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PHYSICS OF SEMICONDUCTOR DEVICES

On the Active Conductivity of a Three-barrier Resonant-Tunneling Structure and Optimization of Quantum Cascade Laser Operation

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Abstract—Within the context of the model of effective masses and rectangular potentials, the theory of active electronic conductivity is proposed for a three-barrier resonant-tunneling structure in a dc electric field, as the active element of a quantum cascade laser. It is shown that the chosen geometrical parameters of the active regions in the first experimentally fabricated quantum cascade lasers are most optimal and the experimental and theoretical values of the radiation energies correlate with each other with an accuracy of up to a few percent.

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1. INTRODUCTION

As is known, the operating principle of a laser based on quantum transitions between the resonance levels of quantum wells, proposed in theoretical works by Kazarinov and Suris [1, 2], was first experimentally implemented in quantum cascade lasers (QCLs) by Faist and Capasso with collaborators [3–5]. Since the main structural elements of QCLs (active region, injector) and quantum cascade detectors [6–8] are planar resonant-tunneling structures (RTS) with nanoscale layers, further significant efforts of researchers have focused on studying the properties of different types of open nanosystems.

Despite active theoretical studies of the physical phenomena and processes in multilayer RTSs, a theory adequately explaining them and completely consistent with experimental results has not yet been developed.

Among the theoretical studies in which various properties of multilayer RTSs were most thoroughly and deeply studied, the works by Pashkovskii and Golanta [9–12] and also Elesin with collaborators [13–15] should be noted. Although the active electronic conductivity of electron fluxes through RTSs was studied mostly in the ballistic mode in the series of mentioned works, and the δ-barrier model of multilayer nanosystems was studied in most cases, the theoretical models and methods developed there appeared to not only adequately explain many QCL properties, but also made it possible to determine at least the qualitatively predictable properties of some nanodevices in the case of the use of a model with rectangular wells and barriers [16].

The objective of this study is to develop the theory of the active conductivity of electrons of a three-barrier RTS (TBRTS) in a dc electric field, based on the model of effective masses and rectangular potentials. Since such a system played the role of the active region in the first QCLs [3–5], analysis of the active conductivity properties depending on the TBRTS geometrical parameters allows estimation, on the one hand, as to how optimal the selected sizes of the layers of the experimental nanosystems were; on the other hand, to what extent the results of theoretical calculations of the laser radiation energy are consistent with the experiment.

2. THEORY OF THE ACTIVE CONDUCTIVITY OF ELECTRONS OF A THREE-BARRIER RESONANT-TUNNELING STRUCTURE

We consider a planar TBRTS in a uniform dc electric field with the strength F (Fig. 1), onto which a monoenergetic flux of non-interacting electrons with

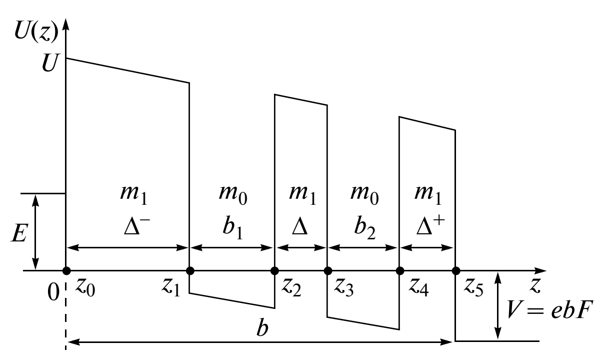

Fig. 1. Geometrical and energy diagrams of the three-barrier resonant-tunneling structure. The quantum well (b_1, b_2) and barrier (Δ^-, Δ, Δ^+) widths are indicated. m_0 and m_1 are the electron effective masses in the quantum well and barrier layers.

the energy E and the concentration n_0 is incident from the left perpendicular to its layers (coordinate z). The known geometrical parameters are shown in Fig. 1. Such a problem can be considered as the one-electron problem. An insignificant difference between the lattice constants of well layers and barrier layers of RTSs allows study of the system in the model of known effective masses

$$m(z) = m_0\left\{\theta(-z) + \sum_{p=1}^{2}[\theta(z-z_{2p-1}) - \theta(z-z_{2p})] + \theta(z-z_5)\right\} + m_1\sum_{p=0}^{2}[\theta(z-z_{2p}) - \theta(z-z_{2p+1})] \quad (1)$$

and rectangular potentials

$$U(z) = U\sum_{p=0}^{2}[\theta(z-z_{2p}) - \theta(z-z_{2p+1})]. \quad (2)$$

Here, $\theta(z)$ is the Heaviside unit-step function.

The one-dimensional Schrödinger equation for an electron in such a system is written as

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t} = [H_0(z) + H(z,t)]\Psi(z,t), \quad (3)$$

where

$$H_0(z) = -\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z} + U(z) - eF\{z[\theta(z) - \theta(z-z_5)] + z_5\theta(z-z_5)\} \quad (4)$$

is the Hamiltonian of the steady-state problem whose solution is known,

$$\Psi_0(z) = \Psi_0^{(0)}(z)\theta(-z) + \sum_{p=1}^{5}\Psi_0^{(p)}(z) \times[\theta(z-z_{p-1}) - \theta(z-z_p)] + \Psi_0^{(6)}(z)\theta(z-z_5)$$
$$= (e^{ik^{(0)}z} + B^{(0)}e^{-ik^{(0)}z})\theta(-z) + A^{(6)}e^{ik^{(6)}z}\theta(z-z_5) + \sum_{p=1}^{5}[A^{(p)}\mathrm{Ai}(\xi^{(p)}) + B^{(p)}\mathrm{Bi}(\xi^{(p)})] \times[\theta(z-z_{p-1}) - \theta(z-z_p)], \quad (5)$$

where $\mathrm{Ai}(\xi)$ and $\mathrm{Bi}(\xi)$ are Airy functions and e is the electron charge,

$$k^{(0)} = \sqrt{\frac{2m_0E}{\hbar^2}}, \quad k^{(6)} = \sqrt{\frac{2m_0(E+V)}{\hbar^2}},$$

$$V = eFb, \quad \xi^{(1)} = \xi^{(3)} = \xi^{(5)} = \rho^{(1)}\left(\frac{U-E}{V} - \frac{z}{b}\right),$$

$$\rho^{(1)} = \rho^{(3)} = \rho^{(5)} = \left(\frac{2m_1Vb^2}{\hbar^2}\right)^{1/3}, \quad (6)$$

$$\xi^{(2)} = \xi^{(4)} = -\rho^{(2)}\left(\frac{E}{V} + \frac{z}{b}\right),$$

$$\rho^{(2)} = \rho^{(4)} = \left(\frac{2m_0Vb^2}{\hbar^2}\right)^{1/3}.$$

The unknown coefficients $B^{(0)}$, $A^{(6)}$, $A^{(p)}$, $B^{(p)}$ (p = 1–5) are determined from the boundary conditions

$$\Psi_0^{(p)}(z_p) = \Psi_0^{(p+1)}(z_p),$$
$$\frac{1}{m_{0(1)}}\frac{d\Psi_0^{(p)}}{dz}\bigg|_{z=z_p} = \frac{1}{m_{1(0)}}\frac{d\Psi_0^{(p+1)}(z)}{dz}\bigg|_{z=z_p} \quad (p = 0\text{–}5), \quad (7)$$

which entirely uniquely defines the wave function $\Psi_0(z)$ in all regions of the system and makes it possible to perform an accurate analytical calculation of the distribution function of the probability of finding the electron in the TBRTS,

$$W(E) = \frac{1}{b}\int_0^b|\Psi_0(z)|^2dz. \quad (8)$$

This function, in contrast to the transmittance, makes it possible to determine the spectral characteristics (resonant energies and resonant widths, hence, the lifetime) of quasi-steady states (QSSs) of the electron in the TBRTS with arbitrary geometrical parameters and in any energy region [17]. The second term in Eq. (3),

$$H(z,t) = -e\epsilon\{z[\theta(z) - \theta(z-b)] + b\theta(z-b)\} \times(e^{i\omega t} + e^{-i\omega t}), \quad (9)$$

is the Hamiltonian of the electron interaction with a time-variable electromagnetic field with the frequency ω and the strength amplitude ϵ of its electrical component.

Considering the high-frequency electromagnetic field amplitude to be small, we seek the solution to Eq. (3) in the single-mode approximation of perturbation theory,

$$\Psi(z,t) = \sum_{n=-1}^{+1}\Psi_n(z)e^{-i(\omega_0+n\omega)t} \quad (\omega_0 = E/\hbar). \quad (10)$$

To determine the corrections $\Psi_{\pm1}(z)$ to the wave function, retaining the quantities of the first order of smallness in (3), we obtain the inhomogeneous equations

$$[H_0(z) - \hbar(\omega_0 \pm \omega)]\Psi_{\pm1}(z) - e\epsilon\{z[\theta(z) - \theta(z-b)] + b\theta(z-b)\}\Psi_0(z) = 0, \quad (11)$$

whose solutions are superpositions of the functions

$$\Psi_{\pm 1}(z) = \Psi_{\pm}(z) + \Phi_{\pm}(z). \quad (12)$$

The functions $\Psi_{\pm}(z)$ as the solutions to homogeneous equations are sought in the form

$$\begin{aligned}\Psi_{\pm}(z) &= \Psi_{\pm}^{(0)}(z)\theta(-z) \\ &+ \sum_{p=1}^{5} \Psi_{\pm}^{(p)}(z)[\theta(z-z_{p-1}) - \theta(z-z_p)] + \Psi_{\pm}^{(6)}(z)\theta(z-b) \\ &= B_{\pm}^{(0)} e^{-ik_{\pm}^{(0)} z}\theta(-z) + A_{\pm}^{(6)} e^{ik_{\pm}^{(6)} z}\theta(z-b) \\ &+ \sum_{p=1}^{5} [A_{\pm}^{(p)}\mathrm{Ai}(\xi_{\pm}^{(p)}) + B_{\pm}^{(p)}\mathrm{Bi}(\xi_{\pm}^{(p)})] \\ &\times [\theta(z-z_{p-1}) - \theta(z-z_p)],\end{aligned} \quad (13)$$

where

$$\begin{aligned}k_{\pm}^{(0)} &= \hbar^{-1}\sqrt{2m_0(E \pm \Omega)}, \\ k_{\pm}^{(6)} &= \hbar^{-1}\sqrt{2m_0[(E \pm \Omega) + V]}, \\ \Omega &= \hbar\omega, \\ \xi_{\pm}^{(1)} = \xi_{\pm}^{(3)} = \xi_{\pm}^{(5)} &= \rho^{(1)}\left(\frac{U-(E \pm \Omega)}{V} - \frac{z}{b}\right), \\ \xi_{\pm}^{(2)} = \xi_{\pm}^{(4)} &= -\rho^{(2)}\left(\frac{E \pm \Omega}{V} + \frac{z}{b}\right).\end{aligned} \quad (14)$$

The partial solutions of the inhomogeneous equations (11) have the exact analytical form

$$\begin{aligned}\Phi_{\pm}(z) &= \pi\frac{\epsilon}{F}\sum_{p=1}^{5}\left\{\mathrm{Bi}(\xi_{\pm}^{(p)})\int_{1}^{\xi^{(p)}}\left(\eta - \rho^{(p)}\frac{U(z)-E}{V}\right)\right. \\ &\times \mathrm{Ai}\left(\eta \mp \rho^{(p)}\frac{\Omega}{V}\right)\Psi_0^{(p)}(\eta)d\eta - \mathrm{Ai}(\xi_{\pm}^{(p)}) \\ &\times \left.\int_{1}^{\xi^{(p)}}\left(\eta - \rho^{(p)}\frac{U(z)-E}{V}\right)\mathrm{Bi}\left(\eta \mp \rho^{(p)}\frac{\Omega}{V}\right)\Psi_0^{(p)}(\eta)d\eta\right\} \\ &\times [\theta(z-z_{p-1}) - \theta(z-z_p)] \mp \frac{e\epsilon b}{\Omega}\Psi_0^{(6)}(b)\theta(z-b).\end{aligned} \quad (15)$$

The continuity conditions such as (7) of the total wave function $\Psi(z, t)$ and corresponding fluxes at all heterojunctions at any time t lead to boundary conditions for the functions $\Psi_{\pm 1}(z)$, from which the unknown coefficients $B_{\pm}^{(0)}$, $A_{\pm}^{(6)}$, $B_{\pm}^{(p)}$, $A_{\pm}^{(p)}$ ($p = 0$–5), hence, the total wave function $\Psi(z, t)$ can be uniquely determined.

Then, having analytically calculated the electron–electromagnetic field interaction energy as the sum of the energies of the electron waves emerging from both sides of the TBRTS, we will define the real part of the active conductivity $\sigma(\omega)$ in the quasi-classical approximation in terms of the flux densities of the electron waves (see [10]) emerging from both sides of the TBRTS,

$$\begin{aligned}\sigma(\Omega, E) = \frac{\Omega}{2be\epsilon^2}\{&[j(E+\Omega, z=b) - j(E-\Omega, z=\mathrm{b})] \\ &- [j(E+\Omega, z=0) - j(E-\Omega, z=0)]\},\end{aligned} \quad (16)$$

which, according to quantum mechanics, are defined by the total wave function,

$$\begin{aligned}j(E, z) = \frac{e\hbar n_0}{2m(z)}\Big[&\Psi(E, z)\frac{\partial}{\partial z}\Psi^*(E, z) \\ &- \Psi^*(E, z)\frac{\partial}{\partial z}\Psi(E, z)\Big].\end{aligned} \quad (17)$$

As a result of calculation of the real part of the active conductivity, it can be written as two terms

$$\sigma(\Omega, E) = \sigma^{-}(\Omega, E) + \sigma^{+}(\Omega, E) \quad (18)$$

which have the exact analytical form

$$\sigma^{-}(\Omega, E) = \frac{\hbar\Omega n_0}{2bm_0\epsilon^2}(k_{+}^{(0)}|B_{+}^{(0)}|^2 - k_{-}^{(0)}|B_{-}^{(0)}|^2), \quad (19)$$

$$\sigma^{+}(\Omega, E) = \frac{\hbar\Omega n_0}{2bm_0\epsilon^2}(k_{+}^{(6)}|A_{+}^{(6)}|^2 - k_{-}^{(6)}|B_{-}^{(6)}|^2) \quad (20)$$

and are partial components of the total active conductivity, caused by electron fluxes interacting with the high-frequency electromagnetic field, facing forward (σ^+) and backward (σ^-) with respect to the initial direction of the flux incident on the TBRTS.

3. PROPERTIES OF THEACTIVE CONDUCTIVITY OF LASER THREE-BARRIER RESONANT-TUNNELING STRUCTURES

Based on the theory developed in the previous section, we calculated the spectrum, lifetimes, and active conductivity of electrons in two TBRTSs composed of the active operating elements of quantum cascade lasers experimentally studied in [4, 5]. The physical and geometrical parameters of both TBRTSs are: $U = 516$ meV, $n_0 = 3 \times 10^{17}$ cm^{-3}, $m = 0.08m_e$; (I) $F = 70$ kV/cm, $\Delta^- = 6.8$ nm, $b_1 = 4.8$ nm, $\Delta = 2.8$ nm, $b_2 = 3.9$ nm, $\Delta^+ = 2.7$ nm; (II) $F = 85$ kV/cm, $\Delta^- = 6.5$ nm, $b_1 = 4.5$ nm, $\Delta = 2.8$ nm, $b_2 = 3.5$ nm, $\Delta^+ = 3.0$ nm.

Before analyzing the obtained results, it should be noted that we took into account two important factors in the calculation. First, since the thicknesses of all the layers are very small in the RTSs under study, the effective mass approximation in each individual layer a priori should be and is indeed rougher than the chosen effective mass averaged over all three components (GaAs, AlAs, InAs). Second, the positions of the

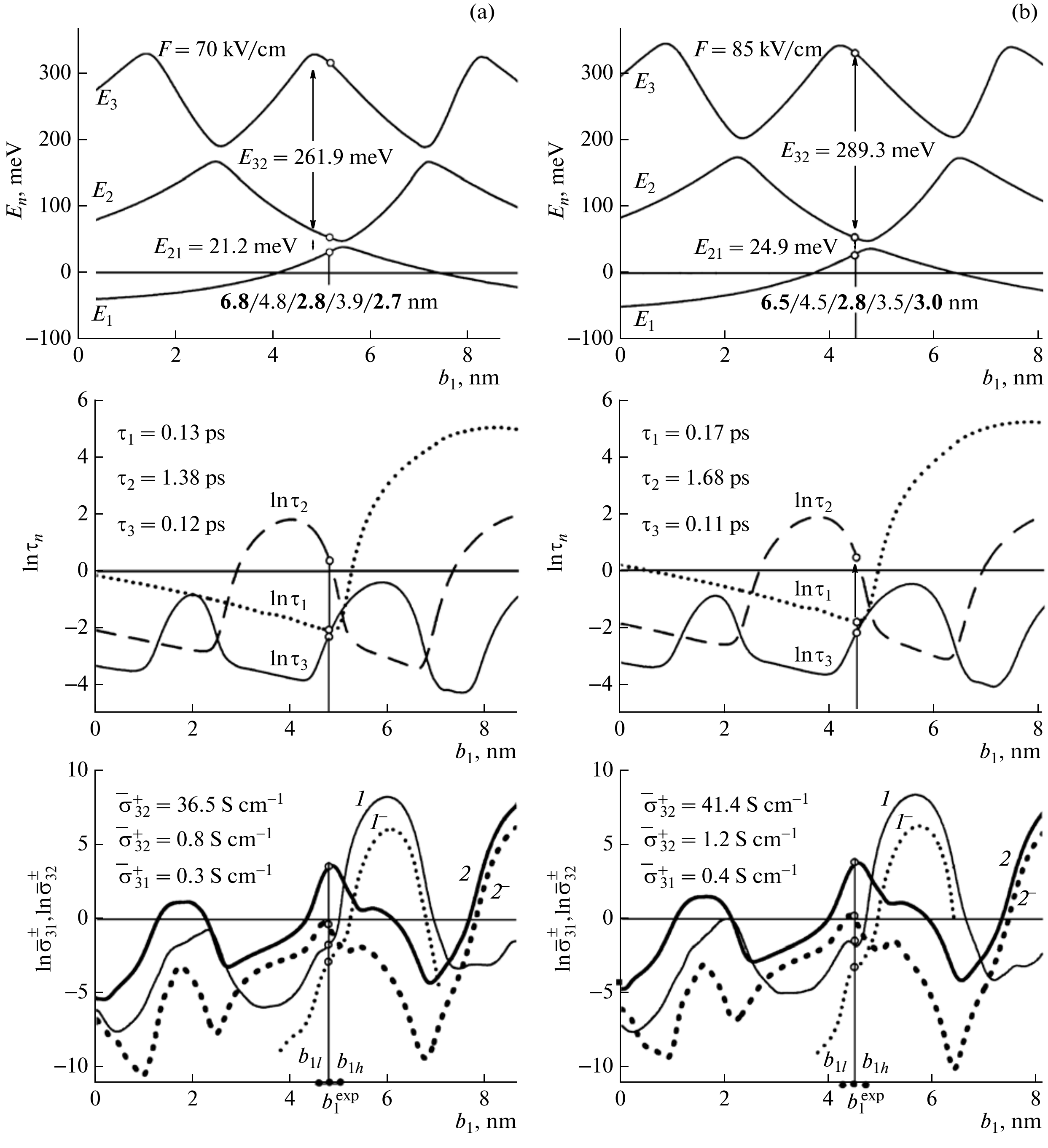

Fig. 2. Dependences of E_n, $\ln\tau$, $\ln\bar{\sigma}_{32}$ and $\ln\bar{\sigma}_{31}$ on the width of the input potential well b_1 for TBRTS I (a) and II (b). (*1*) $\ln\bar{\sigma}_{31}^{+}$, (*1*$^-$) $\ln\bar{\sigma}_{31}^{-}$, (*2*) $\ln\bar{\sigma}_{32}^{+}$, (*2*$^-$) $\ln\bar{\sigma}_{32}^{-}$. The values of τ_n and $\bar{\sigma}_{nn'}$ corresponding to the experimental values of b_1^{exp} are given.

interfaces between both neighboring cascades and between the injector and active region (TBRTS) of each individual cascade are rather conditional, since they are not well defined within the input and output barriers.

Therefore, in the calculation, we varied the sizes of the edge TBRTS barriers so that the ratio of their thicknesses would correspond to the experimental values. It was found that, as the thickness of the smaller (output) barrier is varied by a factor of 1.5–2, all the RTS parameters under study vary within only a few percent. Therefore, we chose such thicknesses of the external TBRTS barriers (indicated in Fig. 2), which correspond to best agreement with the experiment.

As is known from [4, 5], the QCL was designed so that the electron flux from the injector region with the width $\Delta E \approx 230$ meV would be incident on a TBRTS with the energy E corresponding to the resonant energy E_3 of the third QSS. Due to electron interaction with the electromagnetic field, they transfer to the second QSS (energy E_2). In this case, laser radiation with the energy $E_{32} = E_3 - E_2$ and a power proportional to the active conductivity (σ_{32}) arises. To promote electron escape from the second QSS, the geometrical parameters of the active region (of the TBRTS) were selected so that the difference between the resonant energies ($E_2 - E_1$) would be comparable to the energy of phonons, due to interaction with which electrons from the second QSS transferred to the first QSS (E_1) and left the active region.

To clarify, whether the choice of the geometrical parameters of the active region in the experimental QCLs [3–5] is optimal from the viewpoint of the developed theory, we calculated the spectral parameters of the first three QSSs and active conductivities and their partial terms depending on the position of the internal barrier between the external barriers of the TBRTS.

Since the electron flux from the injector region is nonmonochromatic under experimental conditions, it is considered that its electrons are uniformly distributed over energies within the injector region width ($\Delta E \approx 230$ meV [4, 5]); hence, the average maximum active conductivity $\bar{\sigma}_{nn'}$ (and its partial components $\bar{\sigma}^{+}_{nn'}$ and $\bar{\sigma}^{-}_{nn'}$) is calculated by the formula

$$\bar{\sigma}_{nn'}(\Omega) = \frac{1}{\Delta E}\int_0^{\Delta E}\sigma(\Omega, E)dE.$$

The results of calculating the resonant energies (E_n) and logarithmic lifetimes ($\ln\tau_n$) in the first three QSSs and the logarithmic active conductivities ($\ln\bar{\sigma}_{nn'}$) and their partial components ($\ln\bar{\sigma}^{\pm}_{nn'}$) at quantum transitions from the third to the second and first QSSs as functions of the position (b_1) of the internal TBRTS barrier between the external ones are shown in Fig. 2.

We can see that, since the physical and geometrical parameters of the active regions of both RTSs (I, II) are close, the dependences of $E_{n=1,2,3}$, $\ln\tau_{n=1,2,3}$ and $\ln\bar{\sigma}^{\pm}_{32}$, $\ln\bar{\sigma}^{\pm}_{31}$ on b_1 not only qualitatively, but also quantitatively differ slightly.

Since the dc electric field F applied to the TBRTS decreases the potential energy from the input to the output from the system, forward electron fluxes significantly exceed the backward ones; therefore, independent of the position (b_1), as seen in Figs. 2a and 2b, $\bar{\sigma}_{32} \approx \bar{\sigma}^{+}_{32} \gg \bar{\sigma}^{-}_{32}$ and $\bar{\sigma}_{31} \approx \bar{\sigma}^{+}_{31} \gg \bar{\sigma}^{-}_{31}$. We can also see that, as the input well width (b_1) increases from zero to $\sim b/4$, the low conductivities $\bar{\sigma}_{32}$ and $\bar{\sigma}_{31}$ gradually increase, initially $\bar{\sigma}_{32} \gg \bar{\sigma}_{31}$ and then $\bar{\sigma}_{32} \approx \bar{\sigma}_{31}$.

In the range of input well widths $1.5 \le b_1 \le 2$ nm, where $\bar{\sigma}_{32} \approx 1$–$10$ S/cm, $\bar{\sigma}_{32} \gg \bar{\sigma}_{31}$, it is possible that the QCL could also operate in the range of energies lower than $E^{\exp}_{32}$ at the $3 \longrightarrow 2$ transition. In this case, due to short electron lifetimes in both working QSSs ($\tau_2 \approx \tau_3 \le 0.1$ ps), the $2 \longrightarrow 1$ transitions due to phonons would be not so significant.

Upon a further increase in the input potential well width within $b/4 \le b_1 \le b_{1l}$, QCL operation would be impossible because of low active conductivities; however, since $\bar{\sigma}^{+}_{32} \approx \bar{\sigma}^{-}_{32}$, due to commensurate forward and backward electron fluxes, the laser would not operate efficiently.

As the internal barrier position changes with respect to the external ones in the range $b_{1h} \le b_1 \le b$, QCL operation becomes either inefficient or impossible. Indeed, although large $\bar{\sigma}_{31}$ significantly exceeds $\bar{\sigma}_{32}$ in the range $b_{1h} \le b_1 \le 3b/4$), which actualizes the $3 \longrightarrow 1$ transition, in this case, $\bar{\sigma}^{-}_{31} \approx \bar{\sigma}^{+}_{31}$; therefore, the forward and backward fluxes are almost compensated. Furthermore, the lifetime in the first QSS is too large, due to which dissipative processes can violate the coherent state. In the range $3b/4 \le b_1 \le b$, QCL operation at the $3 \longrightarrow 2$ transition is inefficient due to almost total compensation of opposite fluxes ($\bar{\sigma}^{+}_{32} \approx \bar{\sigma}^{-}_{32}$).

As seen in Fig. 2, there exists only a rather narrow range $b_{1l} \le b_1 \le b_{1h}$ in which a change in the internal barrier position with respect to the external ones optimizes the TBRTS operation as an active element of the QCL.

Indeed, if the internal barrier position is in the range $b_{1l} \le b_1 \le b_{1h}$, optimal conditions are satisfied for TBRTS operation in the active-region mode, since $\bar{\sigma}_{32} \gg \bar{\sigma}^{-}_{32}$, $\bar{\sigma}_{31}$, i.e., the forward electron flux at the $3 \longrightarrow 2$ transition significantly exceeds the backward one and both fluxes at the $3 \longrightarrow 1$ transition. In this case, the conductivity $\bar{\sigma}_{32}$ value defining the intensity (or power) of the laser radiation is sufficiently large; furthermore, the electron lifetimes in all three working QSSs are small, which facilitates coherent state retention.

In both experimental QCLs [4, 5], the geometrical parameters of the active region (TBRTS) were chosen so that both devices operated at the $3 \longrightarrow 2$ transition, emitting an electromagnetic field with the wavelength $\lambda = 4.6$ μm corresponding to the energy $E^{\exp}_{32} = 270$ meV. Theoretical calculation of the energies, lifetimes, and active conductivities of the TBRTS with parameters corresponding to the experimental implementation of active regions shows that the radiation energies at the 3 ⟶ 2 transition ((I) $E_{32} = 261.9$ meV, (II) $E_{32} = 289.3$ meV) are in agreement with the experimental value to within 3–4%. The energy differences between the second and first QSSs ((I) $E_{21} = 21.2$ meV, (II) $E_{21} = 24.9$ meV) correlate with the energies of bulk and interface phonons ($\Omega_{ph} \approx 30$ meV), which, according to the idea of the authors of [3–5], facilitates rapid electron escape from the second QSS through the first one, minimizing the effect of dissipative processes which violate coherence.

4. CONCLUSIONS

The developed theory of the active conductivity of electrons in a TBRTS in a dc electric field adequately explains the physical processes in the active region of the QCL.

It was shown that the choice of the geometrical parameters of TBRTSs as active regions of experimental QCLs provided optimal conditions for the emission of electromagnetic waves with $\lambda = 4.6$ μm, since the active conductivities appeared largest in this case, and the lifetimes in the working QSSs appeared short enough, which minimized the effect of dissipative processes.

Since the theoretical and experimental values of laser radiation energies satisfactorily correlate with each other, it can be expected that the developed theory of active conductivity of a TBRTS can be applicable in optimization of the geometrical configuration of multilayer QCL cascades.

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