiaxis of the SOTEQD at a fixed value of the major semiaxis.

Figure 3. Dependences of the AE on the major semiaxis of the SOTEQD at a fixed value of the minor semiaxis.
$b = 0.2a_c$ we have $\omega' = 2.5 \times 10^4 \text{s}^{-1}$, which is 1.35 times as much as before. As it is seen from formula (10), with increasing semiaxes the particle energy decreases, and it is more “sensitive” to the variations of the minor semiaxis due to SQ contribution. It should be noted that with increasing semiaxes the energy levels become closer together, but remain equidistant.

Figures 2 and 3 present the dependences of the AE on the minor and major semiaxes of a SOTEQD, respectively. With decreasing semiaxes the absorption edge increases, which is a consequence of the SQ increase (the “effective” forbidden band width increases). As can be seen from the plots, the change in the AE manifests itself clearly in the dependence on the minor semiaxis. For the same reason the curves corresponding to different values of the minor semiaxis (fig. 2) provide a larger shift than in the opposite case (fig. 3).

Figures 4 and 5. Dependencies of the absorption coefficient on the frequency of incident light for the first two equidistant families in the case of Gaussian distribution (The sum of absorption coefficient for all transitions). The Lifshits-Slezov distribution.

Fig.4 illustrates the dependence of absorption coefficient $K$ on the frequency of incident light for the first two equidistant families in the case of Gaussian distribution, when $\overline{c}_i = 50 \text{Å}$ and $a_i = 250 \text{Å}$. The sum of the absorption coefficients corresponding to the separate transitions are also presented on the top of the right side of the figure.
As it is mentioned above, instead of distinct absorption lines, consideration of size dispersion will give a series of maxima. Fig.5 illustrates the same dependence for the Lifshits-Slezov distribution case. Note that both in the model of Gaussian distribution and in the model of Lifshits-Slezov QDs distribution a single distinctly expressed maximum of absorption is observed. When the frequency of light is increased, the second weakly expressed maximum can be observed. Further increase of the incident light frequency results in a fall of absorption coefficient. Fig.6 illustrates the dependencies of the absorption coefficient on the frequency of incident light for both cases.

Schematic diagrams for appropriate transitions where the absorption of light is present are depicted on the fig.7 to understand in detail the process of absorption. From the comparison of diagram and fig.4 (fig.5), it is obvious that first clear expressed maximum corresponds to the $n = n' = 1$ transition family and weak expressed picks are the result of the transitions between quidistant levels. The second weaker maximum corresponds to the $n = n' = 2$ transition family. It is also obvious from fig.4 (fig.5) that the intensity corresponding to the above mentioned family is weaker than the first maximum. This is a result of the small value of the electron and hole wave functions overlapping integral, which means that the transition probability decreases.

5. Conclusion

The energy levels of electrons in SOTEQD are shown to be equidistant and levels of “slow” subsystem are arranged on the levels of “fast” subsystem. These results are true only for the low levels of the spectrum or for small values of QNs, when the adiabatic approximation is applicable. It is shown that with increasing semiaxes the particle energy decreases, and it is more “sensitive” to the variations of the minor semiaxes due to SQ contribution. Red shift of absorption threshold has been observed depending on the values of geometrical sizes of QD.

6. References

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