Hyerarchial Approach to Resonant-Tunneling Diode Modeling

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Abstract **– Hierarchical approach to resonant-tunneling diode modeling (RTD) is proposed. Hierarchical model's family consists of analytical model, numerical one-band and numerical two-band models. Each model was developed by improving both theoretical and numerical aspects of existing models. Inside each family different assumption could be accepted, depending on the goal of modeling. Flexibility, speed and functionality of modeling are shown to be enhanced by using this approach.**

Keywords – resonant-tunneling diode, hierarchial approach, numerical model, analytical model

I. INTRODUCTION

Due to its unique properties, RTD is a one of the most promising component to be used in terahertz sources, high-frequency logical schemes [1]. Development of RTDs with improved electrical characteristics is now being performing by some intuitive consideration rather than based upon deep understanding of the underlying physical processes. This is due to lack of a tool, allowing adequate modeling with high prognostic ability and making it possible to analyze real processes underlying RTD's electrical characteristics. This paper describes an attempt of developing such a tool, based on hierarchical approach.

II. ANALYTICAL MODEL

Quantitative modeling of electron processes in RTD requires numerical models. General drawback of all existing numerical models is a high intensity of using numerical resources, and lack of analytical, suitable for direct analysis, connections between input (physical and topological parameters) and output quantities (parameters of quantum effects and electron transport). It is clear that general lows of such dependences and quick qualitative estimations are of great value for device fabrication.

Based on [2], we have developed a fast qualitative model, which allows tracing cause-and-effect connections between the width of a well a and barriers b, stoichiometric composition of the layers x, donor's concentration at the reservoirs N_D from one side and levels' position E_i, levels' broadenings Γ_i and Γ_p and applied voltage V from another side. Intermediate quantities, appearing within a given formalism (Fermi energy E_F, single barrier transmission probability T_b, relaxation time τ_p) also have clear physical sense and analytically connected with input quantities. The scheme of the model is shown in fig. 1. Examples of analytical modeling results for RTD with parameters, taken from [3] are given in Fig. 2.

Analytical model serves as a "predictor" for design development of RTD. When the main tendencies have been estimated, one can pass on to more accurate modeling, making use one of the numerical models, described below.

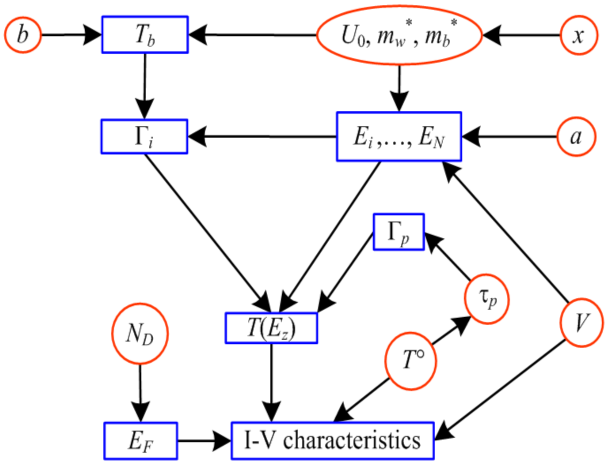

Figure 1. Cause and effect chains between input (circles) and output (rectangles) parameters or characteristics.

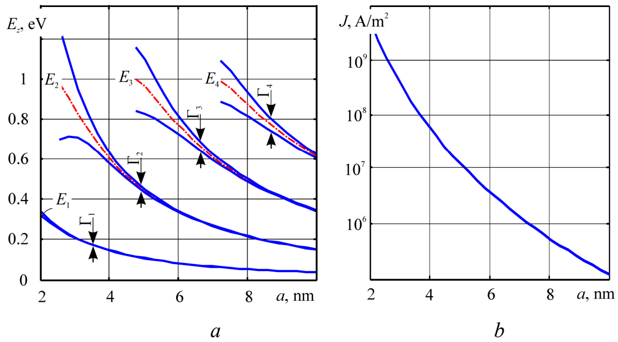

Figure 2. Energy levels' position E_i, their natural broadening Γ_i (*a*) and current density (*b*) versus well's width *a*

III. NUMERICAL MODELS

The key feature of the numerical models is a distinct description of undoped nanoscale region (it consists of double barrier quantum system (DBQS) and spacers) and two bulk regions, surrounding it. The first region is called "device", the latter is known as "reservoirs". Electron gas in each reservoir is considered to be in equilibrium with its Fermi level and distributing according to Fermi-Dirac statistics. Electron distribution function in quantum region is defined by the distribution of electrons, emitting there from the left and right reservoirs; their behavior assumed to be affected by the field of the lattice (within band theory) and interaction with all others electrons within the Hartree approach ("self-consistent field"). The two regions are "sticking together" by so-called quantum transmitting boundary method [4].

It is possible to take into account three scattering mechanisms in RTD: (a) scattering in the quantum well (according to method, described in [5]); (b) inelastic scattering in the emitter quantum well; (c) elastic interface intervalley scattering at the heteroboundaries.

Inelastic scattering into the emitter quantum well is taking into account by original method, developed by us in [6]. It allows avoiding a principal restriction of the envelope function formalism, which is impossibility to take into account inelastic processes. We have bypassed this problem by introduction "virtual" reservoir and some phenomenological notions. Recently, it was proven that electrons, thermalized to the metastable levels in EQW, contribute to the net current in the negative conduction region of I-V characteristics [7]. Our model predicts such changes of I-V curve fairly; underlying physics is in complete agreement with experiment, unlike [8].

The last mechanism of scattering needs higher valley engagement to be realized. We call such a model "*two-valleys*" one as opposed to "*one-valley*" model, which implied to be not accounts for intervalley scattering.

As opposed to standard "rough" approximation of the conduction band wrapping, we apply recent results, obtained within pseudopotential method, which testifies that assumption about two-steps wrapping is more accurate [9].

Electric current through resonant-tunneling diode is calculated according to well-known Tsu-Esaki formula, in which transmission coefficient is to be found, taking into account two channels (coherent and incoherent) in two valleys (usually Γ and X), as well as transport by means of EQW metastable level.

There is a set of visualized quantities, which enables deep analysis of electron processes in RTD: local densities of states, in Γ- and X-valleys, transmission coefficients (as shown in Fig. 3), distribution functions, concentration and potential distributions across the layers in each valley. Numerical experiments were fulfilled by "QuanT ST" application we have designed to simulate quantum-size effects and transverse electron transport in heterostructures. This is free-distributed software with open source, realized in Matlab GUI [10].

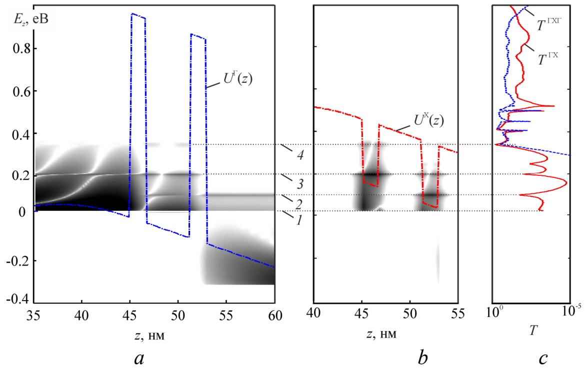

Figure 3. Two-valley numerical model simulation results: electron distribution function in Γ-valley (*a*) and X-valley (*b*); net transmission coefficients (*c*) from Γ to Γ valley ($T^{\Gamma X\Gamma}$) and from Γ to X-valley ($T^{\Gamma X}$). Notes: *1* – bottom of conduction band in the left reservoir, *2*, *3* – interference levels, *4* – second main level. RTD topology was taken from [3]. Darker color corresponds to higher electron density in E_z-space.

IV. CONCLUSION

By using three models, differing by adequacy, functionality and purpose, instead of one, we obtain desirable flexibility and speed of modeling. Better adequacy is also achieved by improvement of existing models. Using proposed approach is expected to speed up designing of RTDs with preassigned properties.

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