Modeling and analysis of functional characteristics of QD-InAs/GaAs heterointerface with multi-barrier layers

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Abstract. The article is devoted to the problem of studying the functional characteristics of heterointerfaces with quantum dots InAs by methods of mathematical and simulation modeling. A solution to the problem in the form of a developed mathematical model of a structure with quantum dots InAs with two types of barrier layers GaAs and AlGaAs is proposed. It is shown that using the quasi-drift-diffusion model in combination with the solution of the Schrödinger equation in the potential well of a quantum dot, it is possible to construct the energy structure of the layer-by-layer heterointerface design with the possibility of modeling functional characteristics, in particular, the spectral dependence of the external quantum efficiency and the dark current-voltage characteristic.

1. Introduction
The development of the scientific direction of using quantum-sized structures in modern devices for converting solar energy (photodetectors) also requires the development of methods for their mathematical modeling as the main tool for pre-growth research. In approaches to mathematical modeling of optoelectronic structures with arrays of self-organizing quantum-sized objects (quantum dots), there are currently two problems of both fundamental and applied nature. First, the mathematical model should reflect as closely as possible the constructive structure of a photoconverter with arrays of quantum-size objects, i.e. be object-oriented, including the ability to controllably change the geometry of the layers, the composition of the matrix (the layer surrounding the quantum dot), the size and shape of the quantum dots [1]. Secondly, the model should provide a high speed of calculations with a minimum number of iterative steps, but at the same time, without violating the reliability of the results [2].

2. Target of research
To construct a mathematical model of functional characteristics, a layer-by-layer heterointerface design based on InAs quantum dots with two types of barrier layers was developed: GaAs and AlGaAs. The thicknesses of the layers of the structure correspond to the technological thicknesses of a real optical device, the impurity components and doping concentrations also correlate with the experimental data on obtaining this type of heterointerfaces. A schematic representation of the structure with an array of InAs quantum dots is shown in Figure 1.
Figure 1. Simulated quantum dot heterostructure

Rear Au contact, $n^+$-GaAs substrate (thickness ~ 500 nm, doping level ~ $10^{18}$ cm$^{-3}$), which is a buffer layer; $n$-GaAs layer (thickness ~ 150 nm, doping level ~ $7 \times 10^{16}$ cm$^{-3}$) - lower matrix layer of the quantum dot array; an array of two layers of InAs nanoislands (~ 6 ML thick) separated by a wetting and barrier layers; GaAs/AlGaAs barrier layers with a technological thickness of 30 nm; spacer passivating layer $n$-GaAs/AlGaAs 150 nm thick. ($doping$ level ~ $7 \times 10^{16}$ cm$^{-3}$), $p^+$-GaAs layer (thickness 300 nm, doping level is $10^{18}$ cm$^{-3}$), frontal Au contact to the $p^+$-region.

3. Mathematical methods of the model

Initially, to build a model, it is necessary to determine the boundary conditions:

- A pyramidal shape of quantum dots in an infinite semiconductor matrix is chosen.
- The deformation inhomogeneity does not change the energy spectrum of electronic states, since InAs quantum dots are electron trapping centers [3].
- The model considers interband transitions; therefore, the model of the electronic structure can be substantially reduced by assuming that the quantum dot contains one discrete level for each of the allowed bands.
- The heterointerface model is based on a pin structure with an intermediate subzone [4].
- We neglect the Coulomb interaction of electrons in discrete bands and the splitting of the valence band into levels of heavy and light holes.
- The following thermal components were not taken into account [5]:
  - a change in the shape of the lines of the photoluminescence spectrum due to the ejection of charge carriers from the quantum dot into the wetting layer;
  - broadening of the spectral maximum due to the non-uniformity of the sizes of quantum dots.
- A quantum dot is a quantum well in a band structure, where the width of the well is equal to the dimensions of the quantum dot [6].

The main approaches to modeling quantum dots should solve two problems: taking into account the influence of elastic deformation forces and determining the electronic structure. Elastic deformation plays a decisive role in the process of self-organization and growth of quantum dots, since it significantly alters the band structure of a semiconductor [8]. To determine the field of elastic deformation forces in the developed model, the model of the field of valence forces was used, which takes into account the position of atomic nuclei and the distance only to neighboring atoms in the lattice. The Keating potential is used to describe the interaction of elastic deformation forces with a semiconductor [9]:

\[
\text{Keating potential} = k_1 \left( \frac{r_{ij}}{a} \right)^{\alpha} \left( 1 - \frac{r_{ij}}{a} \right) - k_2 \left( \frac{r_{ij}}{a} \right)^{\beta}
\]

where $r_{ij}$ is the distance between two atomic nuclei, $a$ is the equilibrium interatomic distance, and $k_1, k_2, \alpha, \beta$ are constants.
The basic equations of photoconversion structures are the Poisson equation and the continuity equation. Taking Gauss and Maxwell’s law:

\[ \nabla E = \frac{\rho}{\varepsilon} \]  \hspace{1cm} (2)

\[ \nabla B = \mu J + \frac{1}{\gamma^2} \frac{\partial E}{\partial t} \]  \hspace{1cm} (3)

where \( E \) is the energy of the electric field, \( \rho \) is the density of charge carriers, \( \varepsilon \) is the dielectric constant of the material, \( B \) is the magnetic field, \( \mu \) is the magnetic permeability, \( J \) is the current density, \( v \) is the speed of light in the medium, we can determine the electric potential in the Poisson equation and the equation continuity [10]:

\[ \nabla^2 V = -\frac{\rho}{\varepsilon} \]  \hspace{1cm} (4)

\[ \nabla J = -\frac{\partial \rho}{\partial \varepsilon} \]  \hspace{1cm} (5)

By including the components of the generation and recombination mechanisms into the continuity equation, we obtain the continuity equations for electrons and holes:

\[ \frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n - R_n + G \]  \hspace{1cm} (6)

\[ \frac{\partial p}{\partial t} = -\frac{1}{q} \nabla J_p - R_p + G \]  \hspace{1cm} (7)

where \( t \) is the time, \( q \) is the electron charge, \( n \) and \( p \) are the concentrations of electrons and holes, \( J_n \) and \( J_p \) are the densities of the electron and hole current, \( R_n \) and \( R_p \) are the rates of recombination of electrons and holes, and \( G \) is the rate of generation of electron-hole pairs. For the subsequent solution, it is necessary to determine the density of states of charge carriers; however, in the quantum model, the Fermi-Dirac distribution undergoes changes associated with the quantum effect. As mentioned above, quantum dots in the model are represented as quantum wells. Therefore, we will deal with a two-dimensional electron gas and the equations for the distribution statistics will take the following form:

\[ N(E) = \frac{2m_e^*}{\pi \hbar^2} \sum_i \Theta(E - E_i) \]  \hspace{1cm} (8)

where \( \Theta \) is the Heaviside step function, \( h \) is Planck’s constant. Next, we get a two-dimensional expression for the electron concentration:

\[ n = \frac{2m_e^* kT}{\pi \hbar^2} \sum_i \ln(1 + \exp(-\frac{E_i - E_F}{kT})) \]  \hspace{1cm} (9)

To take into account the localization of the charge over the entire width of the quantum well, we introduce the corresponding plane wave function (expression for the direction of the growth axis of the structure - \( x \)):
\[ n(x,T) = 2 \frac{m^*_n kT}{\hbar^2} \sum_i \left| \Psi_i(x) \right|^2 \ln(1 + \exp(-\frac{E_i - E_F}{kT})) \] \quad (10)

\[ p(x,T) = 2 \frac{m^*_p kT}{\hbar^2} \sum_j \left| \Psi_j(x) \right|^2 \ln(1 + \exp(-\frac{(E_F - E_j)}{kT})) \] \quad (11)

For further solution, it is necessary to know the band structure (the location of the valence and conduction bands), which is obtained by solving the Schrödinger equation with the participation of the effective masses of charge carriers (below are the expressions for electrons and holes, respectively):

\[ \frac{\hbar^2}{2m_n} \Delta \Psi_i + E_C \Psi_i = -\frac{\partial \Psi_i}{\partial t} \] \quad (12)

\[ \frac{\hbar^2}{2m_p} \Delta \Psi_j + E_V \Psi_j = -\frac{\partial \Psi_j}{\partial t} \] \quad (13)

The potential model is a solution of the Schrödinger equation in the form of two transcendental equations of the form:

\[ \cos k(a + b) = \frac{Q^2 - K^2}{2QK} \sinh(Qb) \sin(Ka) + \cosh(Qb) \cos(Ka) \quad E < V_0 \] \quad (14)

\[ \cos k(a + b) = -\frac{\beta^2 - K^2}{2\beta K} \sin(fb) \sin(Ka) + \cos(fb) \cos(Ka) \quad E > V_0 \] \quad (15)

where \( K, Q, \beta \) are local wave vectors:

\[ K^2 = \frac{2mE}{\hbar^2} \quad V = 0 \quad \forall E \] \quad (16)

\[ Q^2 = \frac{2m(V_0 - E)}{\hbar^2} \quad V = V_0 \quad E < V_0 \] \quad (17)

\[ \beta^2 = \frac{2m(E - V_0)}{\hbar^2} \quad V = V_0 \quad E > V_0 \] \quad (18)

The main criterion in simulating photoluminescence is taking into account the mechanisms of recombination of charge carriers and the concentration of charge carriers in the allowed level. The following mechanisms are included in the developed model [11]:

- Recombination according to the Shockley-Reed-Hall model. In this case, the rate of recombination of electrons and holes is assumed to be equal.
- Taking into account the tunneling of charge carriers through a potential barrier in the conduction band.
- Contribution of the effect of thermionic emission. However, it should be noted here that this mechanism will be taken into account only at elevated temperatures.
- Radiative and nonradiative recombination.

To take into account the contribution of thermionic emission, we will use the model described in [12] with some modifications. Expressions for the densities of charge carriers:

\[ J_n = qn_0(1 + \delta) \left( n_2 - n_1 e^{-\Delta E_C/kT} \right) \] \quad (19)
\[ J_p = -q v_p (1 + \delta) \left( p_2 - p_1 e^{-\Delta E_V/kT} \right) \]  

(20)

where \( \delta \) is the coefficient of thermionic emission, \( v_n \) and \( v_p \) are the rates of thermal motion of electrons and holes, respectively, \( \Delta E_C \) and \( \Delta E_V \) are the differences in energies in the conduction and valence bands. The thermal velocities of the carriers are determined by the following expressions:

\[ v_n = \frac{A_n^* T^2}{q N_C} \quad v_p = \frac{A_p^* T^2}{q N_V} \]  

(21)

\[ A_n^* = \frac{4 \pi k^2 m^*_n}{h^3} \quad A_p^* = \frac{4 \pi k^2 m^*_p}{h^3} \]  

(22)

Thermionic emission coefficient:

\[ \delta = \frac{1}{kT} \int_{E_m}^{E_{C(0)}} dE \exp \left( \frac{E_C(0) - E}{kT} \right) \exp \left( -\frac{2}{h} \int_0^{x_E} dx \sqrt{2m^*_n (E_C(0) - E(x))} \right) \]  

(23)

where \( E_{C(0)} \) is the energy at the initial point of the potential, \( E_m = \max \left[ E_C(0), E_C(W) \right] \) is the maximum value of the energy over the entire width of the barrier \( W \). Recombination according to the Shockley-Reed-Hall model takes into account the traps of capture of charge carriers near the allowed bands. Let us denote as \( N_t \) the density of trapping traps having energy \( E_t \) within the band gap. In this case, the recombination rate will be:

\[ \delta = \frac{1}{kT} \int_{E_m}^{E_{C(0)}} dE \exp \left( \frac{E_C(0) - E}{kT} \right) \exp \left( -\frac{2}{h} \int_0^{x_E} dx \sqrt{2m^*_n (E_C(0) - E(x))} \right) \]  

(24)

\[ R_{SRH} = \frac{\sigma_n \sigma_p v_n N_t (np - n_i^2)}{\sigma_n (n + n_i e^{(E_t - E_i)/kT}) + \sigma_p (p + n_i e^{(E_t - E_i)/kT})} \]  

(25)

where the cross sections for the capture of charged traps \( \sigma_n \) and neutral traps \( \sigma_p \), \( n_i \) is the intrinsic carrier concentration. For the convenience of modeling, we rewrite expression taking into account the lifetime of charge carriers:

\[ \tau_n = \frac{1}{\sigma_n v_n N_t} \quad \tau_p = \frac{1}{\sigma_p v_p N_t} \]  

(26)

\[ R_{SRH} = \frac{np - n_i^2}{\tau_n (n + n_i e^{(E_t - E_i)/kT}) + \tau_p (p + n_i e^{(E_t - E_i)/kT})} \]  

(27)

The equations were solved using the MatLab software package for mathematical and physical modeling [13].

4. Results

In the visible spectrum from 400 to 900 nm, the results of simulating the external quantum yield of classical structures on GaAs give parameters from 50 to 60% and there is a sharp decline at the edge of the absorption boundary at 900 nm. With the introduction of arrays of InAs quantum dots into the simulation model, an increase in the quantum efficiency in the near-IR spectrum beyond the GaAs absorption boundary is observed. Simulation of the external quantum efficiency of the heterointerface showed the effect of the composition of the barrier layer of quantum dots on the spectral characteristics of the device. The use of a higher band gap material makes it possible to increase the contribution of
quantum dots to the capture of photons for the generation and confinement of charge carriers. Figures 2 and 3 show the results of simulation of the spectral dependence of the external quantum yield of a sample with a GaAs barrier and a sample with an AlGaAs barrier. Both barriers had a technological thickness of the order of 30 nm.

![Graph](image1)

**Figure 2.** External quantum efficiency with a barrier GaAs

![Graph](image2)

**Figure 3.** External quantum efficiency with a barrier AlGaAs

When using the classical GaAs barrier, the dark current density is of the order of $10^{-6}$ A/cm$^2$, at zero bias and a temperature of 90 K. The use of a wide-gap energy barrier makes it possible to reduce the dark current density to $10^{-9}$ A/cm$^2$ at a temperature of 90 K. The introduction of a wide-gap barrier reduces the thermionic emission of carriers from a potential well formed by a quantum dot. Figures 4 and 5 show the results of modeling the dark characteristics of the heterointerface.
5. Conclusion
A mathematical model has been developed for constructing the band structure, the spectral dependence of the external quantum yield and dark current-voltage characteristics based on the Kronig-Penny model and the method of effective masses for interband transitions. Numerical modeling was carried out according to the results of which the efficiency of transformation of the structure was shown at the level of 60%. Spectral dependencies of the external quantum efficiency are obtained with the contribution of the array of quantum dots at the levels of 9.9% and 16.5%. It has been found that the use of a wide-gap barrier layer increases the capture capacity of quantum dots and reduces the dark current density to a level of $10^{-9}$ A/cm$^2$ at a temperature of 90 K.
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