Abstract. We present simulation results for two resonant phonon terahertz quantum cascade lasers using a self-consistent energy balance model, which determines the electron temperature for each conduction subband. These temperatures, along with the electron populations and scattering rates, are determined in a manner similar to previously published models. However, the presented model is able to converge through the use of an algorithm that appears to be robust. The predicted individual subband electron temperatures, population densities and scattering rates are compared to previously published Monte Carlo and experimental studies for both lasers, where subband temperature variations were observed. These quantities were chosen since they provided the only comparison to modeling results from other studies.
1. Introduction

Quantum cascade lasers (QCL’s) have become a promising source technology in the mid-infrared and terahertz frequency ranges. However, further study is still needed in order to make terahertz QCL’s a viable choice for many applications and to eventually reach room-temperature operation. Device modeling is an important element in meeting this need and several methods exist for producing QCL simulation results. Once such model, the self-consistent energy balance (SCEB) model [1], has been shown to predict lasing characteristics without the computational demands of Monte Carlo [2] (MC) or non-equilibrium Green’s function [3] (NGF) methods. An improvement to the SCEB model has been suggested [4], which used the energy balance condition for each subband to determine its electron temperature. Additionally, algorithms have been suggested which could find each subband temperature using an iterative procedure. Previous studies have indicated that the multi-subband temperature models did converge, but the algorithms did not converge in all cases [5].

Additionally, few comparisons between the results of SCEB models, which determine subband electron temperatures, and other modeling methods have been done. Comparisons have been made between an average electron temperature and a multi-subband electron temperature SCEB model [1, 5], between an average electron temperature SCEB and a MC model [6, 7], and between a multi-subband temperature SCEB and a MC model [5]. However, the multi-subband temperature SCEB and MC model comparison was done for a p-SiGe/Si material system. Si-based QCLs remain a purely theoretical area of study, and have never been demonstrated experimentally. Therefore, there is still a need for studies of multi-subband models to quantify their success. This is especially true since a successful multi-subband SCEB model would provide an efficient means to determine thermal effects, which can have a significant impact on the transport mechanisms within a QCL (through thermal backfilling, parasitic transitions, etc.) and gain performance [8].

Electrons can acquire a temperature $(T_e)$ different from the lattice temperature $(T_L)$ due to the applied bias and exchanged energy between the electron subbands and the lattice. Additionally, each electron subband can have a different temperature. These differences are vital to the internal physics of QCL’s since the subband energy distributions are dependent on the subband temperature. Therefore, the scattering rates, population densities and all subsequent calculations are also affected by electron temperature. These temperatures can be found through a MC procedure, but not all self-consistent models are capable of calculating subband temperatures. When self-consistent models are modified to account for electron heating, typically only an average $T_e$ for the entire conduction band is found [6]. However, MC simulations [9, 10, 11, 12, 13, 14, 15] and experimental measurements [16, 17] have shown that there is considerable variation among subband temperatures, especially in resonant phonon QCL designs. In order to determine a separate $T_e$ for every subband using the self-consistent model, a multi-subband energy balance condition must be implemented.
A SCEB model which determines the temperature for electron conduction subband as well as the associated algorithm is presented. This simulation tool permits the determination of individual electron subband temperatures and accurately assess the effects of electron subband heating on carrier transport within QCL’s. The results of two resonant phonon device studies are shown and the resulting calculations are compared to published MC simulations and experimental measurements.

2. Subband electron temperature

The subband electron temperatures ($T^i_e$) are determined by a set of energy balance equations [4] similar to the average electron temperature equation [6]. In these equations, the potential energy is defined as the subband energy minimum (or the quantized eigenenergy $E_i$ for subband $i$). The kinetic energy $E^k_i$, which is related to the the electron temperature, is defined as any additional energy above that minimum. If distribution-averaged scattering rates are used in a single temperature SCEB model, the average electron temperature equation can be solved by using just the electron eigenenergies and the population densities. However, regardless of the form of the scattering rates, the multi-subband SCEB model requires the electrons’ kinetic energy in order to find the subband temperatures.

The multi-subband energy balance condition is met when the rate of energy lost from transitions out of each subband is equal to the rate of energy gained from transitions into each subband. For a single particle transition between two states, $i \rightarrow f$, the rate of change of energy out of subband $i$ is the energy transition rate $w^-_{if}$ multiplied by the population density of the initial state $n_i$. However, the same single particle transition also affects subband $f$. In this case, the rate of change of energy of subband $f$ is the energy transition rate $w^+_{if}$ multiplied by $n_i$. The energy transition rates $w^-_{if}$ and $w^+_{if}$ are each a function of the relevant particle transition rate and kinetic energy of the subbands. Any additional scattering particles (such as phonons) also contribute to the rate of change of energy. Therefore, the energy transition rate is defined as

$$w^+_{if} = \frac{\int_{E_i}^{\infty} E^k_i w_{if}(E^k_i) f_i(E^k_i, E^j_f, T^i_e) [1 - f_f(E^j_f, T^f_e)] dE^k_i}{\int_{E_i}^{\infty} f_i(E^k_i, T^i_e) dE^k_i}$$ (1)

where $f_i(E^k_i, T^i_e)$ is the Fermi-Dirac distribution for subband $i$ and the kinetic energy of the final state $E^k_f$ can be found from the conservation of energy. For transitions involving one electron

$$E^f_k = E_i + E^k_i - E_f + \delta E$$ (2)

where $\delta E$ represents the energy of the scattering particle. The single particle scattering mechanisms included in the present study were

$$\delta E = \begin{cases} E_{LO} & \text{for phonon absorption} \\ -E_{LO} & \text{for phonon emission} \end{cases}$$ (3)
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Electron-photon interactions were treated in the same way. When (2) is substituted into (1), the relationship between the energy transition rates is found, as in [4]:

\[ w_{if}^+ = (E_i - E_f + \delta E)W_{if} + w_{if}. \]  

(4)

In the above equations, \( W_{if} \) represents the distribution-averaged particle transition rate from the state \( i \) to \( f \), as defined in section 3.

An approximate average subband kinetic energy was found by averaging over the quasi-Fermi distribution of the electron state. Defining the average kinetic energy for a subband \( i \) as \( \beta_i \),

\[ \beta_i = \frac{\int_{E_i}^{\infty} E_i^k f_i(E_i^k, T_i^e) dE_i^k}{\int_{E_i}^{\infty} f_i(E_i^k, T_i^e) dE_i^k} \]  

(5)

where \( E_i^k \) is the quasi-Fermi energy for subband \( i \), and \( f_i(E_i^k, T_i^e) \) is the Fermi-Dirac distribution function. Then the average energy transition rate has the form

\[ w_{if}^+ \approx W_{if} \beta_i. \]  

(6)

This form for the average energy transition rate has the benefit of being easy to implement since \( W_{if} \) is already calculated to find the scattering rates. However, it has been pointed out to the authors that a more accurate form for the average energy transition rate may be

\[ w_{if}^+ \approx W_{if}(\beta_i) \beta_i \]  

(7)

where \( W_{if}(\beta_i) \) is the scattering rate at the energy \( \beta_i \) and not the distribution-averaged scattering rate.

The balance condition for e-e transitions is more complex since not only does it involve four particle states, but it also has to be determined from a four-dimensional matrix of scattering events. In this case

\[ \frac{dE_{ee}^{em}}{dt} = \sum_{ijg} n_i W_{ijfg}^{ee}(\langle E_{ij}^k \rangle) - n_f \sum_{gij} W_{fgij}^{ee}(\beta_f) \]  

(8)

where \( W_{ijfg}^{ee} \) is the rate for two electrons in the initial states \( i \) and \( j \) that scatter to the states \( f \) and \( g \), respectively, and

\[ \langle E_{ij}^k \rangle = E_i + \beta_i + E_j + \beta_j - E_f - E_g - \beta_g. \]  

(9)

Finally, all forms of scattering which contribute to the rate of change of energy into and out of a subband \( f \) must meet the energy balance condition

\[ \frac{dE_{em}^{em}}{dt} + \frac{dE_{abs}^{abs}}{dt} + \frac{dE_{ee}^{ee}}{dt} = 0. \]  

(10)

Since the scattering rates, population densities and kinetic energies in (10) are temperature dependent, the temperature of each subband has to be varied until the balance condition is met for all subbands. This is accomplished using an iterative procedure with the entire multi-subband SCEB model, as described below.
3. Multi-subband SCEB Model

Simulations were performed using a set of sequential calculations and convergence conditions which ensured all electron wavefunctions, eigenenergies, populations, lifetimes and temperatures were consistent with one another. This sequence, which was repeated until all convergence conditions were met, provided an accurate representation of the lasing device. A schematic flow-chart is shown in figure 1.

The wavefunctions and eigenenergies for three full QCL periods were found using an iterative solution of the one electron Schrödinger and Poisson equations. Doing so took into account space charge effects, which have been shown to significantly affect simulation results [14]. The wavefunctions from the central period were then copied to the surrounding two periods since they most accurately represented an infinite cascade structure [5]. The subbands were evenly populated for the first SCEB iteration; however, all later iterations used the population densities resulting from the solution of population rate equations.

A waveguide mode solver was used to determine all field coefficients and the axial wavenumber of the fundamental mode. A one-dimensional slab waveguide model was used, which coupled the field coefficients with the axial wavenumber via a transfer-matrix approach [18]. The total waveguide loss, confinement factor and gain threshold were then found.

Transition rates were calculated using Fermi’s Golden Rule for electron-photon (e-p), electron-longitudinal-optical phonon (e-LO), and electron-electron (e-e) scattering. These rates were averaged over the in-plane wave vector assuming Fermi-Dirac statistics. All possible transitions within three periods of the active region were found, which included a four-dimensional matrix of rates to describe all possible e-e scattering events. Despite its potentially weak effect [19], state-blocking was included. For e-p scattering, the stimulated emission rate is

$$W_{i\rightarrow f}^{st} = m_{if} \frac{\epsilon^2}{2\pi m^* \epsilon V \Delta \nu_{if}} f_{i\rightarrow f}$$

where $m_{if}$ is the photon population density for this transition, $V$ is the active region volume, $f_{i\rightarrow f}$ is the oscillator strength defined as

$$f_{i\rightarrow f} = \frac{2m^* \omega_{if}}{\hbar} \left( \int \psi_f^*(z)z\psi_i(z)dz \right)^2$$

and $\nu_{if}$ is the transition line width defined as

$$\Delta \nu_{if} = \frac{1}{\pi} \left( \frac{1}{2\tau_i} + \frac{1}{2\tau_f} + \frac{1}{T_2^*} \right).$$

The quantities, $\tau_i$, $\tau_f$, and $T_2^*$ are the initial state, final state, and dephasing lifetimes, respectively. The dephasing lifetime was kept at a constant value of 0.25 ps. For e-LO scattering the phonon emission and absorption rate are

$$W_{i\rightarrow f}^{\text{ems,abs}} = \frac{m^* \epsilon^2 E_{LO}}{8\pi \hbar^3} \left( \frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_s} \right) (n_{LO} + 1/2 \pm 1/2) \int dk_i k_i f_i(k_i) \int_{0}^{2\pi} d\theta \frac{A_{rLO}(q)}{q}$$
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where $\epsilon_\infty$ and $\epsilon_s$ are the high and low frequency permittivities, respectively, $n_{LO}$ is the phonon occupation number, $q$ is the magnitude of the phonon wavevector, $\theta$ is the angle between the wavevectors $k_i$ and $k_f$, and $A_{\text{e-LO}}(q)$ is the form factor integral for e-LO scattering as found in Ref. [20]. The integrals over $k_i$ represent the distribution averaging over the initial state $i$. Finally, for e-e scattering

$$W_{i,j \rightarrow f,g}(k_i) = \frac{m^*e^4}{64\pi^3\hbar^2\epsilon^2} \int dk_j \int d\theta \frac{1}{q^2} |A_{\text{e-e}}(q)|^2 f_j(k_j)(1 - f_g(k_g))(1 - f_f(k_f)) \tag{15}$$

where $q$ is the magnitude of the relative wavevector $k_i - k_f$, $\theta$ is the angle between the wavevectors $k_j - k_i$ and $k_g - k_f$, and $A_{\text{e-e}}(q)$ is the form factor integral for e-e scattering as found in Ref. [20]. This equation was also averaged over the initial state distribution energy as in (14). The Fermi-Dirac distribution functions in equations (14) and (15) are equivalent those in equations (1) and (5). These forms are all in the distribution averaged form and are consistent with those found elsewhere [21, 20, 22, 23].

The effect of screening on e-e scattering rates was also taken into account. A modified single subband model was employed, since it was shown to provide better agreement with the full screening tensor equation than common single subband models [13, 14, 24]. The modified model alters the dielectric function according to

$$\epsilon_r(q) = 1 + \sum_i \frac{e^2}{2\epsilon_s q} \Pi_{ii}(q,T) A_{iiii}(q) \tag{16}$$

where $i$ is an electron state in the central module, $A_{iiii}$ is the intrasubband form factor integral for state $i$, and $\Pi_{ii}(q,T)$ is the polarization function. The temperature-dependent [25] polarization function was found in the static limit [26]. This form of screening had the added benefit of taking into account the separate temperatures of each subband.

A set of iterative rate equations were then solved for each subband in order to modify the subband population densities using the calculated transition rates [27]. The rate equations took into account every transition within three periods of the active region which could possibly affect the subband populations. Additionally, the photon population densities were found according to

$$m_{ij} = \frac{n_i}{W_{ij}^p/(\Gamma W_{ij}^{\text{sp,1mode}}) - V(n_i - n_j)} \tag{17}$$

where $V$ is the active region volume, $W_{ij}^p$ is the photon loss rate (which is a function of the waveguide and mirror losses), $\Gamma$ is the confinement factor, and $W_{ij}^{\text{sp,1mode}}$ is the spontaneous emission rate into a single mode. These photon populations are found self-consistently with the electron populations. This is an approach which was suggested in the literature [24], and has been implemented in semi-classical Monte Carlo models [28] and is intrinsically included in quantum transport models [29]. However, to the authors’ knowledge this has not been implemented in any other rate equation models. This was considered to be a refinement over rate equation models which simply used the current
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density to account for scattering into and out of the lasing transition [30]. Once the population densities reached convergence, the energy balance condition was applied to determine subband electron temperatures.

Initially, the electron temperatures were assumed to be equal to $T_L$ and then all subsequent calculations were performed using this assumption. Then the energy balance equations were calculated, and if any evaluated to be above some threshold value, a new estimate for the electron temperatures was made. Then the scattering rates and population densities were re-calculated using these new temperatures and the energy balance equations were solved again. This process was repeated until all balance equations evaluated to a value below the convergence threshold.

Within each iteration of the multi-subband SCEB model, $2N$ equations had to be solved to find populations and temperatures for all $N$ subbands. Previous publications expressed difficulties associated with these equations reaching convergence using the Broyden method [5]. Therefore a different algorithm was developed to update subband temperatures and reach convergence, based on the secant method. Subband temperatures were updated based on the value of the related energy balance equation. If an energy balance equation evaluated to be much different than zero, then the associated temperature was changed much more than when an energy balance equation was near zero. This relationship can be expressed as a slope $(\Delta(dE_i/dt)/\Delta T_i)$. An initial guess for this slope was made; however, after several iterations of the system of energy balance equations, this slope was calculated from a linear regression of the calculated energy balance values with their associated temperatures. The slopes were calculated from the previous five iterations, which prevented large fluctuations in slope from one iteration to the next.

With each iteration, the energy balance equations were evaluated and compared to a threshold condition, which was also determined from the slope. The threshold used for the current paper was

$$\left| \frac{dE_f}{dt} \right| \leq \left| \alpha T_e \frac{\Delta(dE_i/dt)}{\Delta T_i} \right|$$

(18)

where $\alpha$ was a threshold factor to be chosen by the user. For temperature convergence to within 0.1%, then $\alpha$ was set to 0.001.

Finally, after the first iteration of the complete multi-subband SCEB model, the electron population densities were checked for convergence compared to the results of the previous iteration. If the densities differed by more then a predefined threshold value, the model was repeated using the results of the previous iteration to improve the input parameters. If the populations differed by less than the threshold value on the next iteration of the model, then the output parameters were determined, such as lasing frequency, power and current.
Figure 1. Flow chart of the complete QCL computational model. Conditional steps are indicated by a question mark. After the Schrödinger-Poisson box, electron wavefunctions are checked for convergence. After the electron populations box, electron populations are checked for convergence. After the electron temperature box, the electron temperature is checked for convergence. Finally, the electron wavefunctions are again checked for convergence before the process is repeated again.

4. Results and discussion

The electron subband temperatures have been determined for two resonant phonon structures using the SCEB model as described in Sec. 3. Both structures have exhibited a considerable variation among subband temperatures in either MC simulation or experimental measurement. The dependence of the electron temperatures on either lattice temperature or bias voltage is shown as well as additional quantities such as population densities and transition rates. These quantities were chosen over other parameters (such as current density and power) since they would provide the most direct comparison to other models as well as minimize confounding effects.

4.1. 3.4 THz, three-well design

The first structure studied, shown in figure 2, was the 3.4 THz, three-well, diagonal design [31] which has been shown to lase up to a lattice temperature of 186 K. Due to its exceptional performance, this structure was the subject of an exhaustive MC analysis [15], which allowed for a comparison of modeling results.

The device parameters were taken from those found in reference [31]. For the model, the device dimensions were 170 $\mu$m $\times$ 2.51 mm with a 10 $\mu$m active region consisting of 222 periods. The waveguide was modeled using 50 nm thick contact layers doped to $n = 5 \times 10^{18}$ cm$^{-3}$ above and below the active region with the Au waveguide layers surrounding the contact layers. The SCEB model predicted a slightly higher optimum voltage, at 70 mV/module, than that predicted by the MC study [15]. At this bias, the electron temperature of the upper lasing state as a function of lattice temperature was found and is shown in figure 3(a). At lower lattice temperatures, the electron temperature of the upper lasing state ($T_{el}^4$) was significantly higher than $T_L$. But as $T_L$ was increased to 150 K and above, $T_{el}^4$ and $T_L$ were roughly equal. This behavior was also seen in the MC study of this structure [15], but $T_{el}^4$ was several degrees higher
Figure 2. Calculated potential profile and squared wave functions of the 3.4 THz structure at a bias of 64 mV/module for three periods of the active region. Space charge effects were included, although the band bending may not be obvious in the diagram. The middle period states are labeled such that state 4 and 3 are the lasing states, while 2 and 1 are responsible for depopulation and injection.

than in the present study. The lower $T_e^4$ seen in the present study is most like due to a smaller overall injection rate into the upper lasing state via electron-electron scattering (figure 3(b)) than that predicted in reference [15].

Additionally, the predicted lifetime of the upper laser state was much lower at higher $T_L$ due to increased electron-phonon emission. These discrepancies between the SCEB and MC calculations indicated that the observed differences in electron temperatures for this structure could be due to differences in the calculation of scattering rates and screening. The reduced population ratio between the two lasing states (figure 3(c)) predicted by the SCEB model could be explained using the same arguments. However, since the MC study in reference [15] did not include electron-photon scattering, the electron populations would not have been calculated in the same way as in the SCEB model (see section 3).

It should be noted that the population ratio shown in figure 3(c) reached a minimum at a lattice temperature of 100 K. This is the result of the scattering rate temperature dependencies. For the upper lasing state, the lifetime of the state decreased steadily with lattice temperature as seen in Figure 3(b). However, the lifetime of the lower lasing state remained essentially constant for lattice temperatures up to 100 K due to the cooling influence of phonon emission on the electron temperature of the lower lasing state. This led to a dramatic reduction in the population ratio between states 4 and 3 up to 100 K. Above 100 K, the electron temperature of the lower lasing state was able to increase and therefore the lifetime of this state decreased, reducing the discrepancy between the upper and lower lasing state lifetimes and the population ratio was able to increase.
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Figure 3. Device characteristics as a function of lattice temperature at a bias of 70 mV/module for the 3.4 THz structure. (a) Electron temperature of the upper lasing state 4. (b) Electron-electron scattering rates of the injection ($1' \rightarrow 4$) transition as well as the lifetime of the upper lasing state. (c) Population ratio between lasing levels 4 and 3.

4.2. 2.8 THz, four-well design

Experimental measurements of subband electron temperatures have provided further indications that there is significant temperature variation between subbands in resonant phonon QCL designs [16, 17]. One of these measured structures was a four well, 2.8 THz design [16]. Device parameters were taken from this reference for the sake of modeling. The dimensions used were 40 $\mu$m $\times$ 0.72 mm with a 10 $\mu$m active region consisting of 152 periods. The waveguide structure used was the same as that described in the previous subsection. This structure was also simulated using the SCEB for comparison to experimental results and is shown in figure 4. The electron temperatures of the upper laser level (state 5) and the two injection states (1 and 2) are shown in figure 5(a). At 60 mV/module, the SCEB model predicted a temperature difference between the upper laser state and the two injector states of 25-38%. This is not as large as the almost 100% difference seen experimentally; however, MC simulations have never predicted temperature variations of that magnitude in resonant phonon QCL designs. The SCEB temperature variations are very close to that of MC simulations of a similar
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Figure 4. Calculated potential profile and squared wave functions of the 2.8 THz structure at a bias of 65 mV/module for three periods of the active region. Space charge effects were included, although the band bending may not be obvious in the diagram. The middle period states are labeled such that state 5 and 4 are the lasing states, while 3, 2 and 1 are responsible for depopulation and injection.

device [9], which predicted subband temperature variations of up to 38%. The subband temperatures reported in the MC study were 96, 111, and 102 K for the upper lasing, upper injector, and lower injector state, respectively. The subband temperatures from the SCEB model were 99, 118, and 99 K for the same states, which is in good agreement.

The population inversion ratios determined from the SCEB model are shown in figure 5(b) and are nearly identical to the measured values [16]. However, the MC study of the similar structure [9] yielded a population inversion ratio of 8 at the alignment voltage, which is considerably higher than that from measurement or the present SCEB modeling. This higher population density of the upper laser state is most likely due to the higher lifetime of 3.5 ps reported in that study as compared to the 1.2 ps predicted by the SCEB model. However, the lifetime of the lower lasing states predicted by the MC study and the present one were identical.

5. Conclusions

A self-consistent model containing a multi-subband energy balance condition was presented. This model was used to generate subband electron temperatures as well other output parameters for two resonant phonon QCL designs. Detailed comparisons between MC simulations, experimental measurements and the SCEB model were performed. The SCEB model predicted similar electron temperatures to those of MC studies. The discrepancies observed in population densities were most likely due to differences in scattering rate calculations. When applied to a structure measured experimentally, the SCEB model predicted the upper lasing state to have the highest subband temperature
Figure 5. Device characteristics as a function of bias at a lattice temperature of 100 K for the 2.8 THz structure. (a) Electron temperatures of the upper lasing state (5) and the two injector states (1 and 2). (b) Population ratio between the lasing levels 5 and 4.

within the device, which was verified experimentally. Although the degree of subband temperature variation was not as high as that seen in experiment, the population ratio did match.

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References


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