Temperature dependent high speed dynamics of terahertz quantum cascade lasers

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Temperature Dependent High Speed Dynamics of Terahertz Quantum Cascade Lasers

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Abstract—Terahertz frequency quantum cascade lasers offer a potentially vast number of new applications. To better understand and apply these lasers, a device-specific modeling method was developed that realistically predicts optical output power under changing current drive and chip temperature. Model parameters are deduced from the self-consistent solution of a full set of rate equations, obtained from energy-balance Schrödinger-Poisson scattering transport calculations. The model is thus derived from first principles, based on the device structure, and is therefore not a generic or phenomenological model that merely imitates expected device behavior. By fitting polynomials to data arrays representing the rate equation parameters, we are able to significantly condense the model, improving memory usage and computational efficiency.

Index Terms—Quantum cascade laser, rate equation model, electro-optical dynamics, thermal roll-over, bandwidth, turn-on behavior, free space communication

I. INTRODUCTION

The terahertz (THz) band of frequencies [1] has become increasingly accessible in recent years via emerging technologies for generating and detecting THz radiation. Amongst the many potential applications are broadband short-range communication [2]–[6], heterodyne detection of exogenous THz radiation, imaging, and material analysis [7]. The THz quantum cascade laser, first demonstrated in 2002 [8], is a compact yet powerful semiconductor source of coherent THz radiation. Current devices are able to operate at temperatures as high as 129 K in continuous wave (cw) [9] and 200 K in pulsed mode [10], and emitting peak pulsed optical powers of greater than 1 W [11].

Modeling the dynamic behavior of THz QCLs is vital for understanding the more complex behaviors of these devices and thus for the development of new applications – more so, considering that laboratory investigation of such behavior can be prohibitively expensive and experimentally challenging due to the extraordinarily short timescales on which some phenomena occur. Further, a growing class of THz QCL applications relies on the self-mixing effect [12]–[14], in which emissions from the device are reflected from a target back into the laser cavity, yielding information about the target [15]. Such retro-injected light (optical feedback) alters the device state and behavior, introducing a new dimension of complexity into device behavior [16]. In these applications, a realistic model is an indispensable research tool. It may be necessary to consider the effects of optical feedback even where it is undesirable, as failure to do so can lead to unexpected outcomes in behavior [17], [18].

The exemplar laser modeled in this paper is a bound-to-continuum (BTC) type QCL, a device that is particularly challenging to model and optimize due to the relatively large number of quantum-confined subbands in the active region (AR). Full rate equation (RE) models can be solved in order to extract dynamical information relating to all the intersubband transitions. Since the intersubband scattering processes are both temperature and electric field strength (voltage) dependent, it is necessary to determine these dependencies via first principles in order to properly model a device. However, full RE modeling is computationally intensive and therefore restricted to static solutions. Moreover, solving full REs self-consistently with optical and thermal models is computationally challenging.

Reduced rate equations (RREs), which employ a subset of parameters derived from the full RE model, offer a simple and practical means of predicting a device’s dynamic behavior without the need to repeatedly solve the full set of REs self-consistently. In principle, slight changes in a QCL’s electric field distribution due to dynamical behavior necessitate recalculation of the full self-consistent RE solution. In practice, ignoring the effect of these slight changes in electric field distribution on RE parameters leads to a second-order error in the RRE solution that is commonly considered insignificant. This makes it possible to use RREs for both dynamic and static modeling [19], and self-consistent computation of the emitted THz optical power.

However, a commonly made assumption in the use of the three-level RRE model for QCLs is that RRE parameters have constant values. All the RRE parameters are in fact both temperature- and voltage-dependent. Simulation results
based on the assumption are therefore valid only over the narrow range of voltages and temperatures for which the RRE parameters were calculated.

Various approaches have been taken in dealing with this problem [19]–[22], usually by addressing either temperature-dependent or voltage-dependent device behavior in isolation. Our modeling approach, introduced in [23], overcomes this difficulty by accommodating the temperature- and voltage-dependence of all RRE parameters over the full operating range of the device. With the addition of an AR temperature model to our rate equations, we are able to predict lattice temperature under changing excitation and cold finger temperature, thereby accounting for the temperature-dependence of the RRE parameters. The resulting model is able to correctly reproduce the experimentally observed variations in emitted optical power, from the temperature-dependent threshold current, through rollover to cut-off.

The aim of this paper is to both present our study of the dynamic turn-on behavior of a BTC THz QCL, and to provide a condensed version of our model to enable further investigation. In the following sections we define the model (Section II), setting out the complete generic model and providing device-specific data for a real (exemplar) QCL; discuss the results (Section III) of exemplar model applications to (A) static conditions, to simulate and explore its light–current (LI) characteristics and (B) turn-on behavior to characterize its high speed dynamics; and offer our concluding remarks.

II. MODEL DEFINITION

A. Exemplar QCL

The QCL we chose to model is a single mode GaAs/AlGaAs BTC 2.59 THz device that has been processed into a surface-plasmon Fabry-Pérot ridge waveguide and operates up to temperatures of 50 K in cw. This device has been previously characterized and used in a variety of applications including material analysis [15], [24] and imaging [25]. The band structure is shown in Fig. 1, with the radiative transition’s states labeled ULL and LLL. A complete specification of the active region heterostructure [26] is required to calculate device-specific RRE parameters from first principles.

B. Rate equation model

Our set of RREs reads:

\[
\frac{dS(t)}{dt} = -\frac{1}{\tau_p} S(t) + \frac{\beta_{sp}}{\tau_{sp}(T,V)} N_3(t) + M G(T,V) \frac{(N_3(t) - N_2(t))}{1 + \varepsilon S(t)} S(t)
\]

\[
\frac{dN_3(t)}{dt} = -G(T,V) \frac{(N_3(t) - N_2(t))}{1 + \varepsilon S(t)} S(t) - \frac{1}{\tau_3(T,V)} N_3(t) + \frac{\eta_3(T,V)}{q} I(t)
\]

\[
\frac{dN_2(t)}{dt} = +G(T,V) \frac{(N_3(t) - N_2(t))}{1 + \varepsilon S(t)} S(t) + \frac{1}{\tau_{32}(T,V)} N_3(t) + \frac{\eta_2(T,V)}{q} I(t)
\]

\[
\frac{dT(t)}{dt} = \frac{1}{mc_p} \left( I(t)V(T(t),I(t)) - \frac{(T(t) - T_0)}{R_{th}} \right)
\]

The symbol \( S(t) \) represents photon population, \( \tau_p \) the photon lifetime in the cavity, \( N_3(t) \) the ULL carrier number, \( N_2(t) \) the LLL carrier number, \( I(t) \) the current forcing function, \( q \) the electronic charge, \( \beta_{sp} \) the spontaneous emission factor, \( \tau_{sp} \) the spontaneous emission lifetime (or radiative spontaneous relaxation time), and \( M \) is the number of periods in the structure, 90 in the case of our exemplar QCL. The \( \eta_3 \) term in Eq. (2) models carrier injection efficiency into the ULL and the \( \eta_2 \) term in Eq. (3) models carrier injection efficiency directly into the LLL. The carrier lifetime for non-radiative transitions from the ULL to LLL is \( \tau_{32} \), the total lifetime due to non-radiative transitions for the ULL carrier population is \( \tau_3 \), and the lifetime for transitions from the LLL to the continuum is \( \tau_{21} \). The gain factor is represented by \( G \), as defined in [19]. We make provision for gain compression by including the term in \( \varepsilon \) in Eqs. (1)–(3).

Parameters that depend on temperature \( T \) and voltage \( V \) are expressed as functions of \( V \) and \( T \), \( (V,T) \) in the RREs. These include the gain factor \( G \), injection efficiencies \( \eta_2 \) and \( \eta_3 \), and carrier lifetimes \( \tau_3 \), \( \tau_{32} \), \( \tau_{21} \), and \( \varepsilon_{32} \); the dipole matrix element, which is used to calculate \( \tau_{sp} \). The voltage \( V \) and temperature \( T \) are themselves time-dependent, but for the sake of readability are not written explicitly as functions of time \( t \) in Eqs. (1)–(3).

A requirement of modeling temperature-dependent device behavior is knowledge of the active region (AR) temperature. Changes in AR temperature will occur due to both changes in cold finger temperature and thermal gradients resulting from self-heating in cw operation. Further, any changes in excitation such as steps or ramps create thermal transients [27]–[29] that disturb the thermal circuit’s equilibrium. Therefore in addition to three rate equations, a thermal model capable of predicting AR temperature must be included, and is represented by

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**Fig. 1.** Band diagram of our exemplar 2.59 THz BTC QCL. The radiative inter-subband transition is ULL → LLL (color online).
Table I

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
<th>Meaning (*indicates device-specific)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_p$</td>
<td>9.015</td>
<td>ps</td>
<td>†Photon lifetime in cavity</td>
</tr>
<tr>
<td>$M$</td>
<td>90</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$\beta_{sp}$</td>
<td>1.627e-04</td>
<td>–</td>
<td>†Spontaneous emission factor</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>8.854e-12</td>
<td>m$^{-3}$kg$^{-1}$s$^{-4}$A$^2$</td>
<td>Permittivity of free space</td>
</tr>
<tr>
<td>$\hbar$</td>
<td>1.055e-34</td>
<td>Js</td>
<td>Reduced Planck constant</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>116</td>
<td>$\mu$m</td>
<td>†Wavelength of emission</td>
</tr>
<tr>
<td>$\omega$</td>
<td>1.627e+13</td>
<td>rad s$^{-1}$</td>
<td>†Angular frequency of emission</td>
</tr>
<tr>
<td>$q$</td>
<td>1.602e-19</td>
<td>C</td>
<td>Charge on the electron</td>
</tr>
<tr>
<td>$\eta_{eff}$</td>
<td>3.30</td>
<td>–</td>
<td>†Effective refractive index of the medium</td>
</tr>
<tr>
<td>$R_{th}$</td>
<td>8.2</td>
<td>KW$^{-1}$</td>
<td>†Thermal resistance between active region and submount</td>
</tr>
<tr>
<td>$m$</td>
<td>1.533e-08</td>
<td>$k_B$</td>
<td>†Mass of laser chip</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>330</td>
<td>Jkg$^{-1}$K$^{-1}$</td>
<td>†Effective specific heat capacity of laser chip</td>
</tr>
<tr>
<td>$\alpha_w$</td>
<td>587.9</td>
<td>m$^{-1}$</td>
<td>†Waveguide loss</td>
</tr>
<tr>
<td>$R_1$</td>
<td>0.324</td>
<td>–</td>
<td>†Front facet mirror reflectivity</td>
</tr>
<tr>
<td>$R_2$</td>
<td>0.324</td>
<td>–</td>
<td>†Rear facet mirror reflectivity</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>0</td>
<td>–</td>
<td>†Gain compression factor</td>
</tr>
<tr>
<td>$L$</td>
<td>1.78</td>
<td>mm</td>
<td>†Length of laser chip cavity</td>
</tr>
<tr>
<td>$c$</td>
<td>3.00e08</td>
<td>m.s$^{-1}$</td>
<td>Speed of light in a vacuum</td>
</tr>
</tbody>
</table>

Eq. (4) in our equation set. This equation models the first order thermal behavior of the QCL and produces dynamic temperature response required to determine the temperature-sensitive RRE parameters at each step taken by the RRE solver. In Eq. (4), $m$ represents the effective mass of the laser, $c_p$ the specific effective heat capacity of the laser material in J kg$^{-1}$ K$^{-1}$ and $R_{th}$ the effective thermal resistance in K W$^{-1}$ between the AR and submount, which in this model is assumed to be at the same temperature as the cryostat’s cold finger. The symbol $T_0$ is the temperature, in kelvin, of the cold finger which is usually (but not necessarily) constant.

Although the RREs are expressed in terms of a current forcing function $I(t)$, terminal voltage $V(t)$ is also required by the equations for two reasons: (i) calculation of self heating within the AR, as expressed in Eq. (4) and (ii) calculation of each of the ever-changing voltage-dependent RRE parameters. With $I(t)$ as the independent variable, $V(t)$ may be calculated from the temperature-dependent current–voltage (IV) characteristics of the QCL, shown in Fig. 2. This can be done via a behavioral (or other) model of $V(t)$ expressed in terms of $I(t)$ and $T(t)$. QCLs have IV characteristics somewhat different to, and more difficult to model theoretically, than those of diode lasers. For maximum accuracy we opted for a behavioral model based on measured temperature-dependent IV data, rather than use theoretically predicted IV characteristics.

Initial values for carrier and photon populations, the current forcing function $I(t)$, and $T_0$, serve as independent inputs to the RREs (1)–(4). Given these inputs, the RREs may be solved for carrier and photon populations. The optical output power $P(t)$ can then be found from photon population by [20]:

\[ P(t) = \eta_0 \hbar \omega S(t)/\tau_p, \]

where $\eta_0$ is the power output coupling efficiency, $\hbar$ is the reduced Planck constant, and $\omega$ is the laser’s angular emission frequency. The definition of $\eta_0$ is [20]:

\[ \eta_0 = \frac{(1 - R_1)\sqrt{R_2}}{(1 - R_1)\sqrt{R_2} + (1 - R_2)\sqrt{R_1}} \frac{\alpha_m}{\alpha_m + \alpha_w}, \]

where $R_1$ is the front facet mirror reflectivity, $R_2$ the rear facet mirror reflectivity, $\alpha_w$ the waveguide loss and $\alpha_m$ the mirror loss defined as [21]:

\[ \alpha_m = -\ln(R_1 R_2)/2L, \]

where $L$ is the length of the laser. We calculated the spontaneous emission lifetime $\tau_{sp}$ from the dipole matrix element $z_{32}$ using [21]:

\[ \tau_{sp} = \frac{\varepsilon_0 \hbar \lambda^3}{8\pi^2 q^2 n_{eff}^2 z_{32}^2}, \]

where $\lambda$ is the wavelength of emission and $n_{eff}$ the refractive index of the medium. The photon lifetime $\tau_p$ is calculated from the modal loss via:
dependence. Fall off in η is rapidly with voltage [trace (a)] than temperature [trace (b)], making it the primary cause of roll-over in this QCL.

A well-understood limitation of RE models of QCLs is the prediction of hybridized wave functions extending between periods of the QCL at certain biases [33], resulting in unrealistically large scattering rates being produced. All such non-physical parameters were identified and removed from the data set.

The plot of an example temperature- and voltage-dependent RRE parameter, η3, is shown in Fig. 3.

![Fig. 3. Representation of η3 as a surface, showing temperature and voltage dependence. Fall off in η3 with increasing drive current occurs much more rapidly with voltage [trace (a)] than temperature [trace (b)], making it the primary cause of roll-over in this QCL.](image)

Although each RRE parameter may be realized via interpolation as a function of T and V for use in Eqs. (1)–(4), the bulk of its data structure can be significantly reduced by polynomial fitting. The resulting polynomial coefficients can be viewed as a compressed form of the full RRE data, and polynomials present the additional benefit of de-noising and smoothing the bulk data — an important consideration in solving a set of stiff differential equations. The polynomial we chose for the purpose is a third order polynomial in V and T, fitted using a weighted least-squares method to give simple and smooth RRE parameter functions.

The general form of a polynomial in two independent variables is:

\[ Z(x, y) = \sum_{i,j} a_{ij} x^i y^j, \]

where i and j are permuted subject to \((i + j) \leq k\), and k is the order of the polynomial. The general third order polynomial expanded for variables \(T\) and \(V\) (in lieu of \(x\) and \(y\)) is:

\[
Z(T, V) = a_{00} + a_{10} T + a_{01} V + a_{11} TV + a_{20} T^2 + a_{02} V^2 + a_{21} T^2 V + a_{12} TV^2 + a_{30} T^3 + a_{03} V^3
\]

Table II lists coefficient values for each of the temperature- and voltage-dependent RRE parameters found in (11). Terminal voltage \(V(t)\) was modeled by fitting a third order polynomial of the following form to measured temperature-dependent current–voltage data:

\[
V(I, T) = a_{00} + a_{10} I + a_{01} T + a_{11} IT + a_{20} I^2 + a_{02} T^2 + a_{21} I^2 T + a_{12} IT^2 + a_{30} I^3 + a_{03} T^3
\]

Coefficient values for this \(V(t)\) model are also given in Table II.

### D. Solution process

The derivation of RRE parameters from full REs, fitting of polynomials to RRE data, and calculation of other structure-dependent items indicated in Table I, are a once-off process for each QCL structure. Once done, (1)–(4) may then be repeatedly solved for any chosen current excitation waveform and cold finger temperature. As with any ordinary differential equation (ODE) set, our equations, including the thermal model, have to be solved concurrently. While the solution is in progress, \(V(t)\) is continuously re-calculated using Eq. (12) at every step the solver takes. The result is then fed into Eq. (4) to produce the time-dependent AR temperature \(T(t)\). During this process \(V(t)\) and \(T(t)\) are simultaneously fed into the polynomial coefficients of all seven temperature- and voltage-dependent RRE parameters to update them. We used a well-known commercial ODE solver, Matlab’s `ode23s` function, to produce the results following.

### III. RESULTS AND DISCUSSION

#### A. Static behavior

Characteristics that are easily measured in the laboratory, such as LI curves, are useful as a means of validating a model. We used the model to predict our exemplar QCL’s LI characteristics by excitation with a slow current ramp \(I(t)\) from 300 to 600 mA. The timescale of the ramp, 1 s, was far beyond that of the laser’s electro-optic and thermal dynamics, giving a result that well represents the static response. The simulation was repeated for three cold finger temperatures,
TABLE II

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>$G_0$</th>
<th>$G_1$</th>
<th>$G_2$</th>
<th>$G_3$</th>
<th>$G_{12}$</th>
<th>$G_{21}$</th>
<th>$G_{32}$</th>
<th>$V$</th>
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<tbody>
<tr>
<td>$a_{00}$</td>
<td>+2.5488e+04</td>
<td>+2.1969e+00</td>
<td>+6.7278e-03</td>
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<td>+1.9093e-10</td>
<td>+1.7446e-11</td>
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<tr>
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<td>$a_{30}$</td>
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<td>+2.1744e-03</td>
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<td>+2.1744e-03</td>
</tr>
</tbody>
</table>

$T_0 = 15$ K, 35 K, and 45 K, producing the results shown as solid curves in Fig. 4 (a). Measured characteristics at some of the same cold finger temperatures, for comparison, are shown as dotted traces. The measured data were reduced in magnitude by a factor of approximately four due to the low collection efficiency of the detection optics. The data shown in Fig. 4 (a) has been rescaled to match the simulated curves, for easy comparison. We are not aware of any other THz QCL model, to date, which is able to correctly predict roll-over behavior in QCLs.

As a demonstration of the part played by active region voltage in roll-over behavior, we repeated the simulation using RRE parameters that were temperature- but not voltage-dependent. This was done by assigning a constant value of $V = 2.80$ V in all RRE parameters, effectively making them voltage-independent. The results are shown as dashed lines in Fig. 4 (a) and (b). Although threshold occurs at almost the same points as for the previous simulation, the LI curves are many times broader, with the resulting thermal-only roll-over occurring at far higher currents, demonstrating electric field effects to be the primary cause of roll-over in this type of device. Although the voltage-dependence of RRE parameters was suppressed in this simulation, $V(t)$ continued to be calculated via Eq. (12) for use in Eq. (4). We have previously reported the “full simulation” LI characteristics of this QCL [23], and reproduce them here for comparison with the hypothetical case of “non-voltage-dependent” RRE parameters.

The physical cause of voltage-related roll-over is a misalignment between the injector and ULL at higher voltages [34], that manifests as a rapid drop in injection efficiency $\eta_3$. Figure 3 clearly shows that near roll-over $\eta_3$ drops far more rapidly due to voltage change (see trace (a) in Fig. 3) than due to temperature change [trace (b)].

B. Dynamic behavior

The brief exploration here of our THz QCL’s dynamic behavior aims to both illustrate the effects of temperature and voltage dependence on device behavior, and demonstrate the importance of modeling voltage-dependent device behavior. We chose to investigate basic dynamic behaviors that would be of interest in high speed applications, namely turn-on delay, rise time and overshoot in response to current-step excitation. Our first set of results, shown in Fig. 5, was obtained using
Fig. 5. Effect of cold finger temperature on step response. Response of the QCL to a current step of 0.470 A for six cold finger temperatures (color online) is shown, with both temperature- voltage-dependence of RRE parameters invoked. Both turn-on delay and pulse rise times increase with increasing cold finger temperature.

We then explored the effect of different drive currents on turn-on dynamics, while holding the cold finger temperature constant at 15 K. Figure 9 shows the results as solid lines for the five currents used. As before, we see a correlation between turn-on delay and rise time: starting with long times near threshold (part (a) of the figure), the times reduce to optimum values at about 460 mA and then lengthen again as injection efficiency $\eta_3$ rapidly falls off with increasing current. Optical power output follows the same trend, peaking at $\sim$460 mA and falling off rapidly just before cut-off (part(e) of the figure). When voltage-dependence of the RRE parameters is suppressed in the same way as before, however, response times continue shortening and optical power continues growing (broken lines in Fig. 9). Reduction in optical output power then peaks well after the known cut-off current of the QCL (not shown in figure), due to thermal-only effects, and in accordance with the LI characteristics of Fig. 4(b).

Fig. 6. Dependence of optical output power rise time on temperature for current step excitations of 460, 470, and 480 mA. Circles indicate data points, with curves to guide the eye.

Fig. 7. Relation of turn-on delay and rise time. Inset: turn-on delay as a function of temperature for three currents. Circles indicate data points, with curves to guide the eye.

IV. CONCLUSION

We have presented a complete, computationally simple, dynamic model of an exemplar BTC THz QCL that behaves...
realistically over a wide range of voltages and temperatures. Our simulations reveal temperature- and bias-dependent turn-on characteristics that would be of interest in typically high speed free space communications and pulsed applications. They also demonstrate the importance of temperature- and voltage-dependence modeling, which has an impact on device behavior on timescales from pico-seconds to static. The novelty of our approach is the use of RRE parameters that are functions of device voltage and lattice temperature, derived from first principles by SP solution of the full set of REs. Coupled with a time dependent thermal equation, we obtain an RRE model that is valid over a broad range of device temperatures and voltages, allowing exploration of a QCL’s characteristics over its full operating range of bias currents and temperatures. Although the RRE parameters presented here were derived for an exemplar BTC device, the approach is generic and may be applied to any QCL by extracting appropriate parameters from a full RE model.

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