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LASERS

DYNAMIC CONDUCTIVITY OF RESONANCE TUNNEL STRUCTURES IN THE MODEL OF OPEN CASCADE IN NANOLASERS*

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Abstract. Using the effective mass and rectangular potentials approximations, the theory of dynamic conductivity of electrons for the plane multi-barrier resonance tunnel structure placed into the constant electric field is developed within the model of open cascade. For the experimentally produced quantum cascade laser with four-barrier active region of separate cascade it is proven that the theory of dynamic conductivity in the model of open cascade most adequately describes the process of electromagnetic field radiation during the electronic transport through the resonance tunnel structure placed into the constant electric field.

Key words: resonance tunnel structure, quantum cascade laser, dynamic conductivity.

1. INTRODUCTION

The operation of quantum cascade laser (QCL) [1–4], quantum cascade detector (QCD) [5–7] and other successfully functioning nano-devices is based at the transport properties of open multi-barrier nano-structures. In spite of the long period of the investigation of photon-assisted transport of electrons through the resonance tunnel structures (RTS), taking into account the interaction of electronic current with constant electric and high frequency electromagnetic fields, the present theory correlates to the experimental data not enough.

The main problems for the establishing of consistent theory of electrons transport through the RTS are the mathematical difficulties arising when the non-stationary Schrödinger equation is solved with the Hamiltonians for even comparatively simple models and with open boundaries which allow the quasi-

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particles infinite movement. In order to avoid these problems, the evaluations obtained for the closed analogues of open RTS with rectangular potential wells and barriers were used in early papers [2–4].

Active regions of QCL, such as open two- and three-barrier RTS, were theoretically studied in [8–10]. In these papers the non-stationary one-dimensional Schrödinger equation describing the electrons transport through the RTS with δ-like potential barriers was solved taking into account the interaction with constant electric and high frequency electromagnetic field. The simplified model of constant effective mass of electron along the whole nano-system and δ-barrier approximation of the potentials gave the opportunity to calculate and investigate the electronic currents and, since, the dynamic conductivity in ballistic regime.

The δ-barrier model for the open RTS [11, 12] essentially overestimated the resonance widths of operating quasi-stationary states compared to the more adequate model of rectangular potentials. It explained some properties of electrons transport but could not be used as a reliable base for the comparison with the experiment.

According to the abovementioned and using the effective mass and rectangular potentials approximations, in this paper we develop the theory of quasi-stationary spectrum and dynamic conductivity of the electrons interacting with high frequency electromagnetic field within the model of open multi-barrier RTS. We use the obtained theoretical results in order to calculate the energy of electromagnetic radiation for the experimentally produced QCL [3] with four-barrier active region of the separate cascade.

2. THEORY OF DYNAMIC CONDUCTIVITY FOR RESONANCE TUNNEL STRUCTURE WITH FOUR-BARRIER ACTIVE REGION IN OPEN MODEL

The separate cascade of QCL, such as RTS containing the four-barrier active region and injector consisting of certain number of plane nano-layers (wells and barriers) with fixed sizes, Fig. 1, is studied within the open model. We assume that the constant electric field with intensity F is applied perpendicularly to the RTS planes. The mono-energetic current of uncoupling electrons with energy E, charge e and concentration n_0 falls at RTS from the left side. At these conditions and taking into account the small difference between the lattice constants of wells and barriers, the problem settles to the study of one-dimensional transport of electrons using the models of effective mass and rectangular potentials.

Taking the coordinate system as it is shown in Fig. 1, the electron effective mass and potential energy in RTS (without applied field) is conveniently written as

$$m(z)=\begin{Bmatrix} m_0 \\ m_1 \end{Bmatrix}[\theta(-z)+\theta(z-b)]+m_0\sum_{p=1}^{N_W}\left[\theta(z-z_{2p-1})-\theta(z-z_{2p})\right]+ \\ +m_1\sum_{p=0}^{N_B}\left[\theta(z-z_{2p})-\theta(z-z_{2p+1})\right], \quad (1)$$

$$U(z)=\begin{Bmatrix} 0 \\ U \end{Bmatrix}[\theta(-z)+\theta(z-b)]+U\sum_{p=0}^{N_B}\left[\theta(z-z_{2p})-\theta(z-z_{2p+1})\right], \quad (2)$$

where N_W, N_B are the number of wells and barriers in the RTS which, depending on the model, corresponds to the active region or to the whole cascade.

In order to calculate the dynamic conductivity, we, first of all, solve the stationary Schrödinger equation

$$H(z)\Psi(z)=E\Psi(z), \quad (3)$$

with the Hamiltonian of electron in RTS driven by the constant electric field

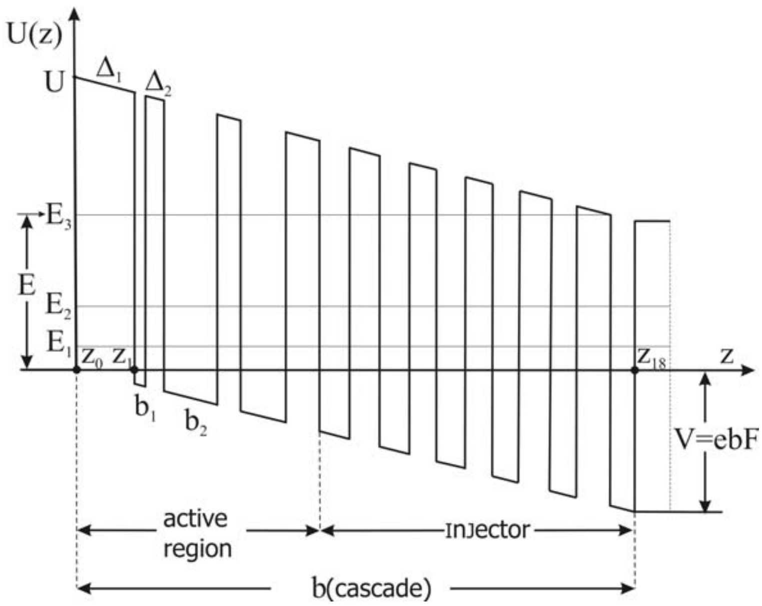

Fig. 1 – The energy scheme of separate cascade with four-barrier active region and injector. The widths of the barriers (Δ_p): 5.0, 1.5, 2.2, 3.0, 2.3, 2.2, 2.0, 2.3, 2.8 and widths of the wells (b_p): 0.9, 4.7, 4.0, 2.3, 2.2, 2.0, 2.0, 1.9, 1.9 are presented from the left to the right in nm units.

$$H(z)=-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z}+U(z)-eF\left[z(\theta(z)-\theta(z-b))-b\theta(z-b)\right]. \quad (4)$$

The solution of equation (3) is written as

$$\Psi(z)=\Psi^{(0)}(z)\theta(-z)+\sum_{p=1}^{N_W+N_B}\Psi^{(p)}(z)\left[\theta(z-z_{p-1})-\theta(z-z_p)\right]+ \\ +\Psi^{(N_W+N_B+1)}(z)\theta(z-b), \tag{5}$$

where the functions

$$\Psi^{(0)}(z)=A^{(0)}e^{\left\{ik \atop \chi\right\}z}+B^{(0)}\mathrm{e}^{-\left\{ik \atop \chi\right\}z};\quad \left(k=\hbar^{-1}\sqrt{2m_0E}\right); \tag{6}$$

$$\Psi^{(p)}(z)=A^{(p)}\mathrm{Ai}(\xi_p(z))+B^{(p)}\mathrm{Bi}(\xi_p(z));\quad (p=1\div N_W+N_B) \tag{7}$$

$$\Psi^{(N_W+N_B+1)}(z)=A^{(N_W+N_B+1)}e^{iKz}\quad \left(K=\hbar^{-1}\sqrt{2m_0(E+V)},\quad V=eFb\right) \tag{8}$$

are the superpositions of the exact linearly independent solutions of equation (3) in the respective ranges of z variable. Here, we introduced the notations

$$\xi_p(z)=\begin{cases}+\left(\dfrac{2m_1\ V\ b^2}{\hbar^2}\right)^{1/3}\left(\dfrac{U-E}{V}-\dfrac{z}{b}\right), & p=1,\ 3,\ 5\ ...\\ -\left(\dfrac{2m_0\ V\ b^2}{\hbar^2}\right)^{1/3}\left(\dfrac{E}{V}-\dfrac{z}{b}\right), & p=2,\ 4,\ 6\ ...\end{cases} \tag{9}$$

$\mathrm{Ai}(\xi)$, $\mathrm{Bi}(\xi)$ are the Airy functions.

The conditions of continuity of wave functions and their densities of currents must be fulfilled at all nanosystem interfaces

$$\Psi^{(p)}(z_p)=\Psi^{(p+1)}(z_p);\qquad \left.\frac{\mathrm{d}\,\Psi^{(p)}(z)}{m\ (z)\mathrm{d}z}\right|_{z=z_p-\varepsilon}=\left.\frac{\mathrm{d}\,\Psi^{(p+1)}(z)}{m\ (z)\mathrm{d}z}\right|_{z=z_p+\varepsilon}; \\ p=0\div N_W+N_B;\quad \varepsilon\to+0. \tag{10}$$

Within the approach of the open model, the reflected wave outside of RTS is absent, since $B^{(N_W+N_B+1)}=0$. All coefficients $A^{(p)}$, $B^{(p)}$ of the wave function $\Psi(z)$ are found from the conditions (10) through the one of them, in its turn, defined by the density of current falling at RTS from the left side. In this case, the electron spectrum is the quasi-stationary one with the resonance energies (E_n) and resonance widths ($\Gamma_n=\hbar\tau_n^{-1}$), where τ_n is the life time in the n-th quasi-stationary state. The resonance energies are fixed by the maxima of probability distribution function of electron location inside of RTS (in energy scale (E))

$$W(E) = \frac{1}{b}\int_0^b \left|\Psi(E,\ z)\right|^2 \mathrm{d}z\,. \tag{11}$$

The resonance widths (Γ_n) are fixed by the widths of this function at the halves of its maxima, placed at the respective resonance energies E_n.

The quantum transitions between the quasi-stationary states occur when the electrons transport through the open RTS driven by the electric field. Consequently, the electromagnetic field with the respective frequency arises. Its intensity is proportional to the magnitude of the dynamic conductivity. During the quantum transitions accompanied by the absorption of electromagnetic energy the positive dynamic conductivity is formed and at the radiation of electromagnetic energy – the negative dynamic conductivity of RTS is formed.

In order to calculate the negative conductivity of open RTS operating in laser regime, one has to obtain the wave functions of electrons interacting with the electromagnetic field. It is found from the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\Psi(z,t)}{\partial t} = \big(H(z) + H(z,t)\big)\,\Psi(z,t)\,, \tag{12}$$

where $H(z)$ is the Hamiltonian (4) of the electrons in RTS without the electromagnetic field and

$$H(z,t) = -e\epsilon\Big[z\ \big(\theta(z)-\theta(z-b)\big) + b\ \ \theta(z-b)\Big]\ \big(\mathrm{e}^{\,\mathrm{i}\omega t} + \mathrm{e}^{-\mathrm{i}\omega t}\big) \tag{13}$$

is the Hamiltonian of electrons interacting with time-dependent electromagnetic field with frequency ω i and its electric intensity ϵ.

Assuming the amplitude of electromagnetic field as a small one, we find the solution of equation (12) in one-mode approximation using the perturbation theory

$$\Psi(z,t) = \sum_{s=-1}^{+1}\Psi_s(z)\,\mathrm{e}^{-\mathrm{i}(\omega_0+s\omega)\,t} \qquad (\omega_0 = E/\hbar)\,, \tag{14}$$

where $\Psi_{s=0}(z) \equiv \Psi(z)$.

Preserving the first order magnitudes in equation (12), we obtain the inhomogeneous equations for the corrections $\Psi_{\pm1}(z)$ to the wave functions

$$\big[H(z) - \hbar(\omega_0 \pm \omega)\big]\Psi_{\pm1}(z) - e\epsilon\Big[z\big(\theta(z)-\theta(z-b)\big) + b\theta(z-b)\Big]\Psi(z) = 0\,. \tag{15}$$

Their solutions are the superpositions of functions

$$\Psi_{\pm1}(z) = \Psi_{\pm}(z) + \Phi_{\pm}(z)\,. \tag{16}$$

The functions $\Psi_{\pm}(z)$, as the solutions of homogeneous equations, are written as

$$\Psi_{\pm}(z)=\Psi_{\pm}^{(0)}(z)\theta(-z)+\sum_{p=1}^{N_W+N_B}\Psi_{\pm}^{(p)}(z)\left[\theta(z-z_{\text{p}-1})-\theta(z-z_{\text{p}})\right]+$$
$$+\Psi_{\pm}^{(N_W+N_B+1)}(z)\theta(z-b)=B_{\pm}^{(0)}\mathrm{e}^{-\mathrm{i}k_{\pm}z}\theta(-z)+A_{\pm}^{(N_W+N_B+1)}\mathrm{e}^{\mathrm{i}K_{\pm}z}\theta(z-b)+ \quad (17)$$
$$+\sum_{\text{p}=1}^{N_W+N_B}\left(A_{\pm}^{(\text{p})}\text{Ai}(\xi_{\pm}^{(p)})+B_{\pm}^{(p)}\text{Bi}(\xi_{\pm}^{(p)})\right)\left[\theta(z-z_{\text{p}-1})-\theta(z-z_{\text{p}})\right],$$

where

$$k_{\pm}=\hbar^{-1}\sqrt{2m_0(E\pm\Omega)};\qquad K_{\pm}=\hbar^{-1}\sqrt{2m_0[(E\pm\Omega)+V]};\qquad \Omega=\hbar\omega;$$

$$\xi_{\pm}^{(p)}(z)=\begin{cases}+\left(\dfrac{2m_1Vb^2}{\hbar^2}\right)^{1/3}\left(\dfrac{U-(E\pm\Omega)}{V}-\dfrac{z}{b}\right), & p=1,3,5...\\ -\left(\dfrac{2m_0Vb^2}{\hbar^2}\right)^{1/3}\left(\dfrac{E\pm\Omega}{V}-\dfrac{z}{b}\right). & p=2,4,6...\end{cases} \quad (18)$$

The partial solutions of the inhomogeneous equations (15) have the exact analytical form

$$\Phi_{\pm}(z)=\pi\frac{\epsilon}{F}\sum_{p=1}^{N_W+N_B}\left\{\text{Bi}(\xi_{\pm}^{(p)})\int_1^{\xi^{(\text{p})}}\left[\eta-\left(\frac{2m(z)b^2V}{\hbar^2}\right)^{1/3}\frac{U(z)-E}{V}\right]\times\right.$$
$$\times\text{Ai}\left(\eta\mp\left[\frac{2m(z)b^2V}{\hbar^2}\right]^{1/3}\frac{\Omega}{V}\right)\Psi^{(p)}(\eta)\,\text{d}\eta-\text{Ai}(\xi_{\pm}^{(p)})\int_1^{\xi^{(\text{p})}}\left[\eta-\left(\frac{2m(z)b^2V}{\hbar^2}\right)^{1/3}\frac{U(z)-E}{V}\right]\times$$
$$\left.\times\text{Bi}\left(\eta\mp\left[\frac{2m(z)b^2V}{\hbar^2}\right]^{1/3}\frac{\Omega}{V}\right)\Psi^{(p)}(\eta)\,\text{d}\eta\right\}\left[\theta(z-z_{p-1})-\theta(z-z_p)\right]+ \quad (19)$$
$$\mp\frac{e\epsilon b}{\Omega}\Psi^{(N_W+N_B+1)}(b)\theta(z-b).$$

The conditions of the continuity of complete wave function $\Psi(z,t)$ and respective densities of currents at all RTS interfaces bring to the fitting conditions, like equations (10), for the functions $\Psi_{\pm 1}(z)$. Also, these equations define the unknown coefficients: $B_{\pm}^{(p)}$, $A_{\pm}^{(p)}$ ($p=0\div(N_W+N_B+1)$) and, consequently, the complete wave function $\Psi(z,t)$.

Using the energy of electron-electromagnetic field interaction, expressed as the sum of energies of electron waves coming out of the both sides of RTS, further, in quasi-classic approximation we calculate the real part of dynamic conductivity (σ) within the densities of currents of these waves

$$\sigma(\Omega, E) = \frac{\Omega}{2be\mathcal{E}^2}\Big\{ \big[j\big(E+\Omega, z=b\big) - j\big(E-\Omega, z=b\big)\big] - \\ -\big[j\big(E+\Omega, z=0\big) - j\big(E-\Omega, z=0\big)\big] \Big\}. \tag{20}$$

According to the quantum mechanics, the densities of currents are determined by the wave function

$$j(E,z) = \frac{ie\hbar n_0}{2m(z)}\left[\Psi(E,z)\frac{\partial}{\partial z}\Psi^*(E,z) - \Psi^*(E,z)\frac{\partial}{\partial z}\Psi(E,z)\right]. \tag{21}$$

Finally, the real part of dynamic conductivity can be expressed as a sum of two terms

$$\sigma(\Omega, E) = \sigma^-(\Omega, E) + \sigma^+(\Omega, E), \tag{22}$$

where

$$\sigma^-(\Omega, E) = \frac{\hbar\Omega\, n_0}{2bm_0\mathcal{E}^2}\left(k_+\left|B_+^{(0)}\right|^2 - k_-\left|B_-^{(0)}\right|^2\right), \\ \sigma^+(\Omega, E) = \frac{\hbar\Omega\, n_0}{2bm_0\mathcal{E}^2}\left(K_+\left|A_+^{(N_W+N_B+1)}\right|^2 - K_-\left|A_-^{(N_W+N_B+1)}\right|^2\right). \tag{23}$$

The physical sense of these partial terms ($\sigma^{\pm}(\Omega, E)$) is evident. They are caused by the electronic currents interacting with electromagnetic field in RTS and flowing out of it in forward (σ^+) and backward (σ^-) directions, with respect to the incident current.

3. DISCUSSION OF THE RESULTS

Using the developed theory we compare two models of QCL: i) the simplified one: the four-barrier active region with passive injector, operating as a conductor which relaxes the electron energy; ii) the model of complete cascade, where four-barrier active region and injector are observed as a sole RTS.

For the comparison with the experiment [3], we used the following physical parameters: U = 516 meV, F = 68 kV/cm, $n_0 = 2\cdot10^{17}$ cm^{-3} and geometrical ones, presented in Fig. 1. We must note that as far as almost equal sizes of all layers in the experimentally investigated cascade in the cited paper contain the small number of unitary cells (2–4) of its composition elements, the approximation of effective mass in different layers of nano-system would be a rough one. At the same time, the whole active region, the whole injector or the whole cascade contains the tens unitary cells in composition elements, thus one can expect that the averaged over all three composition elements (GaAs, AlAs, InAs) effective mass of electron ($m = 0.08\ m_e$, m_e is the mass of pure electron) is more adequate in the present physical situation.

In order to study the influence of geometrical design of separate cascade at the operation of QCL we calculated the resonance energies (E_n), life times (τ_n), active conductivity ($\sigma_{nn'}$) and its partial terms ($\sigma^{\pm}_{nn'}$) within the both models. The results are presented in Fig. 2, as functions of the position (b_1) of inner two-barrier element between two outer barriers of active region at the fixed sizes of all other elements of the cascade, the same as in the paper [3].

From Figs. 2a, 2d it is clear that the first three resonance energies, as functions of b_1, calculated within the model of open four-barrier active region, (Fig. 2a) coincide with the respective resonance energies (E_1, E_2, E_3) of those three states, calculated within the model of open complete cascade (Fig. 2d) where the electron with maximal probability is located in the space of active region. In Fig. 2d one can also see the resonance energies $E_{i1} \div E_{i4}$ (thin curves) of quasi-stationary states, where the electron with bigger probability is located in the injector region of cascade.

The resonance energies (E_n, E_{in}), life times (τ_n), active conductivities (σ_{32}, σ_{31}) and their partial terms ($\sigma^{\pm}_{32}, \sigma^{\pm}_{31}$) are calculated as functions of b_1 for the both open models: i) active region (Figs. 2a, 2b, 2c) and ii) complete cascade (Figs. 2d, 2e, 2f). Before the analysis of the figures we must note that in the model of active region the dynamic conductivities and their terms were calculated through the averaging over those energy diapasons where the levels of injector region ($E_{i4} - E_{i1}$) are uniformly situated. The calculation of these conductivities for the model of complete cascade was performed taking into account that the electrons leave the previous cascade with the energy E_1, which is shifted at the magnitude: $E_3 - E_1 - eFb$, with respect to the resonance energy E_3 of the studied cascade.

The detail analysis of the conditions which optimize the QCL operation due to the geometrical design of active region is performed within the both models. We evaluated the magnitude of dynamic conductivity in the needed quantum transition (for example, 3→2). Besides, this conductivity would be much bigger than the conductivity of the close over the energy magnitude transition (for example, 3→1) at the condition that the partial term of conductivity (σ^{+}_{32}) in forward current would be much bigger than the partial term (σ^{-}_{31}) in backward current. The calculated life times (τ_n) of the operating electron quasi-stationary states give opportunity to guide the natural physical condition: these life times must not exceed the relaxation times of dissipative processes due to the scattering of electrons at the impurities, phonons, imperfections of media interfaces and other factors, which, according to the evaluations [4], are not bigger than twenty picoseconds.

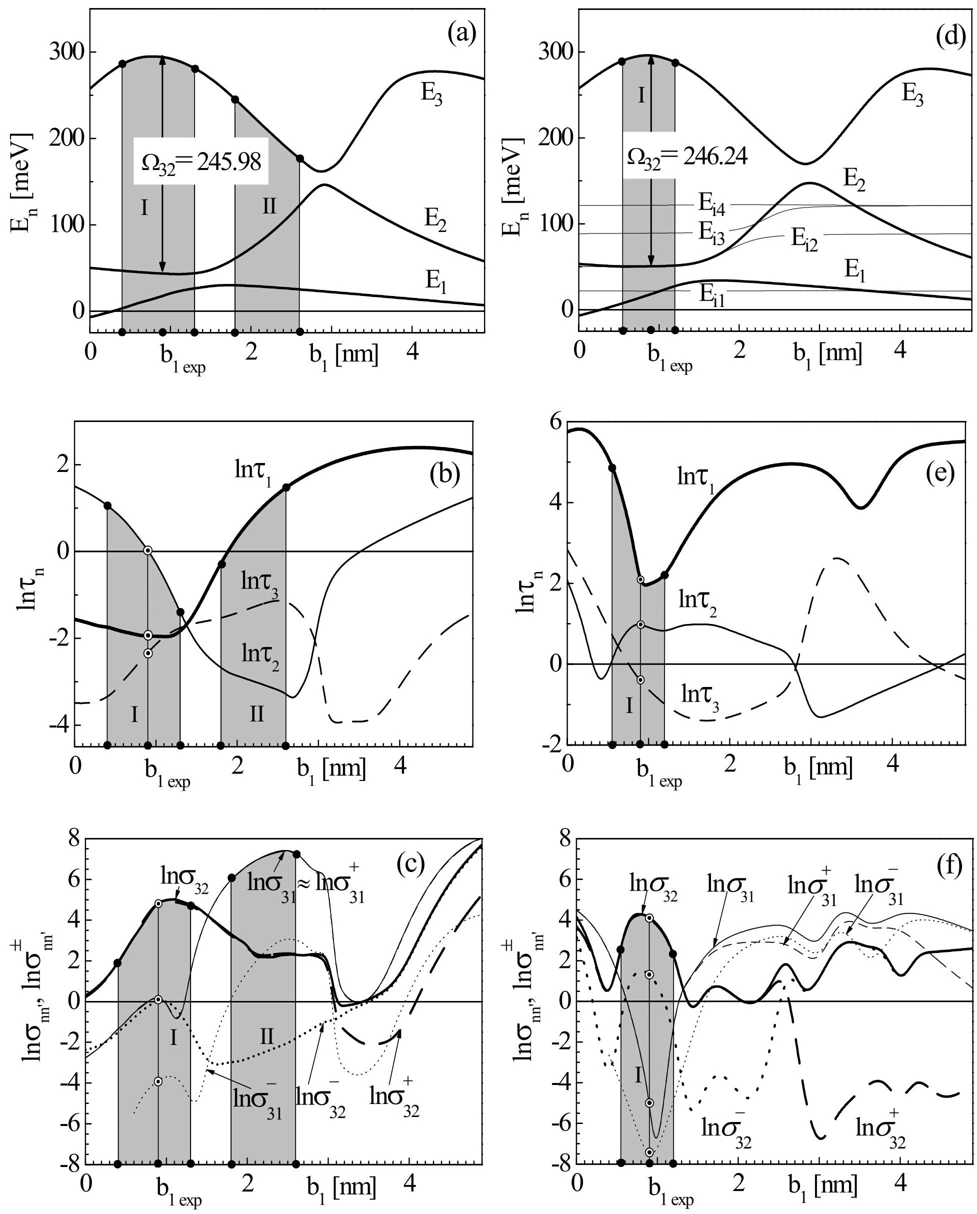

Fig. 2 – Electron energy spectrum (a, d), life times (b, e), and dynamic conductivities (c, f) as functions of input well width (b_1) of QCL active region in two models (i, ii).

The results of numerical calculations of conductivities and life times of electrons in the quasi-stationary states (n = 1, 2, 3) obtained within the both models are presented in Fig. 2. Analysis of τ_n, $\sigma_{nn'}$, $\sigma^{\pm}_{nn'}$ dependences on b_1 proves that there are two regions of b_1 for the model of four-barrier active region, where: I – the optimal is the quantum transition 3→2 (experimentally observed), II – the optimal is the quantum transition 3→1. The latter is possible (model i), Fig. 2b, but in this narrow region (II) for b_1, the life time in the first quasi-stationary state is rather small ($\tau_1 \le 1 \div 3\text{ps} < 10\text{ps}$).

The model of open complete cascade (ii), Figs. 2f, 2g, better describes the properties of photon-assisted transport of electrons through the RTS of QCL. Fig. 2g proves that in this model, the same as in the model of open active region (i), there are also two regions for b_1 varying (I and II) where the conditions of optimal QCL operation fulfill well (the transitions 3→2 and 3→1, respectively). The location and sizes of these regions are almost the same as for the model (i).

However, the analysis of life times τ_1, τ_2, τ_3, Fig. 2f shows that in fact, the region II is not optimal because at such geometrical design the life time $\tau_1 \ge 10$ ps comes up to the time of dissipative processes, breaking the coherent regime of QCL. Thus, the model of open complete cascade (ii) proves that in the experimental QCL [3], only one narrow region (I: 0.55 nm $\le b_1 \le$ 1.2 nm) of the position of inner two-barrier structure between the outer barriers of active region, where laser operates in optimal regime is observed. Only this configuration ensures that the dynamic conductivity σ_{32} in forward current is much bigger than the other conductivities. Herein, not only the life times of both operating quasi-stationary states are small (τ_3, $\tau_2 \le 2$ ps) but the life time of the first quasi-stationary state ($\tau_1 \le 10$ ps) through the which the electrons flow into the next cascade due to the interaction with phonons [3, 4], is minimal.

The geometrical and physical parameters for the numerical calculations within the both theoretical models were taken the same as in paper [3] in order to compare the theoretical and experimental data. These parameters are presented in Figs. 1 and 2. The numeric calculations show that in both models the energies (E_1, E_2, E_3) of operating quasi-stationary states differ between each other not more than at 0.1%. The calculated magnitude of the energy of laser radiation $\Omega_{32} = E_3 - E_2 = 246\text{ meV}$ differs from the experimental one $\Omega_{32}^{\exp} = 238.8\text{ meV}$ at 3% and the difference of the energies $E_2 - E_1 = 34$ meV almost coincides with the phonon energy in [3].

Finally, we should note that the experimental geometrical design of QCL cascade [3] with the input well width $b_1 = 0.9$ nm of four-barrier active region correlates well with magnitude b_1 in both theoretical models. However, only the model of open complete cascade is the most adequate one because it does not contain those geometric configurations of active region, which do not ensure the optimal regime of QCL operation.

4. CONCLUSIONS

We developed the theory of dynamic conductivity of electrons in open multi-barrier RTS placed into the constant electric field, taking into account the interaction between electrons and electromagnetic field. We revealed that the model of complete open cascade confidently ensures the optimal geometrical design of RTS active region, comparing to the experimentally produced QCL with four-barrier active region of separate cascade [3].

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