Analysis of electron energy spectrum in type II core/shell quantum dots

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Abstract. We investigated the peculiarities of the electron energy spectrum in type II core/shell quantum dots. It is shown that the presence of the shell with energy bands shifted relative to the ones in the core gives additional possibilities to control energy level positions.

1. Principal types of core/shell quantum dots

One of the main objects of low-dimension semiconductor heterostructure physics is so-called quasi-zero-dimensional systems or quantum dots (QDs). There have been a lot of experimental [1, 2] and theoretical [3, 4] researches of QDs with various geometrical shapes. Recent nanotechnology trends are related to the generation of core/shell QDs [5, 6]. Like in the classical heterotransition theory, two main core/shell QD types can be pointed out.

Energy gaps in semiconductors forming type II QDs (figure 1) are comparable but the band edges are shifted one relative to another. It is energetically favorable for photo-excited charge carriers to stay within different regions of such a QD, e.g. for an electron to stay inside the shell, and for a hole to stay inside the core.

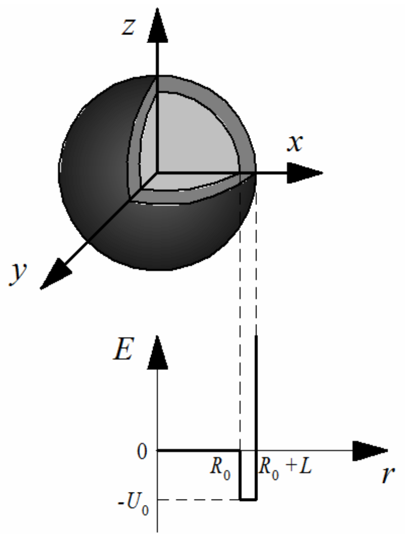

Figure 1. Scheme of type II core/shell quantum dot and the electron potential energy vs distance.

Such quantum dots show the spatial separation of charge carriers and thus they are promising for the systems with a long lifetime of electron-hole pairs due to the reduced overlapping of the electrons

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and holes wave functions. Other effects in type II QDs are an effective energy gap narrowing and a luminescence maxima shift to the red spectral range.

The shell of a type I QD consists of a wide band semiconductor, while the core is a narrow band one. This passivates surface states and localizes electron-hole pairs inside the core. This approach is used to increase the QD luminescence effectiveness.

The aim of this study is to develop a theory of the energy spectrum in type-II core/shell quantum dots.

2. Electron energy spectrum calculations in Type II core/shell quantum dot

The problem under study is being solved using the rigid wall model. The stationary Schrödinger equation in the effective mass approximation is

$$-\frac{\hbar^2}{2m(r)}\nabla^2\psi + U(r)\psi = E\psi . \qquad (1)$$

The potential $U(r)$ and the electron effective mass $m(r)$ inside the QD are expressed in the following way:

$$U(r) = \begin{cases} 0 & r \le R_0 \\ -U_0 & R_0 < r \le R_0 + L \\ \infty & r > R_0 + L \end{cases} , \qquad (2)$$

$$m(r) = \begin{cases} m_1^* & r \le R_0 \\ m_2^* & R_0 < r \le R_0 + L \end{cases} , \qquad (3)$$

where U_0 is the potential barrier height, m_1^*, m_2^* are the effective masses of electrons inside the core and the shell, R_0 is the core radius, and L is the shell thickness.

Using the boundary condition that the wave function vanishes on the QD boundary the solution of the equation (1) determining the energy spectrum of the electrons with energies of $U_0 < E_2 < 0$ can be obtained in the form of:

$$E_2 = \frac{\hbar^2 \xi_{nl}^2}{2m_2^*(R_0 + L)^2} - U_0 , \qquad (4)$$

where ξ_{nl} is the n-th root of the Bessel function of the l-th kind.

The equality and continuity of the wave functions at the QD core/shell border defines the energy spectrum of electrons with energies of $E_1 > 0$:

$$m_2 \left.\frac{dj_l(k_1 r)}{dr}\right|_{r=R_0} = m_1 \frac{j_l(k_1 R_0)}{j_l(k_2 R_0)} \left.\frac{dj_l(k_2 r)}{dr}\right|_{r=R_0} . \qquad (5)$$

Figure 2 shows the results of numerical analysis of expressions (4) and (5) for electrons in the type II core/shell CdTe/CdSe quantum dots with the following parameters: the effective masses of electrons are $m_{CdTe} = 0.14m_0$ and $m_{CdSe} = 0.13\ m_0$, where m_0 is the free-electron mass; $U_0 = 0.60$ eV; $l = 1$. The analysis shows that the number of discrete levels with $U_0 < E_2 < 0$ is finite and, moreover, the increase in core thickness from 2 to 3 nm at a fixed QD radius leads to an appearance of extra energy levels. When R_0 values are low, the probability of the electron location in the QD core is low as well, that leads to energy oscillations (figure 2 (a)). At higher core radius electrons occupy stable positions, oscillations are terminated, and charge carrier energies decrease significantly (figure 2 (b)). Furthermore, it can be seen that as the size of the QD core increases, the energy levels converge, and the quantum size effects at room temperature for $R_0 > 10$ nm become unobservable.

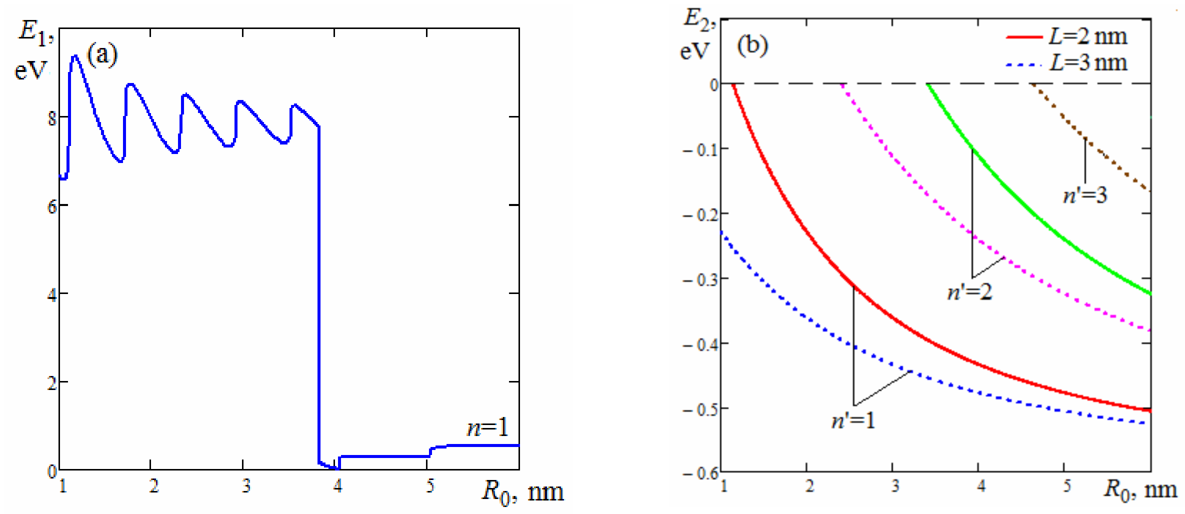

Figure 2. Energy spectrum of the electron as a function of the radius of the type II core/shell quantum dot: (a) $E_1 > 0$; (b) $-U_0 < E_2 < 0$.

The results obtained show a complicated dependence of the electron energy spectrum on the QD radius. Due to the presence of the shell with the energy bands shifted relative to the ones in the core, there appear additional possibilities to control the positions of the energy levels.

3. Conclusions

In this study we suggest a theory of the energy spectrum in type-II core/shell quantum dots, according to which there are two groups of discrete energy levels corresponding to energies of $E_1 > 0$ and $-U_0 < E_2 < 0$. As an example, the numerical calculations for electrons in the CdTe/CdSe QD were made and their results were analyzed. The developed model can be used to obtain quantum dots with electrophysical and optical properties needed for a new generation of optical and nanoelectronic devices.

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