Simplified Analytical Model of Resonant-tunneling Diode

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***Abstract**: Simplified analytical model for analysis of influence of the main parameters of resonant-tunneling diode's (RTD) topology on its static electric characteristics was developed. Analytical relations that relate electric characteristics of RTD with the main design parameters: widths of layers' in active region, chemical compound of layers, doping level of reservoirs, lattice temperature were obtained. The results of modeling were tested for model structures of RTDs with barrier layers formed of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}N$. The model is free of numerical instabilities and adequately expresses the main tendencies in the dependencies of I-V characteristics' parameters on the topology. It has been formulated such, that the computational resources are used efficiently and allow to trace the impact of all listed parameters on the energy structure of active region, and how those changes affect on the shape of I-V characteristics step-by-step.*

1. INTRODUCTION

The modeling of resonant-tunneling diodes has passed several stages since invention. The formalisms of wave functions [1], Green's and Wigner's functions [2,3] were used by different authors since pioneering work [4] by present time. The way of improving consists in the procedure of self-consistency, accurate consideration of band structure of the corresponding materials and taking scattering processes into account [5]. Successive application of all mentioned components leads to enormous complications of modeling procedure. Although the numerical methods could be optimized, the connection between the topology of RTD and its electric characteristics became such that they could not be estimated by analytical relations, and understood intuitively. Under such conditions one should have the model that is complicate enough to reflect all main qualitative tendencies of electric characteristics depending on topology parameters of RTD and connecting them in an analytical way. Such tendencies should be used as a roadmap for device technologists at the initial stage of RTD designing. Then for quantitative analysis the more accurate and numerically extensive model should be used.

2. MODEL

Modeling procedure in the current work is divided into several problems solving successively:

1. Search of the total number and the energy of energy levels in the quantum well, complete neglecting decaying possibility of metastable states.
2. Search of the transmission coefficients for single potential barrier.
3. Search of the quantity of the "natural" and "relaxation" decaying of the energy levels in the quantum well.
4. Using quantities that were calculated for obtaining I-V characteristics of RTD.

2.1. Total number of the levels

If double-barrier quantum system (DBQS) formed by the layers of RTD is considered as a system that is able to decay, then the discrete levels, obtained under complete neglecting of decaying possibility will coincide with the most probable energy of the electron in the correspondent metastable state.

DBQS with infinite barriers' widths is the searched system with zero probability of decaying. Denoting the width of the quantum well by a, and the height of potential barrier by U_0, and solving Schrödinger equation for such system, one can obtain the following two systems of equations, roots of which determine the positions of the energy levels. [6]:

$$\begin{cases} \cos\xi = \pm\gamma\xi \\ \operatorname{tg}\xi > 0 \end{cases}, \qquad (1)$$

$$\begin{cases} \sin\xi = \pm\gamma\xi \\ \operatorname{tg}\xi < 0 \end{cases}, \qquad (2)$$

where $\xi = ka/2$, $k = \sqrt{2m^*E}/\hbar$; $\gamma = \dfrac{\hbar}{a}\sqrt{\dfrac{2}{m^*U_0}}$,

where $\hbar$ is reduced Plank's constant; E is energy of the longitudinal motion of electron; m^* is effective mass of the electron in the well.

The solution of the systems (1) and (2) is possible only if $\gamma\xi < 1$ or $\xi < 1/\gamma$. In such region one of the systems (1) or (2) will have one root in the each of the intervals $\left(\dfrac{\pi}{2}(n-1); \dfrac{\pi}{2}n\right)$, where $n = 1,2,3,\ldots n_{\max}$. The total number of full intervals $s = \operatorname{int}(\dfrac{2}{\pi\gamma})$, where "int" denotes the integer part. Besides, if $\dfrac{2}{\pi\gamma} > s$ (1) or (2) have one more root, belonging to interval $\dfrac{\pi}{2}n_{\max} < \xi < \dfrac{1}{\gamma}$.

Thus, the total number of the discrete levels $N = \operatorname{int}\left(\dfrac{2}{\pi\gamma}\right) + 1$, or, in the usual quantities:

$$N = \frac{\sqrt{2m^*}}{\pi\hbar} a\sqrt{U_0} + 1.$$

2.2. Level's positions.

Graphic interpretation (fig. 1) of the solution of systems (1) and (2) allows to restrict the area of research to the search of one root of one equation for each of intervals $\left(\dfrac{\pi}{2}(n-1); \dfrac{\pi}{2}n\right)$.

It is arising from fig . 1, that eigenvalues of energy E_n for the first four energy levels defined from the following equations:

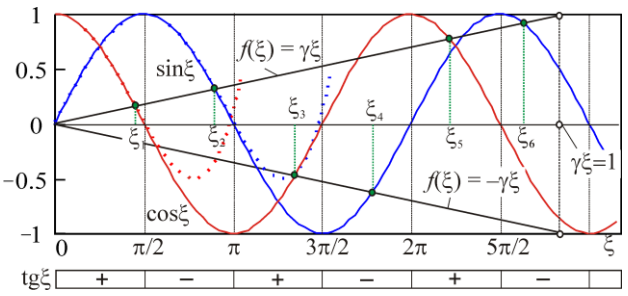

Fig. 1. Illustration for graphycal solving of the systems (1) and (2).

$$n=1: \quad \cos\xi = \gamma\xi, \qquad \xi \in \left(0; \frac{\pi}{2}\right); \qquad (3),$$

$$n=2: \quad \sin\xi = \gamma\xi, \qquad \xi \in \left(\frac{\pi}{2}; \pi\right);$$

$$n=3: \quad \cos\xi = -\gamma\xi, \qquad \xi \in \left(\pi; \frac{3\pi}{2}\right);$$

$$n=4: \quad \sin\xi = -\gamma\xi, \qquad \xi \in \left(\frac{3\pi}{2}; 2\pi\right).$$

As an example, searching the approximate analytical solution of (3), expanding cosine in the neighborhood of $\xi = 0$ and being restricted by two non-zero terms of series, one can obtain:

$$1 - \frac{\xi^2}{2} = \gamma\xi. \qquad (4).$$

Positive root of (4) $\xi = \sqrt{\gamma^2 + 1} - \gamma$, or, moving back to the usual denotes:

$$E_1 = \gamma^2\left(\sqrt{\gamma^2 + 1} - \gamma\right)^2 U_0.$$

Analytical relations for any higher energy level (if such exist) can be found by the same way, expending corresponding function in the neighborhood of any border of interval, inside of which the solutions are searched.

2.3. Transition coefficient

The transition coefficient of potential barrier with the height U_0 and width b could be calculated according to the relation:

$$T = \frac{4k_1^2\chi_2^2}{(k_1^2+\chi_2^2)^2 \mathrm{sh}^2 b\chi_2 + 4k_1^2\chi_2^2}, \quad (5)$$

where $\hbar k_1 = \sqrt{2m^* E}$, $\hbar\chi_2 = \sqrt{2m^*(U_0 - E)}$.

In the present model $T(E)$ considered to be independent from applied voltage *V*. Hereafter we assume that the voltage moves energy levels up by the quantity $\frac{eV}{2}$, so that for *i*-th level:

$$E_i(V) = E_i(0) + \frac{eV}{2}. \quad (6)$$

If $E_i << U_0$ such condition means that the voltage drops uniformly across the structure.

2.4. "Natural" and "relaxation" broadening of metastable levels

Energy spectrum of electron in the potential well, surrounded by potential barriers of the finite width, will be continuous in contrast to the case of barriers with infinite width. Although in such case there is selected magnitude of longitudinal momentum of electron in the well, where electronic wave function's amplitude is much grater, than out of the well. The maximum amplitude of electronic wave in the well corresponds to the energy levels of the same system, but with zero probability of decaying.

These levels are metastable, because electron will eventually leave the well and go to infinity through the one of barriers. Under conditions $|T_i|^2 << 1$ one can obtain the relation for calculation mean life time of electron on the metastable level [7]:

$$\tau_n = \frac{2a}{v_i}\left(\frac{1}{|T_1|^2 + |T_2|^2}\right), \quad (7)$$

where $v_i = (2E_i/m)^2$ is a velocity of electron motion on the *i*-th resonant level, T_1 and T_2 are transition coefficients for 1-st and 2-nd barrier (they are determined by relation (5))

The width of these levels related to the mean life time of electron at this state in accordance with the uncertainty principle for energy: $\Delta E_n = \frac{\hbar}{\tau_n}$, and referred as "natural" broadening of the resonant level.

At the same time, scattering processes, existing in the potential well destroy the coherence of electron wave and appear in additional broadening of energy levels by the quantity of so-called "relaxation" broadening ΔE_p. The former is related to the momentum relaxation time τ_p by the relation:

$$\Delta E_p = \frac{\hbar}{\tau_p}.$$

The main kind of scattering in the intrinsic GaAs is polar optical scattering. Such kind of scattering is nonelastic. The most polar optical phonons have energy $\hbar\omega_o = 0{,}035$ eV. Thus, each scattering event changes electron energy by $0{,}035$ eV that is usually much grater then ΔE_n. This reduces the life time of electron on at the metastable level. That is why each level additionally broadens.

Momentum relaxation time in the present work was calculated using relation for the optical-phonon scattering rate [8]:

$\frac{1}{\tau_p} = \alpha\omega_0\sqrt{\frac{2}{\pi}}\frac{t_e^{1/2}}{\mathrm{sh}t}\mathrm{K}_0(t_e)$, where α is polar constant for GaAs; $t_e = \frac{\hbar\omega_o}{2\mathrm{k_B}T_e}$, $t = \frac{\hbar\omega_o}{2\mathrm{k_B}T}$, where $\mathrm{k_B}$ is Boltzman constant, *T* and T_e are temperature of the lattice and electron's temperature, respectively; K_0 is zero-order modified Bessel function of the second kind.

The total broadening of the energy level $\Delta E = \Delta E_n + \Delta E_p$.

The quantity ΔE has clear physical sense: the probability of finding electron within this interval centered at the energy of the correspondent discrete level is equal to $1/\sqrt{2}$.

Transitional function for DBQS can be approximated by the sum of Lorentz-type functions:

$$D(E)=\sum_{i=1}^{N}\frac{\Delta E_{ni}/\Delta E_i}{1+4\left(\frac{E-E_{ni}(V)}{\Delta E_{ni}}\right)}, \qquad (8)$$

where index *i* denotes the number of discrete level.

The current density was calculated using Tsu-Esaki formulation [9]:

$$J=\frac{4\pi \mathrm{e}\mathrm{k}_\mathrm{B}m^*T}{\mathrm{h}^3}\int D(Å)dE\ln\left(\frac{e^{-\frac{E-E_\mathrm{F}}{\mathrm{k}_\mathrm{B}T}}+1}{e^{-\frac{E-E_\mathrm{F}+eV}{\mathrm{k}_\mathrm{B}T}}+1}\right), \qquad (9)$$

where h is Plank's constant, E_F is Fermi level of the electrons in the emitter of RTD.

Integration passes from the bottom of conduction band till the infinity (in the real cases one can use the level of vacuum as a superior limit)

Assuming $T\to 0$ equation (9) can be rewritten as:

$$J=\frac{\mathrm{e}m^*}{2\pi^2\hbar^3}\int_0^{E_\mathrm{F}}(E_\mathrm{F}-E)DdE,\ V\ge E_\mathrm{F}, \qquad (10),$$

$$J=\frac{\mathrm{e}m^*}{2\pi^2\hbar^3}\left[V\int_0^{E_\mathrm{F}-V}DdE+\int_{E_\mathrm{F}-V}^{E_\mathrm{F}}(E_\mathrm{F}-E)DdE\right],\ V<E_\mathrm{F},$$

Resonance condition is possible in case of $V\ge E_\mathrm{F}$. In case of consideration of quantum well with single energy level E_1, the result of integration (10) is as follows:

$$J=\frac{\mathrm{e}m^*}{2\pi^2\hbar^3}\Delta E_n^2\left\{\frac{E_\mathrm{F}-E_1}{\Delta E}\left[\tan^{-1}\left(\frac{E_\mathrm{F}-E_1}{\Delta E}\right)+\tan^{-1}\frac{E_1}{\Delta E}\right]-\right.$$

$$\left.-\frac{1}{2}\ln\frac{\left(E_\mathrm{F}-E_1\right)^2+\Delta E^2}{{E_1}^2+\Delta E^2}\right\}.$$

The maximum current density will be archived when the bottom of conduction band will coincide with energy level in the well (when $E_1=E_1(0)+\frac{eV}{2}=0$) Under such condition one can obtain the relation for maximum current density:

$$J_\mathrm{max}=\frac{\mathrm{e}m^*}{2\pi^2\hbar^3}\frac{\Delta E_n^2}{\Delta E^2}E_\mathrm{F}\Delta E.$$

3. RESULTS OF MODELING

Parameters of the modeling test structure which where used for model testing cited in the Fig. 2. Reservoirs (emitter and collector of RTD) is formed from heavily doped GaAs (donor's atom concentration $N_D = 10^{24}$ m^{-3}). Barrier layers is formed from $Al_{0.33}Ga_{0.67}As$, quantum well is formed from GaAs. Barrier layers and well layer are both undoped.

Effective mass of the electron in the compound $Al_{xm}Ga_{1-xm}As$ is determined by empirical relation:

$m^*(x_m)=0.15m\cdot x_m+0.067\cdot m(1-x_m)$, where m is the rest mass of electron.

Conductance band discontinuity ΔE_{CB}, that is equal to the height of potential barrier, can be calculated by empirical relation [10]:

$\Delta E_{CB}=0.62(\Delta Å_{\mathrm{BG}_{\mathrm{AlGaAs}}}-\Delta Å_{\mathrm{BG}_{\mathrm{GaAs}}})$ [eV], where $\Delta Å_{BG_{\mathrm{AlGaAs}}}$ and $\Delta Å_{BG_{\mathrm{GaAs}}}$ – energy gap width for AlGaAs and GaAs, respectively. For arbitrary molar fraction of aluminum x_m in the compound $Al_{xm}Ga_{1-xm}As$ the energy gap width could be calculated as: $\Delta E_{BG}(x_m)=(1.42+1.247x_m)$ [eV].

Fermi level E_F relative to the bottom of conduction band is determined as for heavily doped semiconductor:

$E_\mathrm{F}=\left(\frac{h^2}{2m^*\mathrm{e}}\right)\left(\frac{3N_D}{8\pi}\right)^{2/3}$, where N_D is donor's atom concentration (all donor impurity considered to be ionized).

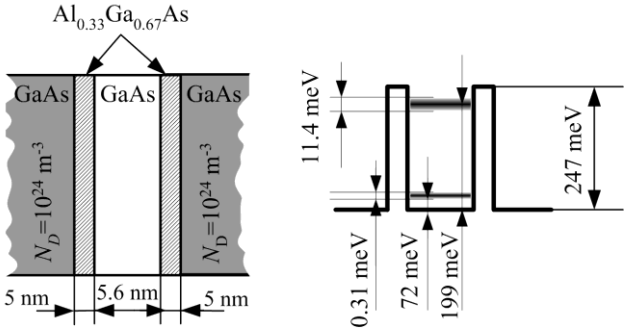

Fig. 2. Topology, position and widths of energy levels for test structure.

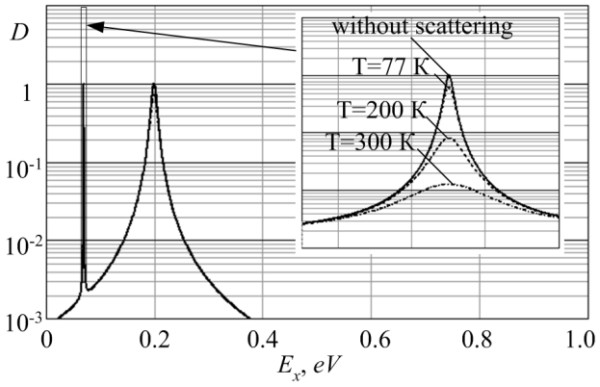

Fig. 3. Transmission probability versus longitude electron energy.

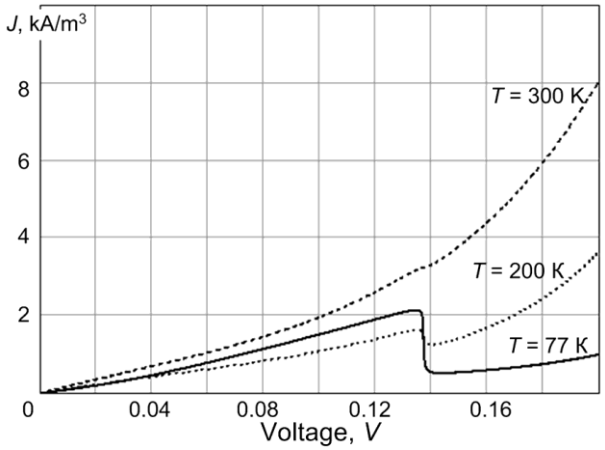

Fig. 4. I-V characteristics of resonant tunneling diode.

4. CONCLUSION

Developed model allows tracing cause-and-effect relations between design parameters of RTD and electric characteristics that expected to show such structure. The model is developed in such a way, that before I-V characteristics calculations the quantities to be computed also have direct physical senses. They are: numbers of energy levels in the quantum well, life time of electron states in the well, their widths (both "natural" and "relaxation" widths and their sum), and transmission coefficients for single barrier and for DBQS as a whole. Maximum pick current can be calculated as an analytical function of all mentioned parameters.

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