Self-Consistent Analysis of Carrier–Transport and Carrier–Capture Dynamics in Quantum Cascade Intersubband Semiconductor Lasers

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Abstract—A methodology for the self-consistent analysis of carrier transport and carrier capture aspects of the dynamics of quantum cascade intersubband semiconductor lasers is described in this paper. The approach is used to analyze two prototype quantum cascade lasers. The self-consistent analysis incorporates the calculation of the electron densities and temperatures in each subband, together with the intersubband relaxation time. In the calculation of the relaxation time, we take into account the electron interaction with polar optical and acoustic phonons, as well as electron degeneracy. In addition, we also calculate the capture time, considering backward processes that play a role in the electron transition from an injection into an active region. The calculations indicate intersubband relaxation times of order 1 ps and capture times of order 100 fs.

Index Terms—Dynamic response, infrared lasers, quantum-well devices, semiconductor heterostructures, semiconductor lasers.

I. INTRODUCTION

This paper describes a theoretical framework for performing calculations of the fundamental time constants that determine the dynamics of carrier transport and carrier capture in intersubband quantum cascade semiconductor lasers. Intersubband lasers have become a topic of active research, particularly following the development by Faist et al. of mid-infrared (MIR) quantum cascade lasers [1], which was the first practical demonstration of a long-standing proposal for the utilization of intersubband transitions to obtain lasing action in semiconductor superlattices [2]. Subsequent research at AT&T, Lucent Technologies [3], [4], and in a growing number of laboratories across the U.S. and Europe has given rise to significant developments in the performance of quantum cascade lasers. In this context, it is of considerable interest to examine the dynamic behavior of quantum cascade lasers with a view, in particular, for evaluating the achievable direct current modulation bandwidth of such lasers. It is noted that the picosecond carrier lifetimes, which are characteristic of the operation of intersubband lasers, may be anticipated to offer opportunities for terahertz bandwidth modulation in such lasers. This aspect has been previously investigated where use was made of a rate equation model described in [5] and [6] to derive expressions for the modulation response of unipolar semiconductor lasers [7]. Subsequent work [8] has generalized that approach to yield a self-consistent rate equation analysis where, in particular, carrier lifetimes are deduced from calculations of electronic wave functions in the structure. Reference [8] indicated that modulation bandwidths of an order of 150 GHz would be obtainable in the chosen structure.

In a recent report [9], it was indicated that unipolar lasers have the potential for achieving terahertz modulation bandwidths, and a detailed description of that analysis has been presented elsewhere [10]. This literature was concerned with the dynamical processes occurring in a single triple-quantum-well (QW) element. In practical intersubband lasers, in order to achieve sufficient optical gain, the active region must contain many copies of such elements so as to achieve the quantum cascade effect, which underpins the successful operation of this class of lasers. In order to analyze the dynamical processes at play in such a quantum cascade laser, attention needs to be given to carrier–transport and carrier–capture processes, which will affect, in particular, the achievable direct current modulation frequency of intersubband cascade lasers. In this paper, a theoretical framework will be established to perform calculations of the pertinent physical factors that govern carrier transport.

In this paper, the generic structure that is assumed to form the building block of the active layer of the electrically pumped intersubband laser of interest is as shown in Fig. 1, i.e., a coupled triple-QW element with an injector well, a central laser well, and an extractor well denoted by QW numbers 1–3, respectively. In general, the carrier transport between the wells is characterized by a tunneling time $\tau_{12}$ describing injection from QW 1 to 2—the lasing well—and a tunneling time $\tau_{23}$ from the lasing well to QW 3—the extractor well. As shown in previous studies [5]–[8], the laser dynamics is further determined by the carrier transit time through the structure $\tau_T$ and the intersubband relaxation time $\tau_S$. The essence of this study is to perform a calculation of the relevant carrier lifetimes with a view to determining the dynamical properties of quantum cascade lasers.

A quantum cascade laser can be considered as being constructed from a series “cascade” of coupled QW structures of the kind illustrated schematically in Fig. 1. In order to describe the dynamical processes in a single element of such a structure, in Fig. 1 we introduce a notation for identifying the energy levels and carrier populations in those levels: subscripts identify the QW number and superscripts identify the energy subband level. As far as an isolated element is concerned, an
electron can be considered to enter the structure by tunneling through the first barrier B1 to the energy level $E_1$ in the first QW, i.e., W1. Tunneling through to $E_2^{(2)}$ in the second QW, i.e., W2, it then makes a vertical transition to $E_2$, after which it rapidly tunnels to $E_3$ in the third QW, i.e., W3, and escapes out of the structure. In order to achieve this, the four lowest energy levels are such that we have one each localized in W1 ($E_1$) and W3 ($E_3$), and two localized in W2 ($E_2^{(1)}$ and $E_2^{(2)}$), when the structure is in an unbiased condition. At an appropriate bias voltage, coupling occurs between $E_1$ and $E_2^{(2)}$, and between $E_2^{(1)}$ and $E_3$.

The dynamics of such a single cell have been examined in some detail in previous work [5]–[9]. The aim of this paper is to study the modifications in predicted dynamical response that arise due to the effects of interelement carrier transport and the finite time associated with the capture of electrons in the well structure. Calculations will thus be performed for the structure described in [7] and [8], where our analysis is based on a structure that is designed for operation at a lasing wavelength of nominally 10 μm, thus, the lasing transition should have an energy of more or less 124 meV. In order to achieve this, it is assumed that a suitable bias voltage is applied to the structure, such that the separation between the two energy levels involved in the transition is of this value.

The framework for analysis developed here is of general applicability, but for the sake of definiteness in prescribing the salient physical processes that are required for accurately predicting the response, this study concerns structures fabricated in the GaAs/AlGaAs system. This material system offers an advantage in terms of the well-advanced state of information concerning fundamental material constants. A recent report [12] of the successful demonstration of intersubband lasing in this material system provides particular motivation for analyzing this structure.
iterations converge rather fast, usually taking no more than five
cycles or so. When that convergence is obtained, an evaluation
of the capture time is performed using the carrier densities and
temperature obtained from the self-consistent calculations. The
self-consistency may be further enhanced by incorporating the
calculation of the capture time within the iteration loop. This,
however, significantly increases the computation time and, for
the present, this has not been undertaken. It is observed that the
calculated capture time has a very reasonable value.

A. Carrier Dynamics

The following rate equations are applicable to four-level
three-well structures with a vertical lasing transition in well
W2 between the subbands \(N_2^{(2)}\) and \(N_2^{(1)}\), as illustrated in the
structure shown in Fig. 1:

\[
\frac{dN_1}{dt} = \frac{J}{cL_1} + \frac{L_2 N_2^{(2)}}{L_1 \tau_{12}} - \frac{N_1}{\tau_{12}} \tag{2}
\]

\[
\frac{dN_2^{(2)}}{dt} = \frac{L_4 N_1}{L_2 \tau_{12}} - \frac{N_2^{(2)}}{\tau_{12}} - aP(N_2^{(2)} - N_2^{(1)}) - \frac{N_2^{(2)}}{\tau_S} \tag{3}
\]

\[
\frac{dN_2^{(1)}}{dt} = aP(N_2^{(2)} - N_2^{(1)}) + \frac{N_2^{(2)}}{\tau_S} + \frac{L_3 N_3}{L_2 \tau_{23}} - \frac{N_2^{(1)}}{\tau_{23}} \tag{4}
\]

\[
\frac{dN_3}{dt} = \frac{L_2 N_2^{(4)}}{L_3 \tau_{23}} - \frac{N_3}{\tau_{23}} - \frac{J}{cL_3} \tag{5}
\]

\[
\frac{dP}{dt} = aP(N_2^{(2)} - N_2^{(1)}) - \frac{P}{\tau_P} \tag{6}
\]

where \(e\) is the electronic charge, \(a\) is the local gain coefficient, \(P\)
is the photon density, and \(L_i\) is the width of the \(i\)th well. \(\tau_{12}\) and
\(\tau_{23}\) are the tunneling times between W1 and W2 and between
W2 and W3, respectively, calculated previously, as shown in
[8]. \(\tau_S\) is the intersubband relaxation time and \(\tau_P\) is the photon
lifetime.

Since the current injection is equal to the rate of total charge
passing through the resonant tunneling QW structure, we can write

\[
J = \frac{e}{\tau_P} \left[ N_1 L_1 + \left( N_2^{(1)} + N_2^{(2)} \right) L_2 + N_3 L_3 \right] \tag{7}
\]

where \(\tau_P\) is the effective transit time of the carriers through the
whole structure, which includes not only the tunneling times
through the barriers and the intersubband transition times, but
also the time delays caused by intrasubband scattering and electron
diffusion. \(J\) is the biasing current density.

B. Carrier Temperature Dynamics

The carrier temperature dynamics can be modeled using the
intersubband energy density equations corresponding to the
structure, following Willatzen’s model for interband lasers [13]

\[
\frac{dU_{1}}{dt} = \frac{N_2^{(2)} \langle E_{21} \rangle}{L_1 \tau_{12}} - \frac{N_1 \langle E_{12} \rangle}{\tau_{12}} + \frac{J \langle E_{p,2} \rangle}{cL_1} - \frac{U_1 - U_{L,1}}{\tau_{\text{heat}}} \tag{8}
\]

\[
\frac{dU_{2}^{(2)}}{dt} = -aP(N_2^{(2)} - N_2^{(1)}) E_{12} - \frac{U_{2}^{(2)}}{\tau_S} + \frac{L_4 N_1 \langle E_{12} \rangle}{L_2 \tau_{12}} - \frac{N_2^{(2)} \langle E_{21} \rangle}{\tau_{12}} - \frac{U_{2}^{(2)}}{\tau_{\text{heat}}} \tag{9}
\]

\[
\frac{dU_{2}^{(1)}}{dt} = aP(N_2^{(2)} - N_2^{(1)}) E_{12} + \frac{U_{2}^{(2)}}{\tau_S} + \frac{L_3 N_3 \langle E_{43} \rangle}{L_2 \tau_{23}} - \frac{N_2^{(1)} \langle E_{34} \rangle}{\tau_{23}} - \frac{U_{2}^{(1)}}{\tau_{\text{heat}}} \tag{10}
\]

\[
\frac{dU_{3}}{dt} = \frac{N_2^{(1)} \langle E_{34} \rangle}{L_3 \tau_{23}} - \frac{N_3 \langle E_{43} \rangle}{\tau_{23}} + \frac{J \langle E_{p,3} \rangle}{cL_3} - \frac{U_3 - U_{L,3}}{\tau_{\text{heat}}} \tag{11}
\]
where $\tau_{\text{ren}}$ is the thermalization time towards the equilibrium energy density $U_{ij} = U_i(N_i, T_L)$ and is assumed to be the same for all subbands. $E_{p,2}$ is the difference in energy between the electrons coming into the structure and the energy level in W1, while $E_{p,1}$ is the difference in energy between the electrons leaving the structure and the energy level in W3, and $E_{\epsilon, i}$ are the quasi-Fermi levels of the upper and lower lasing subbands. $E_{\epsilon, ij}$ denotes the energy difference in electrons coming from subband $i$ to subband $j$. Only electrons coming in from a higher subband are assumed to contribute to the energy of a subband. Finally, $U_i$ gives the energy density in the $i$th subband and

$$U_i = \int dE \rho(E) f_i(E)$$

(12)

where $\rho(E)$ is the density of states function in a QW and $f_i(E)$ is the Fermi distribution function for the $i$th subband.

In the model presented above, free carrier absorption has been neglected.

C. Intersubband Optical Gain

In previous work, we have performed calculations of optical gain in intersubband lasers [14]. Here, we outline the approach taken. Starting from the general standard expression for optical gain per meter in a semiconductor [15], we find that

$$g(\hbar \Omega) = \frac{\pi e^2 \hbar}{m_e^* \epsilon_0^2 \pi^2} |M_T(E_{21})|^2 \rho_T(E_{21}) \int dE \rho_T(f_2 - f_1)$$

(13)

where $|M_T(E_{21})|$ is the transition matrix element, $\rho_T(E_{21})$ is the reduced density of states, $L(\hbar \omega_0 - E_{21})$ is the line-shape function, and $m_0$ is the electron rest mass. The density of states for a QW $\rho_T(E_{21}) = (m_r / \pi \hbar^2 / W)$, where $W$ is the QW width. The transition matrix element is occasionally written as the dipole moment matrix element and the relationship between the two is given by $|M_T(E_{21})|^2 = m_0^2 \Omega^2 |z|^2$. We will be using the dipole moment matrix element

$$g(\hbar \Omega) = \frac{\pi e^2 \hbar}{m_e^* \epsilon_0} \int_0^\infty dE \frac{\hbar \gamma(\epsilon)}{[\hbar \Omega - \hbar \Omega_e]^2 + [\hbar \gamma(\epsilon)]^2}$$

(14)

which is similar to the expression given in [16] and [17], except that (14) above is in MKS units and has the reduced effective subband mass $m_e^*$. $\Omega_e$ is the optical transition frequency for the in-plan electron momentum. $\hbar K = \sqrt{2m_e c \epsilon}$, $\hbar K_e \equiv \hbar K_0 + \epsilon_2 - \epsilon_1$, where $\hbar K$ is the lasing energy at $K = 0$, $\epsilon_2 \equiv \epsilon$ and $\epsilon_1 = \hbar^2 k^2 / 2m_1$ are kinetic energies in the upper and lower lasing subbands, characterized by the effective masses $m_1$ and $m_2$, and the distribution functions $f_1$ and $f_2$. Hence, the reduced mass $m_e^* = m_1 m_2 / (m_1 + m_2)$. The function $\gamma(\epsilon)$ describes the transverse phase relaxation due to intrasubband scattering [16].

In [17], it was assumed that $\gamma(\epsilon)$ is dominated by the interaction with polar optical phonons (pop’s), such that

$$\gamma(\epsilon) = \gamma_0 \times \frac{N_{\mathbf{q}}}{(N_{\mathbf{q}} + 1) \theta(\epsilon - \hbar \omega_p)}$$

(15)

where the top line describes optical phonon absorption and the bottom line describes optical phonon emission

$$\gamma_0 = \frac{\pi e^2}{2\hbar} \left( \frac{1}{\kappa_{\infty}} - \frac{1}{\kappa} \right) q, \quad q = \sqrt{2m_e \Omega / \hbar}$$

The phonon distribution function $N_{\mathbf{q}}$ is Bose distribution in the following form:

$$N_{\mathbf{q}} = \left[ \exp \left( \frac{\hbar \omega_p}{k_B T_L} \right) - 1 \right]^{-1}$$

(16)

where $T_L$ is the lattice temperature and $k_B$ is the Boltzmann constant. The phonon frequency $\omega_p$ in the case of pop’s is dispersionless ($\omega = \omega_p$). $\theta(\epsilon - \hbar \omega_p)$ is a step function, $\kappa$ and $\kappa_{\infty}$ are the static and high-frequency dielectric constants, respectively, and $m_e$ is the electron effective mass.

IV. Electron Relaxation Times

Electron relaxation dynamics in the intersubband lasers are governed predominantly by the electron interaction with pop’s. Nevertheless, in order to verify its contribution, we have also taken into account, via the deformation potential interaction, electron scattering by acoustic phonons. Both phonons are considered to be bulk-like because incorporation of some phonon-confined model affects the overall results to a degree (<10%) comparable to other fine effects such as nonparabolicity [18].

The electron–phonon rates are calculated using Fermi’s golden rule as a transition from the initial subband $i$ with energy $E_i$ to the final subband $j$ with energy $E_j$. The electron rate with an initial energy $E$ can then be obtained for the pop scattering as [19], [20]

$$\Gamma_{ij}^\epsilon(E) = \frac{e^2 \Omega_{\text{PO}} m_e^*}{8 \pi^2 \hbar^2} \left( \frac{1}{\kappa_{\infty}} - \frac{1}{\kappa} \right) \int_0^{2\pi} d\theta \left( N_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2} \right) \frac{F_{ij}(q)}{q}$$

(17)

where the pop wave vector is

$$q = \sqrt{2m_e} \left( 2E - E_{\text{PO}} - 2\sqrt{E + E_{\text{PO}}} \cos \theta \right)^{1/2}$$

(18)

with $E_{\text{PO}} = E_i - E_j \pm \hbar \omega_p$. In (17) and (18), the upper sign stands for the phonon emission, while the lower sign stands for the phonon absorption.

The form factor $F_{ij}(q)$, which plays a crucial role in the rate (17), is defined by

$$F_{ij}(q) = \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \chi(i)(z_1) \chi(j)(z_2) e^{-i (q + \frac{1}{2} \epsilon) z_1} \chi^*(i)(z_1)$$

(19)

with the electron wave functions $\chi(i)(z_1)$ and $\chi(j)(z_2)$ obtained using the APM method [8].

The relaxation rate of an electron with initial energy $E$ scattered by acoustic phonons reads

$$\Gamma_{ij}^\text{Ac} = \frac{D^2 m_e^*}{8 \pi^2 \hbar^2} \int_0^{2\pi} d\theta \left( N_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2} \right) q^2 F_{ij}(q)$$

(20)
where the acoustic phonon wave vector is

\[ q = \frac{\sqrt{2m}}{\hbar} \left( 2E - E_{AC} - 2\sqrt{E + E_{AC}} \cos \theta \right)^{1/2} \]  \hspace{1cm} (21)

with the elastic equipartition approximation given by \( E_{AC} \equiv E_i - E_j \) \cite{19}. Since the lattice temperatures \( T_L \) in our intersubband lasers are sufficiently high (\( T_L \geq 77 \) K), the equipartition approximation works very well. In (20) and (21) for the electron rate, \( D \) is the acoustic deformation potential, \( \rho \) is the mass density, and \( v_{SS} \) is the velocity of sound in the material. The phonon frequency \( \omega \) in the case of acoustic phonons can be approximated by the linear dispersion relation as \( \omega = v_{SS} \sqrt{q} \). Note here that only the deformation potential interaction has been taken into account for the electron-acoustic phonon scattering because the piezoelectric interaction even weaker, and, therefore, can be neglected \cite{21}.

The capture and intersubband relaxation times are sums of the averaged electron intersubband rates

\[ \frac{1}{\tau} = \sum_i \frac{1}{N_{Si}} \sum_j \int_0^\infty \left[ f_i(E) - f_j(E') \right] \left[ \Gamma^+_{ij}(E) + \Gamma^-_{ij}(E) \right] \right) \right] \]  \hspace{1cm} (22)

where \( \Gamma^\pm_{ij} = \Gamma^{PO}_{ij} \pm \Gamma^AC_{ij} \) \cite{23}.

\( N_{Si} \) represents the sheet electron density in the \( i \)th subband, and the electron final energy \( E' = E + E_{PO} \) or \( E' = E + E_{AC} \), respectively. The electron distribution functions \( f_i \) and \( f_j \) are taken as Fermi distributions

\[ f_\alpha(E) = \left[ \exp \left( \frac{E - E_\alpha - F_\alpha}{k_B T_\alpha} \right) + 1 \right]^{-1}, \hspace{1cm} \alpha = i, j. \]  \hspace{1cm} (24)

In (24), \( T_\alpha \) is the electron temperature and \( F_\alpha \) is a quasi-Fermi energy, both in the \( \alpha \)th subband. The quasi-Fermi energy \( F_\alpha \) is a function of the electron temperature and the sheet electron density, which are obtained from rate equations in the following section.

The summations over initial states \( i \) and over final states \( j \) in (22) depends on whether capture or relaxation processes are being considered. In the case of the capture time \( \tau_{ij} \), the sum over \( i \) involves all subbands in the injection region as well as the lowest subband of the previous active region. The sum over \( j \) involves all upper subbands in the active region. In the case of the intersubband relaxation time \( \tau_{ij} \), the first sum goes over all upper subbands and the second one over all lower subbands in the active region only. Further, the second term in (22) does not contribute to the overall sum because the backward processes are negligible in this case. Screening of the electrons is not involved in both of the rates of (17) and (20) because it is greatly reduced for intersubband scattering \cite{22}, especially where the sheet electron densities in the particular subbands are up to \( 2 \times 10^{10} \) cm\(^{-2} \).

V. RESULTS AND DISCUSSION

Using the above quantities, the self-consistency scheme described in the previous section is utilized to perform calculations of the salient features of the laser dynamics. Results presented here are for the lifetimes calculated self-consistently for the structure of Fig. 1, while for the lifetimes of the structure described in [12], we have been used the parameters given in [12].

The electrons in the upper subband levels in the structures of Fig. 1 have high enough sheet densities to achieve a population inversion and, consequently, to participate in laser action. The sheet density in the highest energy subband \( (E_1) \) is also largest. Therefore, we expect that transitions from this level to the lower ones are the most effective. The electron sheet densities in the middle QW indicate that electron transitions between these levels are not as effective as from \( E_1 \). The electron temperatures increase with decrease in the subband energies. We have found an intersubband relaxation time of 1.07 ps after the self-consistent calculations. Further, we have calculated the capture time to be 0.28 ps using the self-consistent results for the electron densities and temperatures. It has been noted in Section III that the capture time was not included in the self-consistent scheme. Performing this calculation self-consistently requires significant additional computation time.

For the structure of [12], we have found a relaxation intersubband time of 4.0 ps at the temperature equal to 77K. The corresponding state lifetimes \( \tau_1, \tau_2, \) and \( \tau_3 \) in the active region (see [12, Fig. 1]) are 0.97, 0.67, and 0.60 ps, respectively. The relaxation intersubband time calculated by us is about two times larger than that of [4], but we believe that our calculations more accurately consider such processes as tunneling between the wells, acoustic phonon interactions, electron degeneracy, and includes also the applied bias. The population inversion conditions \( \tau_S - \tau_3 > 0 \) and \( \tau_S - \tau_3 > 0 \) are even better satisfied in our case. We have also calculated a capture time of 1.8 ps for the structure in [12]. This time, which represents an efficiency of the electron capture from the injection region into the active region, is short enough to encourage the rebuilding of the electron population inversion in the upper level.

The tunneling time \( \tau_{23} \) has also been calculated and found to have an unusually high value of 6.6 ps. This is because the energy difference between levels 2 and 3 is less than the pop energy. In fact, if one wants to find the tunneling time more exactly, the transitions into the following injection region should also be taken into account.

The results obtained here can be used, for example, in order to ascertain the direct-current modulation response of such lasers. Such work is currently in progress.

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