Modeling of Resonant-Tunneling Diode with “Quant ST”

Artem Fedyay and Volodymyr Moskaliuk

Abstract – **Two-valley numerical model of resonant-tunneling diode (RTD) is developed. Coherent and incoherent channels of electron transport and transport through emitter quantum well (EQW) are taken into account. Visualization of the micro- and macroscopic quantities was done, using “QuanT ST” application, developed by the authors and based upon the model.**

Keywords – **quantum transport, resonant-tunneling diode, quantitative simulation, Quant ST.**

I. Introduction

Resonant-tunneling diodes have the potential for use in sources of terahertz frequency range [1]. Successful applications of RTD for a number of applications were shown by now. Although, satisfactory prediction of electric characteristics still achieved only by introducing 5 and more “fitting” parameters [2]. Usability of such models is doubtful.

Quantitative modeling of resonant-tunneling diode is extremely complicated both from theoretical and numerical point of view. Developed model has been shown to be high adequate along with reasonable utilization of numerical resources. We describe its theoretical background and main advantages over analogs and show the result of verification for RTD with complicated emitter structure.

II. The model

The model is derived within envelope functions formalism. The key feature of a model is a distinct description of the 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 are 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, as opposed to [2], where Maxwell distribution were assumed. Electron distribution function in quantum region is defined by the distribution of electrons, emitting there from the left and right reservoirs; particles’ 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 device and reservoirs are “sticking together” by so-called quantum transmitting boundary method [3]; their boundaries are rigidly fixed at the boundaries between high-doped and undoped regions as opposed to [2] or [4].

It is assumed that there are three scattering mechanisms in RTD: (*a*) Quasi-elastic scattering in the quantum well; (*b*) elastic interface intervalley scattering at the heteroboundaries; (*c*) inelastic scattering in the emitter quantum well

Scattering in the quantum well is taking into account by introduction of so-called “optical potential” into Hamiltonian of effective mass Schrödinger equation in the well [5]. In order to preserve current conservation while using “optical potential” model, we apply the single-scatter model [6], which connects reduction of the transmission probability with the transition of electrons from the coherent channel to “incoherent” channel. As opposed to [2], we calculate incoherent transmission, avoiding approximation of the transmission coefficient after scattering event.

Within a known model of interface scattering [7], our model make it possible to take into account the effects of the mixing of the states from the two lowest valleys.

Inelastic scattering in the emitter quantum well is taking into account by original method, developed by us in [8]. It allows avoiding a principal restriction of the envelope function formalism, namely, impossibility of taking 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 [9]. Our model predicts such changes of I-V curve fairly; underlying physics is in complete agreement with experiment [9], unlike [2].

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 [10].

Electric current through the 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.

III. Verification

The model, briefly described above, was verified at the numerous RTD of different structure and composition. Here we demonstrate excellent qualitative coincidence of our modeling results with experimental results for RTD with graded emitter, described in [11]. Substrate orientation is [100]. Topology and stoichiometric composition of the RTD’s layers are shown in Fig. 1.

Physical parameters, accepted by the model are as given in Table 1. In the table T is temperature, $\hbar\omega_{op}$ is optical phonon energy in the quantum well, m and ε denote, respectively, relative effective mass in transverse direction and dielectric permeability. Higher and lower indices, accompanying m and ε, denote the name of a valley and chemical composition, respectively. Coupling constant between Γ and X valley was denoted by α. Parameters of the layers of graded emitter were given according to empirical formulations in [12].

It was shown that the first peak at the I-V curve appeared when the Fermi level coincides with the metastable level in the

Artem Fedyay – Kyiv Polytechnic Institute, Peremohy prosp., 37, Kyiv, 03056, UKRAINE, E-mail: artem.fedyay@gmail.com

quantum well of the DBQS (hereafter "main quantum well", MQW). The second peak corresponds to coincidence of the metastable level in EQW and MQW.

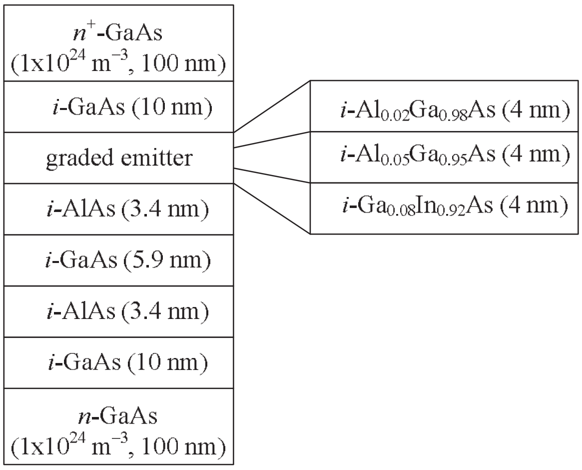

Fig.1. RTD's topology and layers' composition.

Table 1

PHYSICAL PARAMETERS OF RTD LAYERS

parameter	value	parameter	value
T, K	300	m^{Γ}_{GaAs}	0.067
$\hbar\omega_{op}$, eV	0.036	m^{X}_{GaAs}	1.3
S_{op}, $psec^{-1}$	36	m^{Γ}_{AlAs}	0.15
ε_{GaAs}	12.9	m^{X}_{AlAs}	0.97
ε_{AlAs}	10.06	α, eV·Å	0.15

Numerical experiments were fulfilled by our own application "QuanT ST" that was designed for simulation quantum-size effects and transverse electron transport in heterostructures. This is free-distributed open source software, realized in Matlab GUI [13].

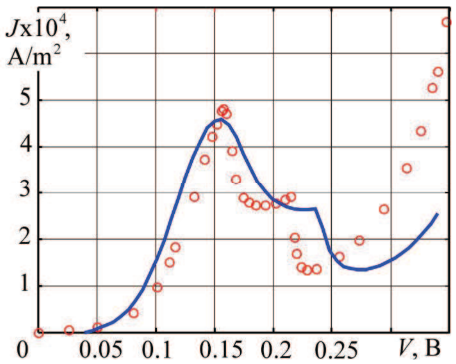

Fig. 2. Comparison of experimental (solid line) and modeled I-V characteristics (circles).

IV. CONCLUSION

We have presented the model of resonant tunneling diode. Standard physical assumptions along with several significant improvements allowed us obtaining fast and adequate physical model. Verification has shown high quantitative and qualitative coinciding with experimental data. As we have used only one fitting parameter, results are among the best obtained by now; therefore, our model can be used for accurate prediction of electrical characteristics of RTD.

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