

1 Introduction

Semiconductor nanostructures have been the subject of intensive research over the last three decades. Due to the fact that the energy spectrum of the nanostructure can be flexibly controlled, the creation of next-generation semiconductor devices with controlled characteristics has become possible.¹ Semiconductor nanostructures are divided into three large classes:²⁻⁵

- quantum wells (QWs),
- quantum wires (QWr), and
- quantum dots (QDs).

An important feature of these systems is the presence of the quantized part of charge carriers in the energy spectrum, which is localized in them. In the case of QWs and QWr, the particle spectrum has a hybrid nature: both continuous and quantized parts of the spectrum exist. The spectrum of charge carriers is completely quantized in the QDs, and in this respect, it resembles individual atoms. It is not accidental that QDs are often called “artificial atoms.” Figure 1 demonstrates the quantization effect on a QW.

QWs were initially called size-quantized films. One of the mechanisms of QW growth is the growth of a thin semiconductor layer with a narrower bandgap on a wide-band substrate with a layer of a wide-band semiconductor deposited from above, for instance, GaAs between $\text{Ga}_{1-x}\text{Al}_x\text{As}$ layers. The band diagram of such a “sandwich structure” is shown in Fig. 2.

As this figure shows, the electron entering the conduction band in GaAs and approaching the boundaries of the QW feels the presence of a quantum confinement due to the jump in energy of the forbidden band at the boundary of the transition QW–surrounding medium. In other words, a certain confining potential arises that leads to particle localization in the region of L , where L is the thickness of the QW. The phrase “thin layer” for the narrowband semiconductor has a fundamental importance. Thicknesses on the order of several tens of angstroms are discussed here. In this case, the effective de Broglie length of the electron becomes a quantity on the order of the thickness of the QW:²⁻⁵

$$\lambda_D^* \sim L, \quad (1)$$

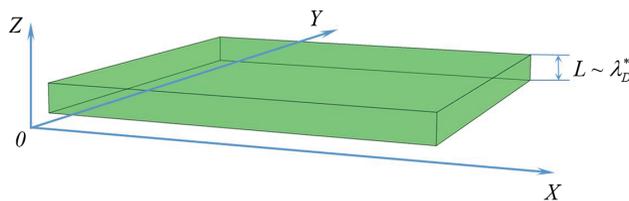


Figure 1 Quantum well.

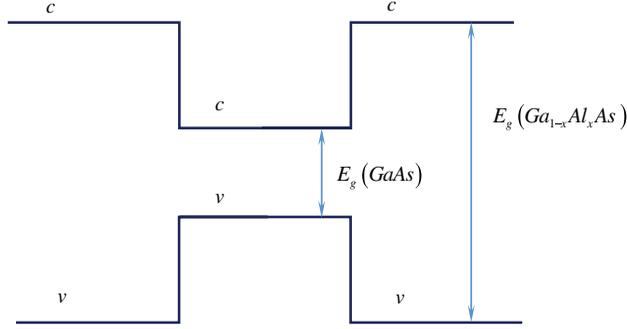


Figure 2 Band diagram of a Ga_{1-x}Al_xAs/GaAs QW.

and therefore, the quantization of energy levels in the given direction becomes significant. Since the quantization of the levels is related to the dimensions of the semiconductor, this quantization is usually called the dimensional.

From a mathematical point of view, the influence of the walls of the QW can be taken into account by introducing the certain confining potential $V_{\text{conf}}(\vec{r})$ into the Schrödinger equation. In the case of QW, this potential will depend only on the z -coordinate. In the simplest approximation of impermeable rectangular walls, $V_{\text{conf}}(z)$ will have the following form:

$$V_{\text{conf}}(z) = \begin{cases} 0, & 0 \leq z \leq L, \\ \infty, & z < 0, z > L. \end{cases} \quad (2)$$

In the plane XOY , the motion of the electron will be quasicontinuous. Thus, the Schrödinger equation will be written as

$$-\frac{\hbar^2}{2\mu_e} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) + V_{\text{conf}}(z) \psi(x, y, z) = E \psi(x, y, z), \quad (3)$$

where μ_e is the effective mass of the electron. The effective mass of the electron as a scalar quantity is considered here. Based on the “separation of variables” method, it can be shown that the wave function has the following form:

$$\psi_n^{k_x, k_y}(x, y, z) = \frac{1}{\sqrt{S}} e^{i(k_x x + k_y y)} \sqrt{\frac{2}{L}} \sin \frac{\pi n}{L} z, \quad (4)$$

and for the energy spectrum,

$$E_n^{k_x, k_y} = \frac{\hbar^2(k_x^2 + k_y^2)}{2\mu_e} + \frac{\pi^2 \hbar^2 n^2}{2\mu_e L^2}, \quad (5)$$

where n is the quantum number, and S is the area of the QW in the XOY plane.

As follows from Eq. (5), one part of the one-electron spectrum is continuous, and the other is discrete. Moreover, the quantized energy has only one degree of freedom (axis OZ). In the case of the QWr, the fraction of the energy of size quantization (SQ) will increase. Finally, in the case of a QD, the region of electron limitation in all three directions becomes a quantity on the order of λ_D^* , and therefore, the spectrum of the electron will be completely quantized. In the case of a rectangular parallelepiped with sides L_1 , L_2 , and L_3 (Fig. 3), taking into account the impermeability of the walls of the QD for the spectrum,

$$E_{n_1, n_2, n_3} = \frac{\pi^2 \hbar^2}{2\mu_e} \sum_{i=1}^3 \left(\frac{n_i}{L_i} \right)^2. \quad (6)$$

The equation shows that the spectrum of the electron can be flexibly manipulated by changing L_1 , L_2 , and L_3 . In this case, the interlevel distances will also vary, and as a result, it will be possible to manipulate various characteristics of the QD. In particular, it will be possible to manipulate the optical parameters of the QD.

Many papers have been devoted to the optical properties of QDs (see, for example, Refs. 6–11). Because of the fundamental rearrangement of the band structure of QDs compared to massive samples, the form of the interband absorption curve changes significantly. Instead of the root function in the case of a bulk semiconductor, the interband absorption curve has the form of alternating delta peaks for a QD, which is a consequence of the nature of the density function of states in zero-dimensional structures (Fig. 4).

One of the most important optical characteristics of the QD is the edge of the interband absorption. It is a certain threshold frequency from which interband transitions can be realized. There, the edge of interband absorption can be flexibly controlled in the QD, changing both the size of the QD and its geometry, and also

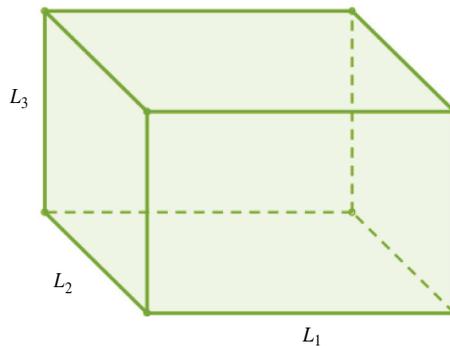


Figure 3 QD in the form of a rectangular parallelepiped.

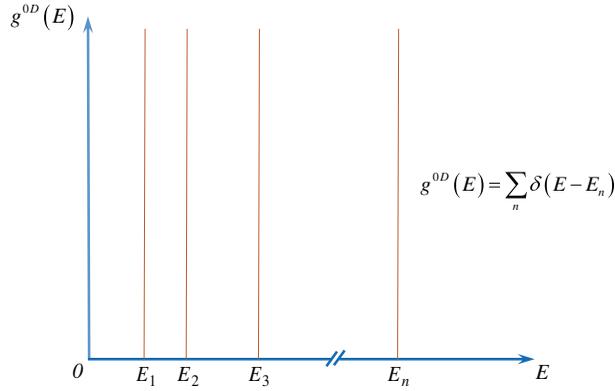


Figure 4 The density of states for QDs.

superimposing external fields. One of the pioneering works devoted to the optics of QDs is by Efros and Efros,¹² in which the interband absorption of light was considered in the semiconductor spheres imbedded in a dielectric matrix.

Within the framework of the infinitely deep spherical well model, interband transitions were considered under different modes of SQ. This work was preceded by experiments on the study of optical absorption in semiconductor spheres imbedded in a dielectric matrix, and the distributions of the balls along the radii were described by Efros and Efros in the framework of the Lifshitz–Slezov theory. The theory developed in the paper¹² was in good agreement with the data of the experiment (see Ref. 5 in Efros and Efros¹²).

The authors also studied the effect of the anisotropy of the band structure on the character of optical transitions in spherical lead sulfide and selenide QDs.¹³ It was shown that a strong anisotropy of the band structure of PbS leads to the appearance of optical forbidden transitions in the isotropic approximation. Direct absorption in a quantum cube was discussed in the work,¹⁴ and the confining potential of a QD was described within the framework of the rectangular, infinitely deep well. Electronic states in ellipsoidal QDs were considered in Refs. 15–18.

In the framework of the adiabatic approximation, the energy levels of the electron and the direct absorption of the light in strongly oblate and prolate ellipsoidal QDs in the presence of electric and magnetic fields were studied in Ref. 15. The energy levels and direct interband absorption of light in strongly oblate and prolate ellipsoidal QDs were studied in Ref. 16. Analytic expressions for the energy spectrum of the particle and the threshold absorption frequency were obtained for three regimes of SQ. In order to facilitate a comparison of the results obtained with the expected experimental data—the dimensional dispersion of the small semi-axis of grown QDs in the modes of strong and weak SQ—we take into account two experimentally realized distributions; Lifshitz–Slezov and Gauss. Electronic states and optical transitions in ring-like and layered structures are considered in various papers.^{19–24}

Interband and intersubband transitions in quantized spherical layers are considered in the presence of external fields (electric and magnetic) in Refs. 19, 23, and 24. For the case of strong SQ, the interband absorption coefficient in a layered cylindrical QD is studied in the presence of magnetic and electric fields in Ref. 25. The absorption coefficient for various orientations of the electric field is calculated. Thus, in the process of the theoretical description of the absorption in an ensemble of QDs at the first stage of the investigation, it is necessary to clarify two important circumstances. First, you need to have information about the geometric form of the QD and its dimensions, and second, you need to find out how strongly QDs are interacting with each other (at least in the pair approximation). If this interaction is weak, then it is possible to consider interband transitions in a separate QD and then average the size distribution of the QDs.¹⁴

2 Fundamental Absorption in Quantum Dots

Before proceeding to specific problems, first let us give some basic concepts of the theory of direct optical absorption in semiconductors.²⁶ The electromagnetic field of a light wave in vacuum can be described by means of the vector potential $\vec{A}(\vec{r}, t)$ and the scalar potential $\varphi(\vec{r}, t)$. Electromagnetic potentials are determined to be accurate within a gradient transformation, which allows us to put the scalar potential equal to zero. Then the electric and magnetic fields are equal:

$$\begin{aligned}\vec{E} &= -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}, \\ \vec{H} &= \text{rot} \vec{A}.\end{aligned}\quad (7)$$

We can additionally subordinate the vector potential to Lorentz's law, $\text{div} \vec{A} = 0$. In this case, $A(\vec{r}, t)$ responds to the wave equation. The Hamiltonian of an electron with charge $-e$ in the periodic field of a crystal $V(\vec{r})$ and the electromagnetic field of a light wave have the following form:

$$\hat{H} = \frac{1}{2\mu_e} \left[\hat{\vec{p}} + \frac{e}{c} \vec{A}(\vec{r}, t) \right]^2 + V(\vec{r}). \quad (8)$$

Neglecting the quadratic term of \vec{A} , we find that the perturbation associated with the action of the light wave in the Hamiltonian equals

$$\hat{H}' = \frac{e}{\mu_e c} \vec{A} \hat{\vec{p}} = -\frac{ie\hbar}{\mu_e c} \vec{A} \vec{\nabla}. \quad (9)$$

For a plane monochromatic wave with a frequency ω , the number of transitions $\nu \rightarrow \nu'$ per unit time for a unit of volume for which the law of conservation of energy $\hbar\Omega = E_g \pm E_\nu \pm E_{\nu'}$, and the law of conservation of the quasimomentum or wave vector $k_1 = k_2$ equals