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Optimization Problems of Nanosized Semiconductor Heterostructures

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Abstract—A new approach is presented that allows solving optimization problems of nanosized semiconductor heterostructures. We have formulated and solved the problem of determining the optimal doping of a barrier layer consisting of a number of sublayers, which provides a preset concentration of electrons in the conduction channel of semiconductor heterostructures. To solve the problem, effective optimization algorithms based on gradient methods are developed. As an example, an $Al_{0.25}GaN/GaN$ heterostructure with a total barrier layer thickness of 30 nm is considered. The results obtained in the numerical experiment are consistent with the modern trend towards the transition from a homogeneous doping profile to a planar δ-doping in field-effect transistor manufacturing technologies. The developed technique of mathematical simulation and optimization can be used in field-effect transistor manufacturing technologies. The approaches presented in the work create the conditions for the automated design of such structures.

Keywords: Ab initio modeling, heterostructure, mobility of charge carriers, two-dimensional electron gas, optimization algorithms, multiscale modeling

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INTRODUCTION

The output characteristics of heterostructural semiconductor microwave devices are determined by a variety of factors that reflect both the structural and technological features of manufacturing heterostructures. In this case, it is extremely important to choose the optimal parameters that determine the basic electrophysical characteristics of the structure—the concentration and mobility of charge carriers in the channels of a two-dimensional electron gas (2DEG) [1].

The problems of the mathematical modeling of such structures are discussed in [2, 3]. The following scheme of multiscale modeling was implemented. Three levels of characteristic scales were allocated. The description of the system at the atomic level is carried out using crystallographic information and a quantum-mechanical model based on the electron density functional theory [4, 5]. The obtained information is transferred to the model of a nanoscale level, where it is used to calculate the distribution of charge carriers in a heterostructure. At this level, a quantum-mechanical description is also used. The mathematical model is a system of Schrödinger and Poisson equations [6]. The data obtained from the solutions of these equations, namely the wave functions and the density distribution of charge carriers across the layered structure enter the next scale model, where the mobility of charge carriers in the longitudinal direction is calculated. In this case, a wide range of electron scattering mechanisms is taken into account: scattering by optical and acoustic phonons, the roughness of the heterointerface, charged centers and dislocations, and piezoelectric scattering. In [7], the scattering by the roughness of a heterointerface was considered. The roughness of the heterointerface was shown to change the width of the quantum well, and, consequently, the position of the energy levels. Such a fluctuation in the potential causes the scattering of charge carriers. The contribution of this scattering process depends strongly on the technological perfection of the heterostructures. A comparison of the results of the calculations with the experimental data [7, 8] showed a sufficiently high simulation accuracy for calculating the carrier concentration and electron mobility of a two-dimensional electron gas. The developed technique and means for numerical simulation allow us to quickly perform a multioptional analysis of multilayered nanosized semiconductor structures. This creates a basis for solving a number of optimization problems that are relevant in modern microwave electronics.

In [9], the results of a multioptional computer analysis of electron density and mobility in nanosized AlGaN/GaN nitride heterostructures are presented. Such compounds have a wurtzite crystalline structure. As a result of spontaneous and piezoelectric polariza-

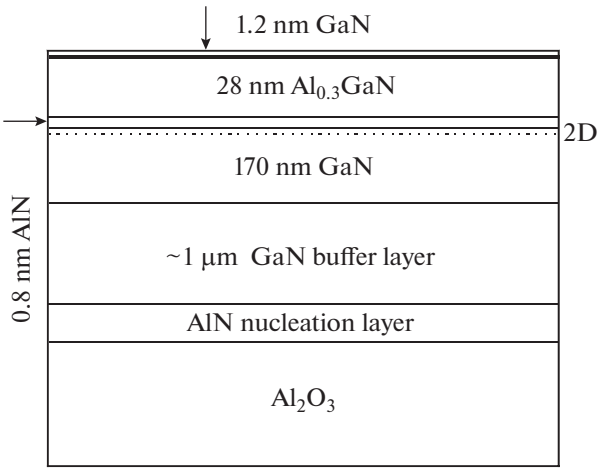

Fig. 1. Multilayer semiconductor heterostructure [7].

tion, uncompensated charges appear on the heterointerfaces playing a decisive role in the formation of 2DEG channels [8]. In [9], the authors used the results of modeling from first principles, or in other words, quantum-mechanical modeling at the atomistic level. In this case, the calculation of the atomic (nuclei) positions and the distribution of the electron density in the internuclear space are determined from the condition for minimizing the potential energy of the system. The ab initio calculation makes it possible to obtain the charge densities on the interfaces, which are then used when calculating the electron density and mobility of the electrons. Computer experiments made it possible to determine the dependence of the concentration and mobility of the electrons on the molar content of aluminum in the barrier layer, on the thickness of the barrier layer, and on a variety of other characteristics. In many cases, such dependences allow us to determine the optimal parameters of the heterostructure from the point of view of the concentration and mobility of the charge carriers. However, problems often arise when it is necessary to use the optimization theory technique. Such problems involve, in particular, inverse problems in determining the characteristics of grown heterostructures that are inaccessible by direct measurement, based on the experimental data on the carrier concentration and mobility in 2DEG. Another class of problems involves the determination of the optimal doping of a barrier layer consisting of a number of sublayers. Such problems are considered in this article.

MATHEMATICAL MODEL

A typical scheme of a nanosized semiconductor heterostructure is shown in Fig. 1 [7]. This heterostructure is based on gallium nitride and ternary solutions. It was grown at the Institute of Semiconductor Physics of the Siberian Branch, Russian Academy of Sciences (SB RAS).

The presence of layers grown from semiconductor materials witha different width of the forbidden band, in combination with polarization effects, provides the formation of a quantum-dimensional well for electrons with a width of the order of several nanometers in the vicinity of a heterointerface in the layer with a smaller width of the forbidden band (GaN). The electron motion in a direction normal to the heterointerface is limited, and the energy levels are quantized. Electrons at these levels can freely move in the plane of the heterointerface, and a two-dimensional electron gas is formed (schematically, the region of the 2DEG formation is shown in Fig. 1 by the points).

The mathematical model to describe the distribution of electrons in such structures is a system of Schrödinger and Poisson equations:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*(z)}\frac{d\psi}{dz}\right)+V(z)\psi(z)=E\psi(z); \quad (1)$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\phi}{dz}\right)=-e\left[u(z)-n(z)\right]+\sum_{l=1}^{M}\sigma_l\delta(z-z_l); \quad (2)$$

$$V(z)=-e\varphi(z)+\Delta E_c(z); \quad (3)$$

$$n(z)=\sum_{i=1}^{I}\left(\psi_i(z)\right)^2 n_i(z); \quad (4)$$

$$n_i(z)=k_BT\frac{m^*(z)}{\pi\hbar^2}\ln\left[1+\exp\left(\frac{E_F-E_i}{k_BT}\right)\right], \quad (5)$$

where E_i and $\psi_i(z)$ are the energy levels and the corresponding wave functions, $\int_0^I \psi_i^2(z)\mathrm{d}z = 1$; I is the number of meaningful energy levels from the point of view of their contribution to sum (4); $n(z)$ is the electron density; $\hbar$ is Planck's constant; e is the electron charge; m^* is the effective mass of the electron; E_F is the Fermi level position; $\varphi(z)$ is the electrostatic potential; σ_l are the charge densities at the interfaces (boundaries); δ is the delta-function; z_l is the interface location; M is the number of heterointerfaces with an uncompensated charge; ε is the dielectric permittivity of material; ΔE_c is the conduction band shift; k_B is Boltzmann's constant; and T is temperature. Function $u(z)$ describes the distribution of dopant impurities in the system, $u(z) = N_d(z) - N_A(z)$, where $N_d(z)$ and $N_A(z)$ are the concentrations of the donor and acceptor impurities, respectively. This function will be further considered as a control function. Model (1)—(5) incorporates the fact that the values m^*, ε, and ΔE_c can vary from layer-to-layer, i.e., functions $m^*(z)$, $\varepsilon(z)$ and $\Delta E_c(z)$ belong to the class of piecewise-constant functions. In this case, the temperature of the heterostructure is assumed to be constant.

On the boundaries of the system ($z = 0$ and $z = L$, where L is the total thickness of the layered structure), the wave functions should take the zero values

$$\psi(0) = 0, \quad \psi(L) = 0. \tag{6}$$

On the left boundary ($z = 0$), the potential barrier φ_b is set. It is formed in the subcontact layer of the semiconductor, which borders the metal (Schottky barrier). In addition, it is possible to set the offset φ_s due to the applied voltage. On the right boundary ($z = L$), the natural condition is the absence of an electric field. Therefore, the boundary conditions for the Poisson equation become

$$\varphi(0) = \varphi_b + \varphi_s, \quad \varphi'(L) = 0. \tag{7}$$

The solution of the spectral problem (1) (the Schrödinger equation), the definition of the eigenvalues and eigenfunctions/vectors of the differential/matrix operator, depends on the electrostatic potential φ. The distribution $\varphi(z)$ in the structure is determined by Poisson's equation (2).

In addition, the electron density $n(z)$ enters the right-hand side of the Poisson equation. The electron density is determined by the energy levels E_i and the wave functions $\psi_i(z)$, according to the Fermi-Dirac statistics (see Eqs. (4)–(5)). The self-consistent solution of this system yields the required energy levels E_i and the corresponding wave functions $\psi_i(z)$ yield the potential well profile $V(z)$ and the electron density distribution in the heterostructure $n(z)$.

The algorithms used for solving problem (1)–(7) are described in detail in [3]. Note that the main computational complexity is associated with the convergence of the global iterations needed for matching the solutions of the Schrödinger and Poisson equations. In order to speed up the computational process, an approach based on the approximation of the nonlinear dependence of the electron density on the potential in combination with the linearization of the Poisson equation was realized. The development of an effective algorithm for solving direct problem (1)–(7) is an important basis for solving optimization problems.

We now turn to the formulation of the optimization problem. The most important indicator of the efficiency of a heterostructure is the concentration of electrons in the 2DEG channel, $N = \int_0^L n(z)\mathrm{d}z$. As shown in [9], this quantity is crucial in many cases for the mobility of electrons. Although the mobility decreases with an increasing concentration (as a rule), the product of the concentration and mobility (conductivity) increases, which causes an increase in N. It should be noted that an excessive increase in concentration may be accompanied by negative effects [1]. Due to this, a reasonable compromise is usually to set the desired level of electron concentration N^*. The main controlling factor affecting N^* is the concentration of donors in the barrier layer. The barrier layer is the region to the left of the 2DEG channel (see Fig. 1), $0 \le z \le z_b$, where z_b is the barrier layer thickness; $z_b < L$.

It is desirable to reduce the average doping level (or total ionization) of the barrier layer. This can help avoid excessive scattering of electrons on distant charged centers. Thus, the functional to be minimized can be written in the form

$$J(u) = \left[\int n(z)\mathrm{d}z - N^*\right]^2 + w\left[\int u(z)dz\right]^2, \tag{8}$$

where w is the weight factor. Hereinafter, the limits of integration are omitted, since integration is always implied throughout the entire region.

There may be technological limitations on the doping of individual layers during the growth of the heterostructure, which is reflected in the constraints on the control function:

$$0 \le u(z) \le x(z). \tag{9}$$

Here the constraint $u(z) \ge 0$ means that only donor doping is considered. This is due to the fact that just such doping facilitates increasing the electron concentration in 2DEG. Moreover, when striving to achieve the highest possible electron concentration (high value of N^*), the restriction on the state of the system becomes significant:

$$V(z) - E_f \ge 0; \quad z \le z_b. \tag{10}$$

This restriction allows us to avoid the formation of parallel conduction channel in the barrier layer ($z \le z_b$).

Thus, the problem of finding the dopant distribution in the barrier layer, which provides a preset concentration of electrons in the 2DEG conducting channel, has been formulated. In many cases, the solution of such a problem is not unique: different doping options may correspond to a preset electron concentration. In this case, the heterostructure designer can use different options; however, the choice is substantially narrowed by the imposed restrictions and the influence of the second term of the functional.

Gradient methods are effective for solving problem (1)–(10).

Let us consider the problem of determining the gradient of a functional. Here the principal point is the previously established relationship between the increments of the electron density and potential [3, 10]. We use the notation $R(z)$ for shortening the expression for the dependence of the electron density increment on the potential increment:

$$dn(z) = R(z)\delta\varphi(z);$$
$$R(z) = \frac{m^*(z)e}{\pi\hbar^2}\sum_i \psi_i^2(z)\frac{\exp\left(\frac{E_F - E_i}{k_B T}\right)}{1 + \exp\left(\frac{E_F - E_i}{k_B T}\right)}. \tag{11}$$

A detailed derivation of this formula is given in [3].

The use of expression (11) substantially simplifies the procedure for determining the gradient of the functional.

Following the traditional scheme of the calculus of variations [11], we multiply Eq. (2) by the Lagrange multiplier $p(z)$, integrate the result over the thickness of the heterostructure and add to functional (8):

$$J(u) = \left[\int n(z)\mathrm{d}z - N^*\right]^2 + w\left[\int u(z)\mathrm{d}z\right]^2 \int p(z) \times \left[\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\varphi}{\mathrm{d}z}\right) + e\left(u(z) - n(z)\right) - \sum_l \sigma_l \delta(z - z_l)\right]\mathrm{d}z. \quad (12)$$

The variation of functional (12) has the form

$$\delta J = 2\left(N - N^*\right)\int \delta n(z)\mathrm{d}z + 2wU\int \delta u(z)\mathrm{d}z + \int p(z)\left[\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}\right) + e\left(\delta u(z) - \delta n(z)\right)\right]\mathrm{d}z, \quad (13)$$

where $U = \int u(z)\mathrm{d}z$.

We integrate the term $\int p(z)\left[\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}\right)\right]\mathrm{d}z$ twice in parts. With allowance for the boundary conditions (7), we obtain

$$\int p(z)\left[\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}\right)\right]\mathrm{d}z = \int \frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}p}{\mathrm{d}z}\right)\delta\varphi\mathrm{d}z - p(0)\varepsilon(0)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}(0) - \frac{\mathrm{d}p}{\mathrm{d}z}(L)\varepsilon(L)\delta\varphi(L).$$

Then Eq. (13) becomes

$$\delta J = 2(N - N^*)\int \delta n(z)\mathrm{d}z + 2wU\int \delta u(z)\mathrm{d}z + \int \frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}p}{\mathrm{d}z}\right)\delta\varphi + p(z)e\left(\delta u(z) - \delta n(z)\right)\mathrm{d}z - p(0)\varepsilon(0)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}(0) - \frac{\mathrm{d}p}{\mathrm{d}z}(L)\varepsilon(L)\delta\varphi(L),$$

or, with allowance for expression (11),

$$\delta J = 2(N - N^*)\int R(z)\delta\varphi(z)\mathrm{d}z + 2wU\int \delta u(z)\mathrm{d}z + \int \frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}p}{\mathrm{d}z}\right)\delta\varphi + p(z)e\left(\delta u(z) - R(z)\delta\varphi(z)\right)\mathrm{d}z - p(0)\varepsilon(0)\frac{\mathrm{d}\delta\varphi}{\mathrm{d}z}(0) - \frac{\mathrm{d}p}{\mathrm{d}z}(L)\varepsilon(L)\delta\varphi(L).$$

Let us compose a system of equations for determining $p(z)$ in order to zero out all terms that do not contain the vafiation δu:

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}p}{\mathrm{d}z}\right) - eR(z)p(z) + 2R(z)\left(N - N^*\right) = 0; \quad (14)$$

$$p(0) = 0, \quad \left.\frac{\mathrm{d}p}{\mathrm{d}z}\right|_{z=L} = 0. \quad (15)$$

As a result, we obtain the following expression for the variation of the functional

$$\delta J = \int p(z)e\delta u(z)\mathrm{d}z + 2wU\int \delta u(z)\mathrm{d}z = \int \left(p(z)e + 2wU\right)\delta u(z)\mathrm{d}z. \quad (16)$$

Now we can write down the required gradient of the functional:

$$J' = p(z)e + 2wU. \quad (17)$$

This approach allowed us to construct a relatively simple problem (14)–(15) for determining the function $p(z)$. Thus, to find the gradient of the functional, it is possible to avoid solving the most computationally complex spectral problem. This allows us to construct effective optimization algorithms based on gradient methods in which the direction of the movement toward the point of the minimum at each step coincides with the direction opposite to the gradient vector of the function to be minimized.

In particular, the results presented in the next section were obtained using the simplest method of gradient descent. The constraints in this work were taken into account by using the projection of the solution onto the subspace of constraints at each iteration step.

RESULTS OF CALCULATIONS

As an example, consider the $Al_{0.25}GaN/GaN$ heterostructure with a total barrier layer thickness of $Al_{0.25}GaN$ 30 nm. To illustrate the effect of doping additives, we present the variants of an undoped and uniformly doped donor impurity barrier layer. The initial data for the calculations are as follows.

The effective electron masses were assumed equal to $0.228m_0$ for both materials (m_0 is the mass of an electron at rest). The charge density at the $Al_{0.25}GaN/GaN$ heterointerface determined by the quantum-mechanical calculation is $1.08 \times 10^{13} e$ Q/cm^2. Note that here we consider a problem with one channel of 2DEG or, in other words, with one heterointerface on which an uncompensated charge is formed ($M = 1$). The rest of the data were determined from approximate expressions [5]:

$$\varepsilon_{\mathrm{AlGaN}}(x) = (0.03x + 10.28)\varepsilon_0;$$
$$\Delta E_c(x) = 0.7\left(E_g(x) - E_g(0)\right),$$
$$E_g(x)\ 6.13x + 3.42(1 - x);$$
$$-e\varphi_b = 1.3x + 0.84;$$

where ε_0 is the electric constant and x is the mole fraction of Al in the AlGaN alloy. The boundary condition $\varphi(0) = \varphi_b$ for the potential was used.

The calculation results are shown in Fig. 2. Figure 2 shows the distributions of the potential energy and

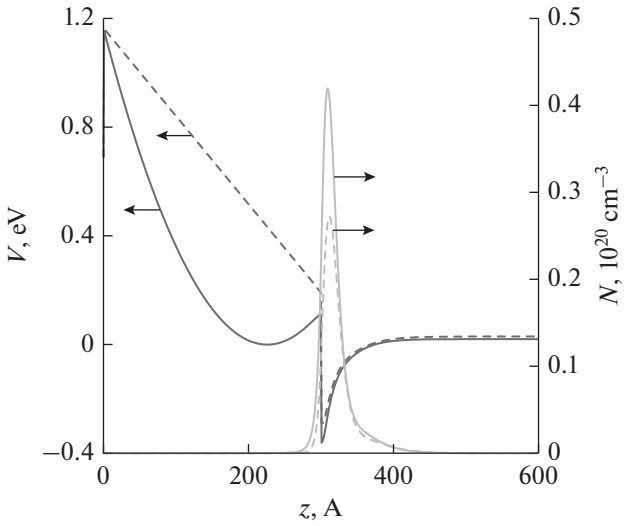

Fig. 2. Potential energy distribution (left scale) and electron density (right scale) across heterostructure for undoped (dashed curve) and doped (solid curve) barrier layers.

electronic energy over the thickness of the heterostructure. The dashed curves correspond to an undoped barrier layer and the solid curves correspond to barriers doped by donors with a constant concentration of 2.61×10^{18} cm^{-3}. Note that this is the maximum permissible concentration to satisfy constraint (10). From Fig. 2 we can see that in the second case the profile of the potential energy acquires a characteristic flexure and the electron density increases. As a result, the layered electron concentration N in 2DEG increases from 8.3×10^{12} to 1.27×10^{13} cm^{-2}.

Now we pass to the results of solving optimization problems. Let it be required to provide the 2DEG electron concentration $N^* = 1.1 \times 10^{13}$cm^{-2}. We will seek the solution in the class of piecewise-constant functions, which corresponds to the technology of manufacturing layered structures. Consider a barrier layer consisting, for example, of five sublayers. The possible number of sublayers in the model is not limited. For simplicity, all the properties of the layers, with the exception of doping, we assume to be identical, including their thicknesses, and we impose the following restrictions:

$$0 \le u_m \le 2.5 \times 10^{18} \text{ cm}^{-3};\ m = 1,\ldots 4;\ u_5 = 0.$$

The last restriction means that the layer immediately adjacent to the 2DEG channel is not allowed to be doped. This is a fairly common restriction, which is dictated by the need to reduce the scattering by alloy inhomogeneities. Such sublayers are usually called spacers. The value 2.5×10^{18}cm^{-3} is taken as an example, although it can be higher. In this case, the model can be applied to arbitrary doping options. The results of solving this problem are shown in Fig. 3a. The distribution of the dopant in the sublayers of the barrier layer $x_d(z) = n_d(z)/\overline{n}_d$ obtained after optimization (the impurity concentration is $\overline{n}_d = 5 \times 10^{18}$ cm^{-3}), the potential energy profile x, and also the distribution of the electron density N in the heterostructure (the density corresponds to a value of 10^{20} cm^{-3}) are shown in this figure.

Next, consider a somewhat modified problem. Let us remove the restrictions on sublayers 1–4, while at the same time we increase the influence of the second term in the functional to be minimized. In other words, we will try to achieve the given electron concentration with the minimal total ionization of the barrier layer. The results of the solution are shown in Fig. 3b. We can see that the maximum doping of layer *3* is the most advantageous. In this case, the total ionization of the barrier layer U in the second option of the calculation turns out to be substantially lower than in the case of relatively uniform doping. This result agrees with the modern trend towards a transition

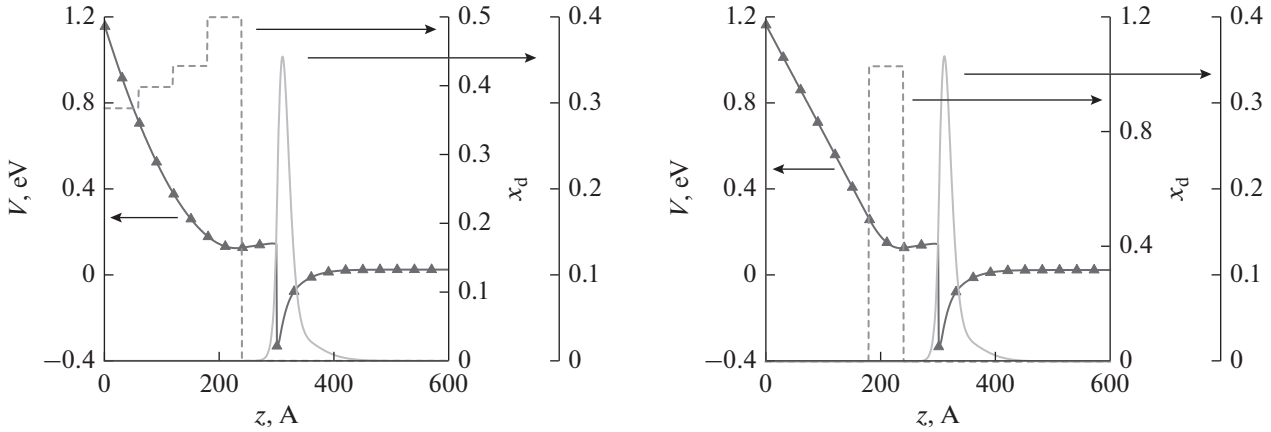

Fig. 3. Distribution of optimal donor concentration (dashed curve, right scale 1), potential energy (marked curve, left scale) and electron density (solid curve, right scale 2) across heterostructure.

from a homogeneous doping profile to planar δ-doping in field-effect transistor manufacturing techniques [1, 12].

CONCLUSIONS

The means of mathematical modeling and optimization, which can be used in field-effect transistor manufacturing technologies, are developed. We present approaches with the help of which the conditions can be created for the automated design of such structures.

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