Comparative Analysis of Electronic Structure of Heterostructures with Quantum Wells and Delta-Layers by Capacitance Methods and Self-Consistent Simulation

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***Abstract*— We present the results of activity in the field of complex analysis of nanoheterostructures, contained quantum well and delta-doped layers. The experimental research by methods of capacitance spectroscopy with following numerical processing and self-consistent simulation of key electronic parameters and quantum confined energy levels brings full information about the emission behavior of the quantum system. With the help of the method we investigate the influence of delta-layer location on the quantization levels and charge carrier concentration in quantum well.**

Keywords: semiconductor heterostructure; delta-layer; self-consistent calculation; Schrödinger and Poisson equation; numerical modeling; capacitance spectroscopy

I. INTRODUCTION

Owing to intense advancement of nanotechnology in the recent decades, the impressive results have been attained in design and fabrication of quantum-confinement heterostructures and high efficient devices based on them. Continuing technological progress in microelectronic requires the development of modern techniques for deep analysis of nanoscale structures, and the role of numerical modeling is permanently growing. We present here the achievements in comprehensive characterization of electronic properties of semiconductor devices by mutual experimental measurements and numerical simulation with subsequent fitting.

Capacitance-voltage (C-V) characteristics are known as a very effective tool for obtaining the charge carrier concentration profiles in semiconductor structures [1]. When a heterostructure contains a quantum-confinement region (quantum well, array of quantum dots or delta-doped layer), the corresponding free carrier profile becomes quite complicated, reflecting the inhomogeneous distribution of electrostatic potential. Here the numerical simulation should include the self-consistent solution of nonlinear Poisson and Schrödinger equations for estimation of potential distribution along the heterostructure and obtaining the true carrier concentration in the quantum-sized area. The subsequent fitting of simulated C-V characteristics to the experimental ones enables determining heterostructures' main electronic parameters, in particular, the energy-band offset at the heterointerface, energies of bound levels in quantum well and corresponding wave functions.

II. SELF-CONSISTENT CALCULATION OF POTENTIAL AND SIMULATION OF CAPACITANCE-VOLTAGE CHARACTERISTICS

The first step in the calculation of C-V characteristics for semiconductor heterostructures containing a quantum well or another quantum confined region is the self-consistent solution of Schrödinger equation in the effective mass approximation on a non-uniform mesh [2, 3]

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*(z)}\frac{d}{dz}\psi_i(z)\right)+V(z)\psi_i(z)=E_i\psi_i(z) \qquad (1)$$

and non-linear Poisson equation

$$\varepsilon_0\frac{d}{dz}\left(\varepsilon(z)\frac{d\phi(z)}{dz}\right)=e\left[N_D^+(z)-n(z)\right]. \qquad (2)$$

In Eqs. (1), (2) N_D^+ is the concentration of ionized donors, $m^*(z)$ is the coordinate-dependent electron effective mass, $\varepsilon(z)$ is the relative permittivity, E_i is the energy of i-th confined in the QW level, $\psi_i(z)$ is the electron wave function at the corresponding level, and $V(z)$ is the potential energy profile with regard to the conduction band offset at the heterojunction.

The numerical solution is a "field–particles" iteration procedure, where at each stage the abovementioned differential equations are subsequently solved to find a corrected distribution of electrostatic potential and concentration of free charge carriers [3, 4]. A requirement for the solution is that the maximum of the correction to the potential at the subsequent iteration should not exceed a preset small quantity (10^{-8} V).

We have carried out the numerical solution of Schrödinger equation in a quantum box, at its boundaries the wave functions should be vanished according to the Dirichlet

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conditions [3]. The Poisson's equation, in which the mobile charge carriers $n(z)$ are taken into account, was linearized and solved using Newton's algorithm with respect to the potential-correction term.

Then, once the eigenenergies and eigenfunctions were determined, the charge carrier density in the corresponding two-dimensional quantum-confinement subbands can be obtained using 2D statistics [3, 4]

$$n(z) = \frac{m^* kT}{\pi\hbar^2} \sum_i \ln\left[1 + \exp\left(\frac{E_F - E_i}{kT}\right)\right] \left|\psi_i(z)\right|^2 . \qquad (3)$$

The position of the Fermi level E_F at given temperature T was determined from the solution of electroneutrality equation. Next, to calculate the capacitance–voltage characteristic we used the quasi-static approach [3, 4]. The barrier capacitance is defined as the ratio of charge to voltage increments

$$C = \frac{\Delta Q}{\Delta U} . \qquad (4)$$

According to the Gauss theorem, the total charge in a closed system is related to the electric field F_S at the surface (at the Schottky barrier) for one-dimensional system by the expression

$$Q = \varepsilon\varepsilon_0 \oint F_S dS = S\varepsilon\varepsilon_0 F . \qquad (5)$$

Thus, the problem of calculation of C–V characteristic can be reduced to finding the dependence of the electric field at the surface of a semiconductor structure on the external applied voltage. Further, using the simulated capacitance–voltage characteristics, we have calculated the profile of mobile charge carrier concentration using the standard differentiation procedure

$$n(x) = 2\left[\varepsilon\varepsilon_0 e \frac{d}{dU}\left(\frac{1}{C^2}\right)\right]^{-1} . \qquad (6)$$

III. Results of Investigations and Simulation of Heterostructures with Quantum Well and Delta-Layer

We have applied the procedure of numerical self-consistent simulation to HEMT-oriented heterostructures with $In_xGa_{1-x}As/GaAs$ quantum wells with closely located delta-doped claddings and to the simplified heterostructures with only single $In_xGa_{1-x}As/GaAs$ quantum well. To generate the experimental C-V characteristic, the self-consistent procedure was repeated about 300 times at sweeping reverse biases, applied to the sample. After the getting simulated C-V characteristic we do fit it to the experimental one. If the coincidence the simulated and experimental curves doesn't occur, the calculations were repeated using another conductance band offset. As a result, for the compositions $0.06 < x < 0.3$ the simulations state only one level, confined in the well. In this case, the experimentally observed profile of majority charge carrier density in the QW region represents the squared wave function of the confined state. One should note that the existence of only one level in the quantum well is important for fabrication of high-efficient single-mode semiconductor lasers.

Upon the numerical solution of Schrödinger's equation within the boundaries of quantum box, the energy states confined in the QW are calculated correctly, while the continuous spectrum of states in the free band above the quantum well is replaced by a set of discrete levels, whose spacing is determined by the size of the box. To calculate the correct carrier concentration in the QW region, we took into consideration 16-20 lowest energy levels within the quantum box. The calculations show that the charge carrier density in the lowest quantization subband (corresponding to the confined level) amounts to about 95% of the total carrier density in the QW region, and the 8-th subband contains no more than 10^{-6} of the total charge carrier density. This fact attests to the high degree of spatial confinement of the charge carriers by the quantum well.

The introduced algorithm of self-consistent solution using the quantum box for Schrödinger equation has the preferences over the commonly used technique of separate calculation 3D- and 2D-electrons in the QW region [2]. Particularly, our method correctly takes into account the quasi-resonant level, positioned between the pure bound and free energy states; the squared wave function of this state is concentrated predominantly in the quantum well.

Besides, the developed simulation and fitting technique has been applied to the characterization of samples, containing both a quantum well and a delta-doped layer. In Fig. 1 the experimental C-V-characteristics are presented, measured in the temperature range 20 – 300 K for the heterostructure with QW $In_{0.22}Ga_{0.78}As/GaAs$ and a delta-layer doped with carbon. With lowering temperature two horizontal plateaus become perceptible in capacitance-voltage curves, which occurred due to the presence in the heterostructure two regions with high concentration of free charge carriers (the regions of quantum well and of delta-layer).

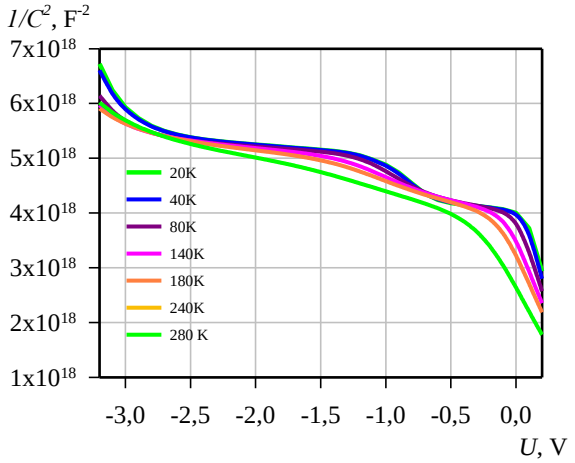

Fig. 1. C-V-characteristics of the structure with QW $In_{0.22}Ga_{0.78}As/GaAs$ and carbon delta-layer in temperature range 20 – 300 K

From the experimental C-V characteristics the concentration profiles of free charge carriers at different temperatures were calculated, Fig. 2. At lowering temperature we noticed decreasing the width and growing the intensity of the concentration peak as from the quantum well, as well as from the single delta-doped layer. Such behavior is in accordance with observed earlier effects for the structure with single quantum well and structure with a single delta-layer doped by carbon and can be explained by the strengthening of localization of charge carriers in the region of QW and delta-layer at reduced temperatures.

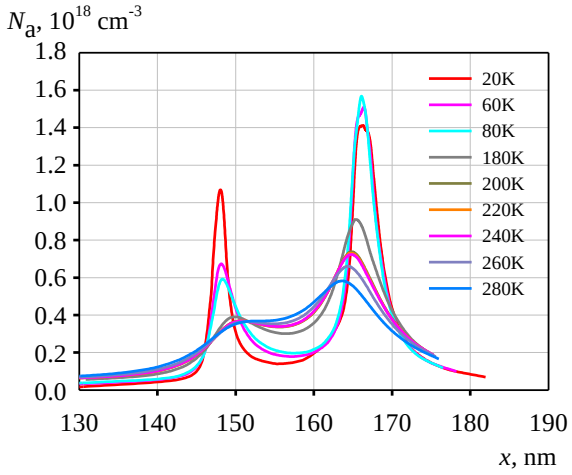

Fig. 2. Apparent concentration profiles of majority charge carriers for the heterostructure with QW $In_{0.22}Ga_{0.78}As/GaAs$ and carbon delta-layer in the temperature range 20 – 300 K

For the structure with a single QW InGaAs/GaAs the temperature increase from 75 up to 250 K leads to significant (about 5 times) lowering of majority charge carrier peak concentration, the reason for it is the increasing probability for thermally activated escape of charge carriers from the quantum well at elevated temperatures. For the heterostructure, contained QW and delta-doped layer, we noticed quite weak (no more than 2 times) amplitude decreasing of apparent charge carrier concentration at increasing temperature from 75 up to 250 K (Fig. 2). This can be the consequence of the fact that the delta-layer positioned near the quantum well acts as an effective charge carrier emitter for the QW. This fact weakens the temperature dependence of charge carrier concentration in QW, as at elevated temperature along with the increase probability for thermally activated escape the charge carriers from the quantum well there is the increase of probability for capture by the QW charge carriers from delta-layer as a result of decrease for localization of charge carriers near the delta-layer.

We have carried out the numerical simulation of apparent concentration profile of charge carriers for the heterostructure, containing a QW and a delta-doped by carbon layer for different distances between the QW and delta-layer. It was revealed, if the delta-layer locates at the distance 40 nm and more from the quantum well, it practically doesn't influence the charge carrier distribution and the shape of the potential around the QW. At close distance between the quantum well and delta-layer the penetrated from the delta-layer free charge carriers do modify the potential, changing the shape of wave function for the bound state and its energy (Fig. 3). Decreasing temperature leads to the enhancement of the interaction.

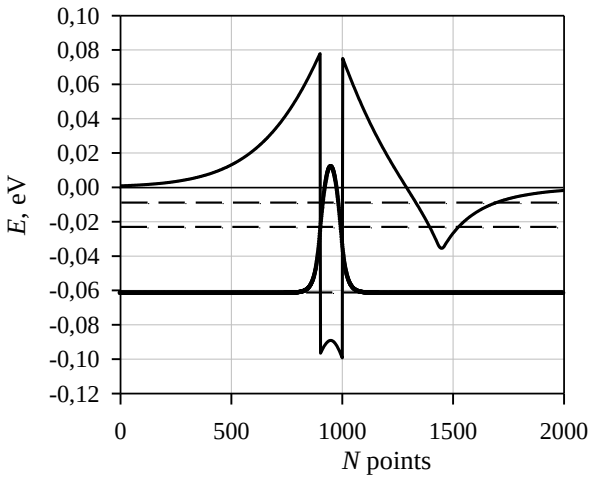

Fig. 3. Self-consistent Hartree potential, obtained during the simulation of the heterostructure with QW $In_{0.22}Ga_{0.78}As/GaAs$ and a delta-layer

The existence of delta-doped layer in vicinity of quantum well not only affects its filling by charge carriers, but also influences on energy of quantized levels in the QW. In Fig. 4 the dependence of bound quantization level in QW from the distance between the quantum well and delta-doped layer is presented, which was obtained during the simulation of electronic spectra of a heterostructure with QW $In_{0.22}Ga_{0.78}As/GaAs$. The point is, the more closely the delta-layer locates to the quantum well, the more intensively the QW does capture the charge carriers from it. This leads to stronger bending of the electrostatic potential that, in turn, leads to shift of quantized levels in the quantum well.

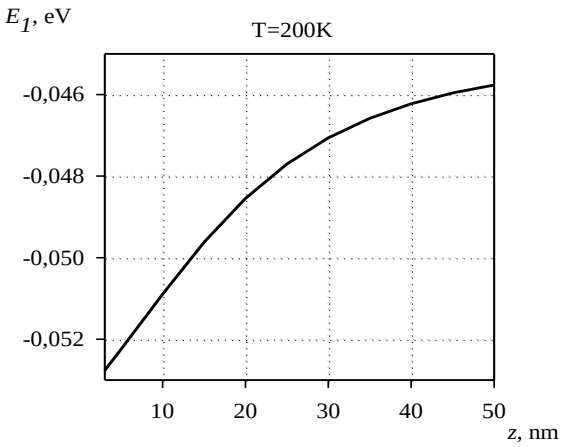

Fig. 4. Self-consistent potential Hartree, obtained during the simulation of the structure with QW In0.22Ga0.78As/GaAs and delta-layer

IV. Conclusions

A method is developed for complex characterization of heterostructures with quantum-confined regions by numerical self-consistent solution of Poisson and Schrodinger equations, followed by the fitting to the experimental data, which are obtained from capacitance-voltage profiling. The algorithm was successfully applicated to investigations of the samples with single quantum well InGaAs/GaAs, and for the heterostructures with simultaneous presence of a quantum well and a delta-doped layer. The comparative analysis allows to reveal the influence of delta-layer location at the filling the quantum well by charge carriers and other important properties of QW.

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