Quantum-mechanical models for calculating the electrical characteristics of semiconductor 2-d structures for technological optimization of nanoelectronics devices based on them

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Abstract. In this paper, a computational algorithm has been developed for the quantum-mechanical model for predicting the electrical properties of 2-d semiconductor structures of nanoelectronics devices with a low-dimensional channel. The most important advantage of the developed algorithm is its scalability for the problems of technological optimization of nanoelectronics devices. An example of application of the developed software to solving the problem of predicting the electrical properties of a low barrier detector sub-terahertz diode with zero-bias in the framework of solving the problem of its technological optimization is presented.

1. Introduction
The current practice in the design of integrated circuits assumes that the circuit is first synthesized and the electrical parameters of its elements are selected according to the criterion of the best fit of the operational characteristics to the specified values. Assignment of electrical parameters is assigned based on the required accuracy of operational characteristics. The next step in the development of the integrated circuits (IC) is the calculation of nominal values and permissible deviations of the construction parameters. The problems of implementing this stage for designing nanoelectronic device structures on semiconductor 2-d structures [1] are due to the fact that, on the one hand, libraries of modern computer-aided design systems do not have the latest nanostructured elements, on the other hand, the models developed to date, although they allow to evaluate the electrical characteristics using heterostructure parameters, they are not adapted for the inverse problem. In most cases, engineers are forced to use rather rough models (allowing to evaluate only the qualitative character of the I-V curve) with a large number of empirical coefficients (for example, methods based on equivalent circuit diagrams [2, 3], phenomenological methods of semiclassical approximation [4]); and / or focus on nomograms [5], which systematize for a particular class of nano-devices the relationship between structural parameters and electrical ones; or use inefficient computational algorithms that require time-consuming calculations on supercomputers [6].

However, it should be noted that studies of physical processes in low-dimensional channels of nanodevices today provide a fairly wide range of formalisms, within which you can take into account the main factors determining quantum transport in nanostructures [1]. Especially promising for integration into the parametric stages (with the aim of reducing methodological error) and technological (reducing not only methodical, but also production and technological errors) optimization (Fig. 1) of
nanoelectronics devices, the authors present combined models of current transfer with quantum-mechanical modeling of a low-dimensional channel [7, 8, 9].

Figure 1. The structure of the process of designing and manufacturing nanoelectronic devices.

Thus, the actual task is to develop quantum-mechanical models for calculating the electrical characteristics of semiconductor 2-d structures, as the most accurate and physically based models, to account for manufacturing technology and gerontological processes causing the most important operational parameters, including indicators of the durability of hybrid and monolithic integrated circuits.

2. Quantum mechanical models for electrical characteristics
The basis of quantum mechanical approaches to the description of electron transport is the representation of semiconductor low-dimensional heterostructures as an open quantum system in the framework of the Landauer – Buttiker formalism [10]. To obtain the electrical characteristics of a nano-device, it is necessary to determine the transmission function of the heterostructure, which can be obtained using quantum-mechanical approaches. As approaches that meet the requirements for current transfer models for design and technological optimization and for reasons of maximum scalability, the authors analyzed the method of plane waves, the matrix method of plane waves, and the Green's function method. Space charge accounting for all methods was carried out within the framework of the concept of self-consistency.

When implementing the method of plane waves, it is necessary to determine the transmission matrix characterizing the relationship between the amplitudes of the waves incident and transmitted through the structure. For this, the potential profile is divided into regions with a constant value of potential energy. In each such domain, the solution of the Schrödinger equation is a superposition of the forward and backward waves. At the boundaries of the regions, with a constant potential, use the conditions for the continuity of the wave functions and the current density in a matrix form. With the help of the full transfer matrix, obtained as a product of the transfer matrices of all adjacent layers, it is possible to determine the amplitudes of the envelopes of the wave functions, on the basis of which to obtain the transmission of the structure.

$$M_{1,N} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \prod_{j=1}^{N} M_{j,j+1},$$

$$T = \frac{1}{|M_{11}|^2} \frac{K_j m_j}{K_j m_N},$$

where $M_{1,N}$ – full transfer matrix, $M_{j,j+1}$ – transfer matrix between layers j and j+1, N – number of layers, $m$ – the effective mass of an electron in layer j, $K_j = \sqrt{2m_j(E-U_j)/\hbar}$ – electron wave number in j layer.

To implement the matrix method of plane waves and the method of Green's functions, it is necessary to perform a discretization of the simulated structure. The finite difference approximation of the Schrödinger equation for grid nodes was obtained using the integro-interpolation method. To take into account the boundary conditions used the conditions of the second kind. In order to avoid lowering the
accuracy of the finite-difference scheme with respect to the grid step, the balance method was used in the approximation of the boundary conditions.

\[
\tilde{z} = \{z_i = i\Delta z, \Delta z > 0, \ i = 0..., N, \ z_i = z_{LB}, \ z_N = z_{RB}\} = z^{in}\cup z^{ex},
\]

\[
-t_{i1}\Psi_{i1} + \left(t_{i1} + t_i + \frac{U_i + U_{i1}}{2} - E\right)\Psi_i - t_i\Psi_{i1} = 0, \ z \in z^{in},
\]

\[
\Psi_{i}(t) = iK_{L}\Delta z - 1 + t_{i}\Psi_{iz} = 2iK_{L}\Delta z e^{ik_{i1}}, \ z \in z^{ex},
\]

where \(\Delta z\) – discrete grid step, \(N\) – number of split points, \(z\) – uniform grid on the interval \([z_i, z_{i+1}]\), \(z^{in} = \{z \in z | z_{RB} < z < z_{LB}\}\) – internal nodes of the grid, \(z^{ex} = \{z \in z | z_{BB} < z < z_{LB}\}\) – external nodes, \(\Psi_i\) – discretized electron wave function, \(t_i = h^2/2\Delta z^2 m_i\) – bound operator, \(m_i = 1/\Delta z\int_{z_i}^{z_{i+1}}m(z)dz\) – average effective mass per interval \([z_i, z_{i+1}]\); \(U_i = h^2/\Delta z\int_{z_i}^{z_{i+1}}U(z)dz\) – average value of potential energy per interval \([z_i, z_{i+1}]\), \(U(z) = E_v - eV\) – potential energy, \(E_v\) – conduction band profile, \(e\) – elementary charge, \(K_{R(L)} = \sqrt{2m_i(E-U_{R(L)})}/h\) – electron wave number in the right (left) reservoir, \(V\) – the potential energy of an electron in the space charge field and the applied external voltage, resulting from the solution of the Poisson equation.

Thus, the finite-difference scheme for solving the Schrödinger equation for an open system is presented in a matrix form.

\[
[H - EI + \Sigma_{L} + \Sigma_{R}][\Psi] = [S],
\]

where \(H\) – Hamilton operator in the matrix form, describing the electron behavior in the active region, \(\Psi\) – discretized wave function, \(\Sigma\) – o matrix operator, describing the outflow of electrons from the active region, \(E\) – energy, \(I\) – identity matrix, \(S\) – the term describing the electron influx into the active region reservoirs.

In the matrix method of plane waves, the resulting system of linear equations, which is the discretized Schrödinger equation, is solved by the modified Thomas method. The amplitudes of the envelopes of the wave functions obtained as a result of the solution are used to determine the transmission of the structure.

\[
T = |A_\beta|^2 \begin{bmatrix} K_{L} & m_i \\ A_\beta^* & K_{R} \end{bmatrix} |\begin{bmatrix} K_{L} & m_i \\ A_\beta^* & K_{R} \end{bmatrix} | \begin{bmatrix} K_{L} & m_i \\ A_\beta^* & K_{R} \end{bmatrix},
\]

When using the Green function formalism, the main parameters, including the structure transmission and electron concentration, are determined using the nonequilibrium Green function, which describes the quantum system's response to an external perturbation. The transmission of the structure is determined by:

\[
T = \sum_{j} G_{jj}^{\Gamma_{L}(R)}\Gamma_{j}^{\Gamma_{R}(L)}\Gamma^{\Gamma_{L},\Gamma_{R}} G_{jj}^{\Gamma_{L}(R)},
\]

\(\Gamma \equiv \Gamma_{LR} = i\left[\Sigma_{L}(R) - \Sigma_{R}(L)\right]\) – matrix characterizing the broadening of energy levels at the border of the left (right) contact channel, \(G = [H - EI + \Sigma_{L} + \Sigma_{R}]^{-1}\) – Green's nonequilibrium function, in matrix form.

The verification of the developed computational algorithm was carried out on a triangular potential barrier and confirmed the correctness of the numerical methods used in the model. The choice of a potential profile for verification was due to the presence of an analytical solution obtained using Airy functions of the first and second kinds. The results of the simulation of the transmission function are presented in Fig. 2 (a). Analysis of the accuracy (Fig. 2 (a)), as well as temporal and spatial complexity.
(Fig. 2 (b)) of the computational algorithms developed for each of the described methods, made it possible to choose as the most effective and satisfactory to the mathematical model of electrical prediction characteristics of semiconductor structures with a low-dimensional channel for design and technological optimization, an algorithm that implements the Green function method.

![Graph](image)

**Figure 2 (a, b). (a)** The dependence of the transmission function of the potential structure on the value of the electron energy; **(b)** Dependence of the computation time of the transmission function on the number of split points of the structure.

Thus, the developed computational algorithm for the quantum mechanical model for predicting the electrical properties of 2-d semiconductor structures of nanoelectronics devices with a low-dimensional channel: 1) verified, and the error in calculating the structure transmission does not exceed 0.3 %; 2) optimized by the criterion of efficiency: a) minimization of temporal and spatial complexity was carried out, resulting in linear asymptotic complexity $\sim O(N)$, including by taking into account the features of the implementation of the Green function method for calculating the current density - see Fig. 2 (b)); b) selection of the optimal grid step was carried out for the construction of a finite-difference scheme, so that the error in determining the electrical parameters was below 0.5% with the minimum execution time of the algorithms; 3) it has a high degree of scalability, which allows integrating it into the software package of technological optimization of nanoelectronics devices with quantum limitations of various types.

3. Application of the developed methods to obtain the electrical characteristics and operational parameters of the detector diode

Validation of the developed quantum-mechanical model was carried out on Heterostructure low barrier diodes (HLBD) based on lattice-matched AlGaInAs triangular barrier used for zero-bias millimeter-wave and submillimeter-wave detection. Perspective of the device is determined, on the one hand, by the attractive performance characteristics of detectors on such diodes that could be obtained on test-made samples [4], on the other hand, by potentially wide application area [11, 12] (for example, in detector receivers, in vision systems, including in mm-wave cameras). Difficulties in the design of such diodes [4] are associated with the problems mentioned in the introduction. Experimental data for a diode with an active region made of materials $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ and $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ are given in [4]. It was obtained that the results of the simulation of electrical characteristics and experimental data converge with an error of less than 3% in the voltage range $[-0.1,0.1]$ V (Fig. 3).
Figure 3. Application of the phenomenological approach and the Green function method for modeling the I-V curve of HLBD [4]; $J$ – current, $J_0$ – saturation current, $\eta_f$ and $\eta_r$ – ideality factors of diode.

4. Algorithm for optimization of design and technological parameters

The results of integrating the developed quantum-mechanical model for calculating electrical characteristics into the HLBD technological optimization procedure are shown in Fig. 4 (with a limited number of technological factors of production and modes of operation). The target function is the probability of production of operability product. The arguments of the objective function are the fraction of the substitution of Ga atoms by Al ($x$) atoms and the barrier width ($w$).

Figure 4. The probability of production of operability product (indicated by color) depending on the fraction of the replacement of Ga atoms by Al atoms ($x$) and the barrier width ($w$), at temperature and heat exposure time $T = 800^\circ C$ and $t = 800$ s respectively [13].

5. Conclusion

The high efficiency of the developed computational algorithm and the accuracy of estimating the I-V curve of 2d semiconductor structures of nanoelectronics devices with a low-dimensional channel were
confirmed in the process of verification and validation. The scalability of the proposed computational algorithm provides practical significance and the possibility of applying the technological optimization of such devices to solve problems. The developed algorithm of design and technological optimization can be scaled to account for an arbitrary number of operating, design and technological parameters. It is possible to increase the accuracy of predicting electrical properties and operational parameters, including absolute values, by considering coherent and incoherent channels with different dissipative processes, taking into account the influence of a greater number of technological factors of manufacturing, taking into account the conditions and modes of operation, taking into account gerontological processes in heterostructures including influence of harsh conditions and operating modes.

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