

Architecture of composite multilayer semiconductor nanostructures

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Abstract. The problem of ensuring the operational parameters of composite multilayer semiconductor nanoscale structures at the design technology stages is solved. A mathematical model based on the physics of processes occurring in the structure during operation is developed. The problem is solved for the resonant-tunnelling AlGaAs nanoheterostructures.

1 Introduction

Composite semiconductor multilayer single-crystal nanostructures based on AlGaAs/GaAs, InAlAs/InGaAs, AlGaN/GaN, InAlN/GaN, etc. are widely used in electronics, radio engineering, and optics devices. Due to a number of quantum-size effects, such as tunneling, resonant tunneling, the formation of a two-dimensional electron gas, one-electron transitions, it is possible to significantly improve the characteristics of devices based on these nanoheterostructures (NHS) [1-10]. The key tasks of designing such structures are to provide indicators of purpose and reliability under given production and operating conditions.

However, the design results cannot be considered optimal, and the potential of such NHS cannot be fully disclosed due to the lack of adequate mathematical models. The mathematical model of the NHS can be divided into 2 components: the model of current versus voltage (CVC) and the full impedance model, which describes the behavior of the NHS in the range of radio frequencies, external voltages and temperatures. The subject of this work is the CVC NHS model.

A CVC model capable of providing the required adequacy and accuracy should be based on the physical processes occurring in the structure during operation. It should include consideration of dissipative processes, multielectron interaction, other processes determined by the design of a particular structure, as well as degradation processes under the influence of external technological and operational factors.

Numerical calculation of NHS CVC, based on the physics of processes, is a labor-intensive task. The problem of time costs becomes especially acute when moving from the analysis problem to the problem of designing an NHS with given performance characteristics, based on an iterative optimization procedure. This problem acquires special

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significance at the stages of modeling technological errors and the kinetics of the current-voltage characteristic due to degradation, which is provided for by the reliability assessment method based on the gradual failure model [11-18]. Thus, an urgent task is to develop a model based on the physics of current transfer and having a relatively small dimensional and time complexity.

2 Materials and methods

In this paper, the problem is solved using the example of resonant tunneling AlGaAs NHS [19-22]. The basic idea of developing a compact model is that a system of integral and differential equations of the verification basis, can be transformed into algebraic and transcendental ones by linearization and decomposition. These methods are based on splitting systems of coupled equations into several simpler independent equations. Decomposition greatly simplifies the qualitative investigation and interpretation of important physical properties described by coupled equations, allowing one to study their wave and dissipative properties effectively. In addition, decomposition in some cases makes it possible to find exact analytical solutions of the corresponding boundary and initial boundary value problems and greatly simplifies the application of numerical methods, which fully corresponds to the goal of developing a compact model of current transfer in resonant-tunneling structures, taking into account the interelectronic interaction.

The construction of an effective model will be based on three assumptions:

1. Current density and concentration of electrons in quantum well is caused by energy charged electrons in vicinity of the lowest resonance level, formed in RTS quantum well in conduction zone.
2. The width of the resonant levels is negligibly small compared to the thermal energy.
3. The tunnel transparency coefficient and local density of states as a function of energy in the vicinity of resonant levels can be approximated by a function proportional to the Lorentz distribution function.

A self-consistent model of current transfer based on the formalism of wave functions was chosen as a verification basis. This model takes into account the interelectronic interaction using the self-consistent field method, the potential of which is the solution of the Poisson equation. To calculate the electron concentration and current density, it is necessary to find the wave functions of electrons, which are the solution of the Schrödinger equation for an open system

$$\left[-\frac{\hbar}{2} \frac{d}{dz} \frac{1}{m(z)} \frac{d}{dz} - E + E_c(z) - q_e \varphi(z) + \Sigma(z) \right] \psi(z) = S(z) \quad (1)$$

where $\hbar$ is the Dirac constant, q_e is the elementary charge, $m(z)$ is the effective electron mass, E is the electron energy, $E_c(z)$ is the bottom of the conduction band, $\varphi(z)$ is the self-consistent field potential (SFP), $\Sigma(z)$ is the operator describing the outflow of electrons from the active region of the structure into the reservoirs, $S(z)$ is the function describing the injection of electrons into the active region, $\psi(z)$ are the envelope wave functions of electrons.

The current density is calculated using the formula:

$$J = \frac{q_e}{h} \int_{E_s}^{\infty} T(E, V) D(E, V) dE \quad (2)$$

where $T(E, V)$ is the tunnel transparency coefficient, $D(E, V)$ is the supply function, E_s is the minimum energy in the source conduction band.

The tunnel transparency coefficient is related to the wave function by the following relation

$$T(E, V) = |\psi(z_l)|^2 \frac{|k_R| |m_L|}{|k_L| |m_R|} \quad (3)$$

where z_l is the coordinate of the “active region - sink” boundary, k_R is the wave number in the drain, k_L is the wave number in the source, m_R is the effective mass of electrons in the drain, m_L – is the effective mass of electrons in the source.

An important factor influencing the RTD CVC is the interelectronic interaction. Usually, the method of taking it into account is the self-consistent field method, in which the SFP is determined from the Poisson equation. The electron density depends on the wave functions and is calculated by the formula:

$$n_{L(R)} = \frac{\sqrt{2}kT}{(2\pi)^2\hbar^3} m^{\frac{3}{2}} \int_{U_{l(r)}}^{\infty} |\psi_{L(R)}|^2 \ln \left(1 + e^{\frac{-E+E_{FL(R)}}{kT}} \right) \frac{1}{\sqrt{E-U_{l(r)}}} dE \quad (4)$$

where kT is the thermal energy, m is the effective mass of electrons in the reservoirs, $\psi_{L(R)}$ are the wave functions of electrons entering the channel from the source (drain), $E_{FL(R)}$ is the Fermi level in the source (drain), $U_{l(r)}$ is potential energy of electrons at the “channel-source (drain)” boundary.

The electron concentration and the potential of the self-consistent field are related by the Poisson equation

$$\frac{d}{dz} \varepsilon(z) \frac{d}{dz} \varphi(z) = q_e [n(z) - N_d(z)] \quad (5)$$

where $\varepsilon(z)$ is the permittivity, $N_d(z)$ is the concentration of donor impurities, $n(z) = n_L + n_R$ is the electron concentration.

With the help of the introduced assumptions on the basis of equations (1)-(5) of the ab initio model, the equations of the effective compact model were obtained, which make it possible to maintain the accuracy of the ab initio model, while achieving less time complexity. Thus, it is proposed to estimate the current density in accordance with the relation:

$$J = \frac{q_e}{h} \sum_{i=1}^N \Gamma_i D(\varepsilon_i, V) \quad (6)$$

where ε_i и Γ_i are the energy and width of the i resonant level, N is the number of resonant levels.

The energy of the resonant level in the developed model is represented as

$$\varepsilon_i(V) = \varepsilon_{0_i} + \phi(V) \quad (7)$$

where ε_{0_i} is the position of the resonant level at zero voltage without taking into account self-consistency, $\phi(V)$ is the correction to the resonant levels due to the external voltage and interelectronic interaction.

In this case, the self-consistent correction $\phi(V)$ is the same for all resonant levels, since it depends on the electron concentration in the well, which is the sum of the electron concentrations at individual resonant levels

$$n_{L(R)} = \sum_{i=1}^N n_{L(R)_i} \quad (8)$$

where $n_{L(R)_i}$ is electron concentration at the i resonant level.

Within the assumptions of the model formula (4) was transformed into the following expression for the electron concentration in the quantum well at the resonant level

$$n_{L(R)_i} = A_{iL(R)} g_{L(R)}(\varepsilon_i) \quad (9)$$

where $A_{i_{L(R)}}$ are constant coefficients, $g_{L(R)}(E) = \ln \left(1 + e^{\frac{-E+E_{FL(R)}}{kT}} \right)$

From the general solution of the Poisson equation and the assumptions of the model, the following equation is obtained, which relates the electron concentration in the RTS quantum well and the self-consistent correction to resonance levels for the case of symmetric structures

$$\phi(V) \approx q_e \frac{V}{2} - E_0(n_L + n_R) \quad (10)$$

where E_0 is constant factor.

Equations (7), (8), (9) and (10) form a system from which a self-consistent correction to resonant levels is found, after which the current density at a given voltage is calculated by formula (6).

3 Results and discussion

As part of the assessment of the adequacy of the obtained mathematical and numerical models, the calculations were verified (with confirmation of the correctness of the discretization of the computational domain and the obtained discrete solution). The verification of the program code was also carried out (with the recognition of the insignificance of the discrepancy (less than 0.5%) of the results obtained with the estimates of the test results of conditionally analytical approaches). To validate the developed model, experimental studies of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructures were carried out. The agreement between the calculation results and the experimentally measured current-voltage characteristics was confirmed. In particular, the value of the relative deviation of the initial section of the calculated CVC from the experimental one does not exceed 2%. Thus, based on the results of verification and validation of the developed model, a conclusion was made about high efficiency (high accuracy with a relatively low time complexity of the computational algorithm). An example of calculating the CVC of a test structure is shown in Figure 1.

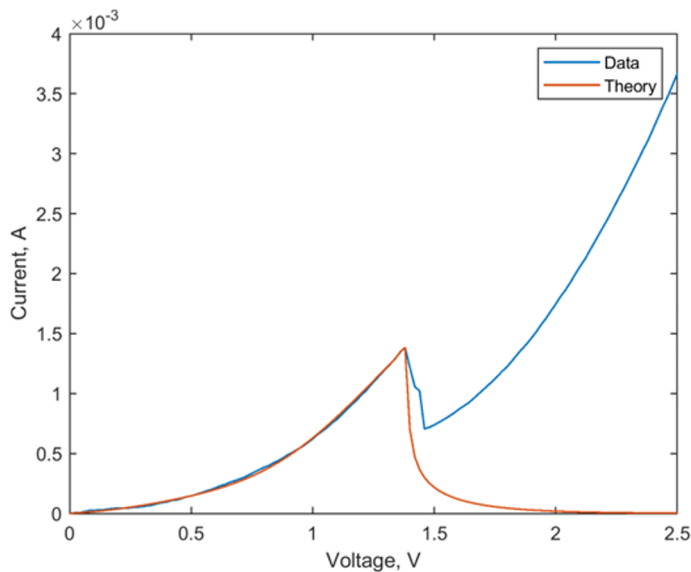


Fig. 1. Experimental RTD current-voltage characteristics in comparison with use of the compact model

The transition to an efficient model from the *ab initio* self-consistent field model made it possible to significantly reduce the time complexity of the calculation. The calculation time for one test CVC using a compact model on an AMD Ryzen 7 2700X Eight-Core Processor with a clock speed of 3.90 GHz, 16.0 GB x64 RAM is 2-5 seconds, while the calculation using the first-principles model (in within the one-valley approximation) is ~15 minutes. Most of the execution time of model algorithms based on wave function formalisms is occupied by solving a system of linear algebraic equations by the sweep method, calculating the local density of states, and calculating integrals. A single call to these functions does not take much time, however, to calculate one CVC these functions need to be executed millions of times, which leads to a large time required for the calculation.

4 Conclusions

A mathematical model is proposed for predicting the current-voltage characteristics of resonant tunneling diodes based on nanosized A_3B_5 heterostructures. A feature of the developed model is the explicit consideration of the processes of interelectronic interaction by adding the energy of this interaction to the energy of resonant levels in the RTS. As a result of the validation, it was proved that the developed model makes it possible to estimate the RTS CVC with an accuracy sufficient for engineering applications. The developed effective model makes it possible to predict non-stationary phenomena in the area of negative differential conductivity, such as hysteresis. A significant gain in calculation speed is shown in comparison with traditional models of current transfer. Thus, the developed model does not have the above disadvantages of traditional approaches and is promising for use in modern E-CAD systems when designing nonlinear radio signal converters.

However, at the moment, it has not been possible to achieve good agreement between the results of calculation and experiment in the area of negative differential conductivity, which is due to the fact that the verification basis model does not take into account the physics of the processes that have a decisive influence in the formation of this area. In this regard, the main direction of further research is the generalization of the model for the NDC section. It should be noted that the shape of this area is significantly influenced by the temperature factor. In this regard, it is planned to study in detail the consideration of temperature in the simulation of current transfer, which is an urgent task in predicting the reliability parameters and the test acceleration factor.

Acknowledgements

The study was supported by the grant from the Russian Science Foundation № 22-19-00455, <https://rscf.ru/project/22-19-00455/>.

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