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# Modeling of current-voltage characteristics of resonant tunneling structures for solving the problems of studying objective functions in the problems of synthesizing resonant tunneling diode

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**Abstract.** The resonant tunneling diode (RTD), due to the possibility of targeted synthesis of the current-voltage characteristic, is one of the most attractive non-linear elements of signal converters. To realize the advantages of the RTD, a model of its current-voltage characteristic (CVC) is needed, however, the existing models do not allow for a physical and mathematical interpretation of the relationships between the CVC parameters and the RTD design, which makes it impossible to analyze the objective functions and, as a result, the choice of optimization method. Hence, the problem of studying objective functions arises, which makes the choice of the optimization method unreasonable. To solve this problem, a compact analytical model of current transfer has been developed, the distinguishing features of which are the allowance for interelectronic interaction and the absence of undetermined empirical correction factors. Estimates of the electron density in the quantum well of the RTD heterostructural channel and the self-consistent correction to resonant levels are obtained. The developed model makes it possible to obtain estimates comparable in accuracy with estimates of distributed models over the entire area of the positive differential resistance of CVC with a relative error for AlGaAs structures not exceeding 1%, which meets the requirements of the design problems of modern radio electronic devices, in particular, devices for converting the frequency of radio signals for receiving - transmitting systems for various purposes. Thus, the presented compact model is promising for integration into RTD-based device design systems.

**Keywords:** mathematical modeling, resonant tunneling structures, self-consistent potential, electron density, oscillators

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# Моделирование вольт-амперных характеристик резонансно-туннельных структур для решения задач исследования целевых функций в задачах синтеза резонансно-туннельных диодов

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**Аннотация.** Резонансно-туннельный диод (РТД) благодаря возможности целенаправленного синтеза воль-амперной характеристики является одним из наиболее привлекательных нелинейных элементов преобразователей сигналов. Для реализации преимуществ РТД необходима модель его вольт-амперной характеристики (ВАХ), однако существующие модели не позволяют проводить физико-математическую интерпретацию связей между параметрами ВАХ и конструкцией РТД, что делает невозможным анализ целевых функций и, как следствие, выбор метода оптимизации. Отсюда возникает проблема исследования целевых функций, что обуславливает необоснованность выбора метода оптимизации. Для решения обозначенной проблемы разработана компактная аналитическая модель токопереноса, отличительными чертами которой являются учет межэлектронного взаимодействия и отсутствие неопределяемых эмпирических поправочных коэффициентов. Получены оценки концентрации электронов в квантовой яме гетероструктурного канала РТД и самосогласованной поправки к резонансным уровням. Разработанная модель позволяет получать оценки, сравнимые по точности с оценками распределенных моделей на всем участке положительного дифференциального сопротивления ВАХ с относительной погрешностью для AlGaAs-структур не превышающей 1%, что соответствует требованиям задач проектирования современных радиоэлектронных устройств, в частности, устройств преобразования частоты радиосигналов для приемо-передающих систем различного назначения. Таким образом, представленная компактная модель является перспективной для интеграции в системы проектирования устройств на основе РТД.

**Ключевые слова:** математическое моделирование, резонансно-туннельные структуры, самосогласованный потенциал, концентрация электронов, осцилляторы

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## Introduction

The resonant tunneling diode (RTD) is one of the most promising devices as a non-linear element of the next generation of signal converters for a wide range of applications. The possibility of optimizing the shape of the current-voltage characteristics (CVC), as well as the presence of a falling section on it, makes it possible to create a whole range of nonlinear radio signal converters with improved characteristics. However, the problem of design and technological optimization of resonant tunneling diodes for nonlinear signal converters is not completely solved today, due to limitations in the choice of optimization methods [1–4] due to the difficulties of analyzing objective functions. The problem of such an analysis lies in the impossibility of studying the form and unimodal objective functions, which calls into question the choice of the objective function and the optimization method. The indicated problem is due to the specifics of CVC models used in the process of optimizing the RTD design [5, 6], which do not allow establishing “transparent” relationships between the CVC parameters and RTD parameters, which does not allow for the study of objective functions. Thus, the problem of constructing a qualitative and quantitative model of current transfer is relevant, the structure of which allows one to analytically study the local properties of objective functions.

## Materials and Methods

For design and technological optimization of the RTD, the criterion for the compliance of the RTD CVC with the required one, as a rule, is formulated in the form

$$K = \int_{V_1}^{V_2} K_V\left(J_T\left(V\right), J\left(V\right)\right) dV \tag{1}$$

here $J(V)$ is RTD CVC, $J_T(V)$ is target CVC, $K_V(J_T(V), J(V))$ is kernel, $V_1$, $V_2$ are boundaries of the section of the optimizing CVC.

Traditionally, as a core in RTD optimization problems, for example, for microwave converters of radio signals, they use an integral estimate of the divergence of the normalized initial participations of the CVC (with a 10–15% offset from the peak current value) or an absolute error at the CVC operating point [1–4]. Herewith the problem arises of calculating the derivatives K with respect to the parameters of the CVC model, from which, obviously, the calculation of the derivative of the CVC follows, which is an unsolvable task for the currently used models. The scheme of optimization approach is shown in Figure 1. To synthesize the resonant tunneling structure (RTS) as solution of the inverse problem at the design stage in [1, 2], enumeration methods or stochastic methods are used, which in most cases actually replace the optimization problem with the problem of choosing a rational design to obtain the target CVC, which, in turn, greatly blurs the mathematical formalization of compliance with the requirements for CVC. The solution to this problem is a reasonable choice of the optimization method based on the characteristic features of the objective function. The core of the criterion (1) is determined by the type of functional dependence of the CVC, and therefore, if instead of an implicitly given function, a compact model that operates with explicit links between the RTD design and the destination parameters is significantly simplified, the rationale for applying one or another optimization method is greatly simplified.

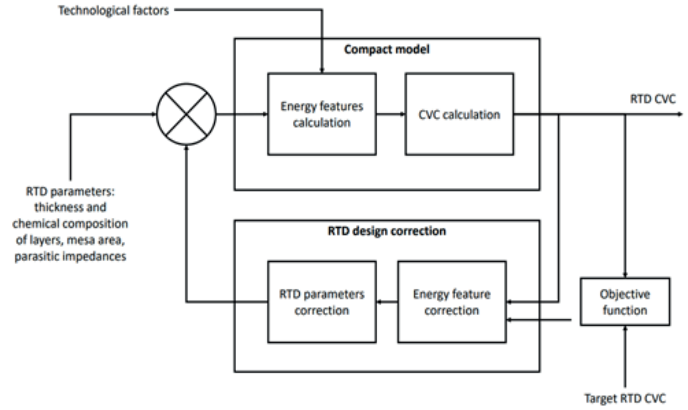

Fig. 1. RTD Design Optimization Scheme

To carry out studies of object functions, a CVC model is required that has the following properties:

1. Acceptable accuracy of CVC prediction should be provided in a wide voltage range;
2. Adequacy of modeling of non-stationary processes in the RTS and, as a result, the impossibility of predicting hysteresis phenomena of the CVC of the RTD;
3. Low temporal and spatial complexity of existing computational CVC algorithms, taking into account dissipative processes in RTS.

Existing CVC models [5–8] have the listed properties only partially, which limits their effectiveness both for solving the problem of synthesizing RTS according to the criterion of a given level of indicators for assigning signal converters, and for studying the properties of objective functions, which makes it relevant to develop an effective compact model of current transfer in RTS.

Based on the results of numerical experiments with various structures, assumptions were formulated, on the basis of which an effective compact model was built:

1. The current density and electron concentration in a quantum well are due to electrons with energy in the vicinity of resonant levels;
2. The width of the resonant levels is negligible compared to the thermal energy (at a temperature of 300 K);
3. The coefficient of tunnel transparency and the local density of states in the vicinity of the resonant levels is approximated by the Lorentz distribution for all designs that provide resonant tunneling at typical operating temperatures of signal converters (from 300 K and above).

Figure 2 shows the results of calculating the local density of states (LDOS) of RTD#1 using the combined model [6,8] (descriptions of the structures are given in the next section), illustrating the assumptions of the compact model.

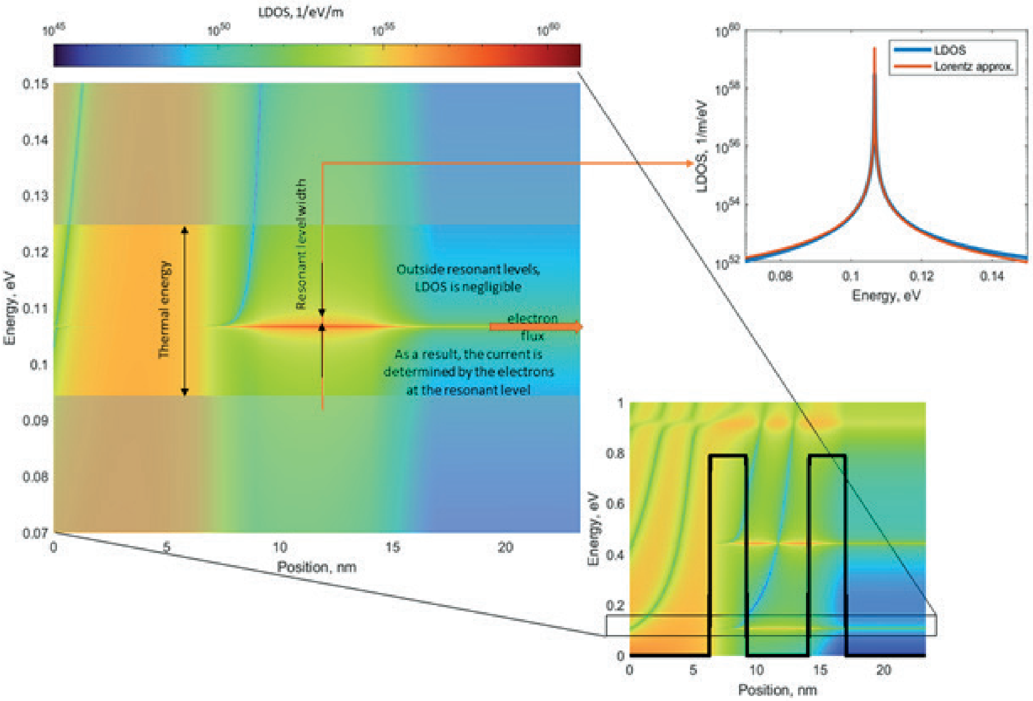

Fig. 2 Characteristic view of the LDOS, explaining model assumptions: on the left side is a plot of LDOS in a narrow energy range, is a more detailed representation of the LDOS dependence in the lower right side; in the upper right part – a view of the approximating Lorentzian curve for LDOS in the vicinity of the resonant level

Within the framework of the formulated assumptions, the following equations were obtained to describe the initial section (from zero to peak) of the CVC of the RTD

$$J(V)=\frac{q_e}{2\hbar}\Gamma\left(f_{2D}(\varepsilon)-f_{2D}(\varepsilon+q_eV)\right)$$
$$\varepsilon=\varepsilon_0-q_e\frac{V}{2}-E_0\left(C_Lf_{2D}(\varepsilon)+C_Rf_{2D}(\varepsilon+q_eV)\right) \tag{2}$$

here $\varepsilon(V)$ – resonant levels energy, $V$ – voltage, $\Gamma$ – resonant levels width, $f_{2D}(\varepsilon)$ – 2D electron gas distribution, $\varepsilon_0$, $E_0$, $C_L$, $C_R$ – internal parameters of the model, $q_e$ – elementary charge, $\hbar$ – Dirac constant.

Model (2) makes it possible to analytically calculate the derivatives of CVC with respect to the model parameters, which makes it possible to analytically study the objective functions.

## Results and Discussion

To validate the developed model and its software implementation, experimental studies of $Al_xGa_{1-x}As$ heterostructures were carried out. RTDs of 3 types grown by the MBE method served as experimental samples (Table 1). Measurements of the current-voltage characteristics of the diodes were carried out on a measuring software and hardware complex, consisting of a SIGNATON S-1160 PROBE STATION microprobe device, an Agilent 3640A DC Power Supply, an Agilent 34401A multimeter, and a personal computer. The stand allows you to measure the CVC in the voltage range from 0.1 μV to 20 V and currents from 10 nA to 3 A with an error of no more than 0.05% for voltage and no more than 0.15% for current. Comparison of the results of modeling and experimental measurements are presented in Fig. 3 and Table 2. As can be seen from the graph and table, for all test RTDs, it was possible not only to maintain the agreement on the peak point of the CVC, but also to obtain good agreement (the error does not exceed 1.5%) along the curvature of the CVC RTD.

Table 1

**RTD's structures**

| № | Layer | Compound | Alloying | Doping, см$^{-3}$ | Layers thickness RTD#1, Å | Layers thickness RTD#2, Å | Layers thickness RTD#3, Å |
|---|---|---|---|---|---|---|---|
| 1 | Waffer | GaAs | – | – | 4 500 000 | | |
| 2 | Buffer layer | GaAs | ud | – | 2 000 | | |
| 2a | Buffer layer | GaAs | Si | 4–5×10$^{18}$ | 15 000 | | |
| 3 | | GaAs | Si | 2×10$^{17}$ | 500 | | |
| 4 | Transition layer | GaAs | Si | 7×10$^{16}$ | 500 | | |
| 5 | Spacer | GaAs | ud | – | 63 | 22.6 | 22.6 |
| 6 | | AlAs | ud | – | 29 | 22.6 | 28.3 |
| 7 | | GaAs | ud | – | 49 | 101.7 | 28.2 |
| 8 | | AlAs | ud | – | 29 | 22.6 | 28.3 |
| 9 | Spacer | GaAs | ud | – | 63 | 22.6 | 22.6 |
| 10 | Transition layer | GaAs | Si | 7×10$^{16}$ | 500 | | |
| 11 | | GaAs | Si | 2×10$^{17}$ | 500 | | |
| 12 | Contact layer (Tsub –> 500C) | GaAs | Si | 4×10$^{18}$ | 500 | | |
| 13 | Contact layer (Tsub = 500C) | Grad InGaAs 0.05 –> 0.5 | Si | 4–5×10$^{18}$ | 500 | | |
| 14 | Contact layer (Tsub = 500C) | $In_{0.5}Ga_{0.5}As$ | Si | 5×10$^{18}$ | 200 | | |
| Mesa diameter, μm | | | | | 10 | | |

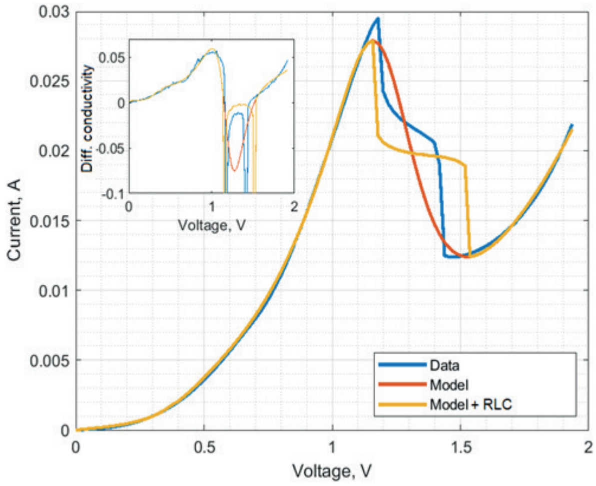

Fig. 3. Calculated CVC and differential conductance of RTD#1 in comparison with experimental ones

The developed model demonstrates a high degree of agreement with the experiment in the initial section of the CVC and in terms of the degree of contrast in the section of negative differential conductivity (NDC), the error usually does not exceed 5% (see Fig. 3 and Table 2). The high accuracy of the model in the initial section was also confirmed by differential conductivity calculations (see the inset in Fig. 3, the colors of the lines correspond to the colors of the legend of the CVC plot). Standard methods for taking into account the external impedance with the inclusion of the LC component in the calculation scheme [9,10] make it possible to improve the correspondence in terms of differential conductivity in the NDC section.

Table 2

**Errors in the calculation of RTD's CVC**

| Parameters | RTD #1 | RTD #2 | RTD #3 |
|---|---|---|---|
| Experimentally measured value of peak current, mA | 29.45 | 1.38 | 5.05 |
| Theoretically calculated value of peak current, mA | 28.00 | 1.38 | 5.45 |
| Peak current calculation error, % | 4.92 | 0.00 | 8.00 |
| Measured peak position, V | 1.19 | 1.38 | 2.48 |
| Theoretically calculated peak position, V | 1.18 | 1.38 | 2.56 |
| Peak position calculation error, % | 0.84 | 0.00 | 3.23 |
| Average absolute error in the calculation of the initial section of the current-voltage characteristic, mA | 0.22 | 0.01 | 0.08 |
| Maximum absolute error in the calculation of the initial section of the CVC, mA | 0.47 | 0.02 | 0.21 |

## Conclusion

A compact model of current transfer in an RTD is presented, taking into account the self-consistent field. As a result of the analysis of current transfer processes in RTDs, taking into account the interelectronic interaction, estimates of the electron density in the quantum well of the heterostructural channel and the self-consistent correction to resonance levels were obtained, which made it possible to solve the problems that traditionally arise when optimizing the RTD design. The developed model, due to the reduction in the time complexity of the algorithm by several orders of magnitude and the preservation of the accuracy of distributed models of current transfer, makes it possible to solve the problems of synthesizing the RTD CVC and investigate the objective functions of design and technological optimization methods in order to increase their efficiency. As a continuation of research for the next stage of research under the grant from the Russian Science Foundation No. 22-19-00455, it is planned to use the developed model to analyze the properties of the objective functions used in RTD synthesis methods, including those modified for RTD synthesis with operating points in various sections of the CVC.

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