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**Article:**

Indjin, D., Harrison, P., Kelsall, R.W. et al. (1 more author) (2003) Self-consistent scattering model of carrier dynamics in GaAs-AlGaAs terahertz quantum-cascade lasers. *IEEE Photonics Technology Letters*, 15 (1). pp. 15-17. ISSN 1041-1135

<https://doi.org/10.1109/LPT.2002.805801>

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# Self-Consistent Scattering Model of Carrier Dynamics in GaAs–AlGaAs Terahertz Quantum-Cascade Lasers

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**Abstract**—Intersubband electron scattering transport in terahertz GaAs–AlGaAs quantum cascade lasers is analyzed, using a full 13-level self-consistent rate equation model. The approach includes all relevant scattering mechanisms between injector–collector and active region states in the cascade structures. Employing an energy balance equation which includes the influence of both electron longitudinal optical phonon and electron–electron scattering, the method also enables evaluation of the average electron temperature of the nonequilibrium carrier distributions in the device. The electron temperature is found to give a strong influence on the output characteristics, particularly at very low temperatures. The threshold currents and electric field-current density characteristics are in very good agreement with experiment, implying that the model has a strong predictive capability.

**Index Terms**—Electron temperature, intersubband transitions, quantum-cascade lasers, terahertz.

THE QUANTUM-cascade laser (QCL), since its first realization [1], has demonstrated an impressive extension of the mid-infrared frequency range [2]–[5] and until recently could be operated at wavelengths as long as  $24\ \mu\text{m}$  [6]–[8]. This has stimulated a number of experimental [9], [10] and theoretical [11] studies of QCL structures designed for emission at terahertz frequencies well below the forbidden phonon Reststrahlenband. Considerable research effort has recently resulted in theoretical prediction of population inversion by Monte Carlo studies [12], followed by luminescence measurements [13], and finally the laser action [14] at  $\lambda \sim 69\ \mu\text{m}$  (4.4 THz) in a GaAs–AlGaAs QCL. Most recently, lasing at  $\lambda \sim 66\ \mu\text{m}$  has been demonstrated in similar structures with very low waveguide losses [15].

Successful experimental developments have stimulated further interest in theoretical work in order to indicate routes to optimized layer design for improved output characteristics, particularly at higher working temperatures. The charge transport in QCLs is due mainly to incoherent-scattering mechanisms [16], and all principal electron longitudinal optical (LO) phonon and electron–electron scattering mechanisms have to be included [17], [18]. This applies not only to the active region, where laser emission takes place, but also to the injector–collector region. The analysis of the operating characteristics of terahertz QCLs is more complex, i.e., computationally demanding, than for mid-infrared devices. This is because the energy separation between most of subbands is smaller than the LO phonon

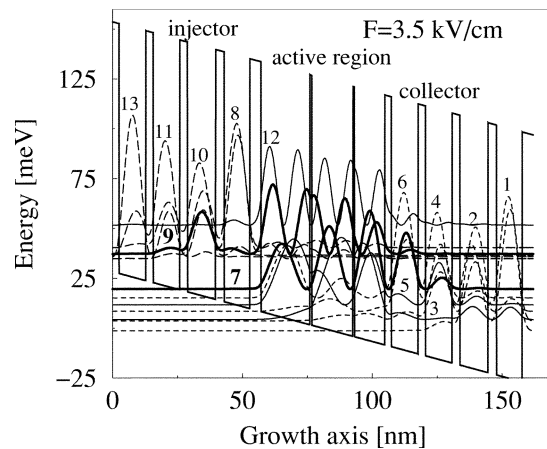


Fig. 1. A schematic diagram of quasi-bound energy levels and associated wave functions squared for  $1(1/2)$  periods of a GaAs–Al<sub>0.15</sub>Ga<sub>0.85</sub>As terahertz QCL: injector (levels 8, 10, 11 and 13) active region (3, 5, 7, 9 and 12) collector (1, 2, 4 and 6). The layer sequence of one period of the structure, in nanometers, from left to right starting from the injection barrier is **4.3**, **18.8**, **0.8**, **15.8**, **0.6**, **11.7**, **2.5**, **10.3**, **2.9**, **10.2**, **3.0**, **10.8**, **3.3**, **9.9**, ([14]). The normal script denotes the wells, bold script denotes the barriers, and underscore denotes the doped region, with a nominal donor sheet density  $N_s = 4.08 \times 10^{10}\ \text{cm}^{-2}$  per period.

energy and electron–electron scattering becomes the dominant scattering mechanism [9], hence necessitating a large number of possibly relevant scattering processes to be accounted for. Additionally, the electron temperature is expected to exceed significantly the lattice temperature. In this letter, two main topics are addressed: 1) development of a technique to analyze terahertz QCLs as an alternative to the full microscopic, but computationally more demanding, Monte Carlo method [12], [16]; 2) extraction of the QCL output characteristics and exploration of the influence of electron temperature thereon.

The electronic structure of a terahertz QCL [14] is illustrated in Fig. 1. Radiative transitions occur between states 9 and 7, while levels 3, 5, and 12 are the ground, the first excited and higher states of the active region, respectively. Simulating electron flow in a cascade requires one to have scattering rates for all intra- and inter-period processes, and an assumption is made that each period of the cascade behaves in the same manner (periodic boundary conditions). Calculation of all these scattering rates formally necessitates for energy states/wavefunctions in two full periods, but in view of negligible active-to-active region coupling,  $1(1/2)$  period (Fig. 1) suffices. Periodic boundary conditions imply that the wavefunctions in the two injector are shifted in space and energy versions of each other, though we have checked that using explicitly evaluated wave functions for the structure in Fig. 1 with hard boundary conditions gives a negligible difference in device output character-

Manuscript received July 9, 2002; revised September 23, 2002. This work was supported by the Engineering and Physical Science Research Council under Grant GR/R04485.

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Digital Object Identifier 10.1109/LPT.2002.805801

istics (less than 3%). To implement periodic boundary conditions, the rate equations were written so that carriers were cycled around the 13-level system, i.e., electrons scattering outside the considered period reappear in equivalent states inside. Electron–electron scattering is calculated using Fermi golden rule within static screening approximation. The  $k$ -space averaging is done assuming Fermi–Dirac distribution within each subband individually, with common value of electron temperature in all subbands. All processes which, compared with electron-LO phonon scattering, make a nonnegligible contribution to the transport ( $\sim 400$ ) are included: the accuracy of this approximation has been confirmed in one-off calculation in which every electron–electron process ( $\sim 8000$ ) was considered. The steady state subband populations of the active region are written as

$$n_i = \left[ \sum_{j=1, j \neq i}^{13} \frac{n_j}{\tau_{ji}} \right] \left[ \sum_{j=1, j \neq i}^{13} \frac{1}{\tau_{ij}} \right]^{-1} \quad (1)$$

where  $i = 3, 5, 7, 9, 12$ . The population of the ground collector level 1 is written as

$$n_1 = \left[ \sum_k \frac{n_k}{\tau_{k1}} + \sum_s \frac{n_s}{\tau_{s8}} \right] \left[ \sum_k \frac{1}{\tau_{1k}} + \sum_s \frac{1}{\tau_{8s}} \right]^{-1} \quad (2)$$

where  $k = 2, \dots, 7, 9, 12$  and  $s = 3, 5, 7, 9, 12$ , and similarly for other injector and collector states. The scattering time  $\tau_{if}$  is a function of both  $n_i$  and  $n_f$ , the initial and final subband populations. Hence, this set of equations has to be solved self-consistently using an iterative procedure [11], [19], [20].

At equilibrium, the rate at which the electron distributions gain kinetic energy (relative to the particular subband minimum) through scattering, will balance with the rate at which they lose kinetic energy to the lattice. Despite the fact that electron–electron scattering is elastic as far as total energy is concerned, inter-subband electron–electron transitions do convert potential energy into kinetic energy (or vice-versa). This work this would lead to an increase (decrease) in the total kinetic energy of a subband population, because the potential energy as defined here includes the quantised component of the kinetic energy. Hence, the kinetic energy balance condition can be written as [21]

$$\sum_{\text{em.,abs.,e-e}} \sum_f \sum_i \frac{n_i}{\tau_{if}} (E_i - E_f + \delta E) = 0 \quad (3)$$

where  $E_i - E_f$  is the subband separation, and the change in energy  $\delta E$  is equal to  $-E_{LO}$  for phonon emission (em.),  $+E_{LO}$  for absorption (abs.) and zero for electron–electron ( $e$ - $e$ ) scattering. The next step of the procedure, is to vary the electron temperature until (3) is satisfied self-consistently.

From the self-consistent solution, the population inversion  $\Delta n_i = n_9 - n_7$  in the steady-state condition is obtained and the modal gain can be calculated [2], [20]

$$G_M = \frac{4\pi e^2}{\epsilon_0 \underline{n}} \frac{z_{97}^2}{2\gamma_{97} L_p \lambda} \Gamma(n_9 - n_7) \quad (4)$$

where  $\lambda$  is the laser emission wavelength,  $2\gamma_{97}$  is the experimental full-width at half maximum (FWHM) of the electroluminescence spectrum below threshold,  $\underline{n}$  is the mode refractive

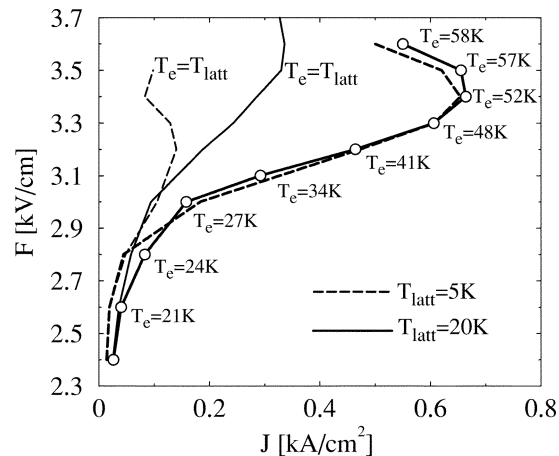


Fig. 2. Electric field versus current density characteristics at lattice temperature  $T_{\text{latt}} = 5$  K and  $T_{\text{latt}} = 20$  K.

index,  $\epsilon_0$  is the vacuum dielectric permittivity,  $L_p$  is the length of one period (injector + active region),  $\Gamma$  is the modal overlap factor, and  $z_{97}$  is the radiative transition matrix element. To extract the output characteristics of QCLs, one has to change the electric field  $F$  (i.e., the applied voltage) and calculate the modal gain  $G_M$  and the total current density  $J$  for each value of the field. The threshold current density  $J_{\text{th}}$  is found according to  $G_M(J_{\text{th}}) = \alpha_M + \alpha_W$ , where  $\alpha_M$  and  $\alpha_W$  are the mirror and waveguide losses, respectively.

Fig. 2 shows the calculated electric field-current density characteristics at lattice temperatures of  $T_{\text{latt}} = 5$  K and 20 K for the terahertz QCL [14], with the electron temperature assumed equal to that of the lattice ( $T_e = T_{\text{latt}}$ ; (2) and (1) only), and, on the other hand, using the full-model calculation with the kinetic energy balance equation included (3). Under the assumption  $T_e = T_{\text{latt}}$ , the  $F - J$  curves show current density saturation and negative differential resistance (NDR) features at very low currents; i.e.,  $\sim 150$  A/cm<sup>2</sup> at 5 K, and  $\sim 350$  A/cm<sup>2</sup> at 20 K, which are not consistent with experimental results [13], [14]. Instead, measurements show only a small sensitivity of  $F - J$  on lattice temperature, which we indeed find with the full calculation, which includes the energy balance. The current is predicted to saturate at  $\sim 680$  A/cm<sup>2</sup> in reasonable agreement with that measured at  $\sim 820$  A/cm<sup>2</sup> [13], [14]. The discrepancy of about 20% is probably related to the fact that we have restricted consideration to a 13-level system, i.e., the parasitic leakage currents from the injector to higher states are neglected. For example, those could be up to 30% of total current density under the higher field/higher current operating conditions in mid-infrared QCLs [22]. The average electron temperature are also shown in Fig. 2.  $T_e$  increases from the lattice temperature, under very low injection, up to  $\sim 60$  K when the NDR occurs. The electron temperatures are more sensitive to the current density than in mid-infrared devices [21]. This is due to the fact that electron–electron scattering is by far the fastest scattering mechanism in terahertz QCLs, with their relatively small spacing between states. Therefore, the inelastic electron-LO phonon scatterings, which couples electron distributions to the lattice heat bath, does not manage to cool electrons as efficiently as in mid-infrared devices. The calculations

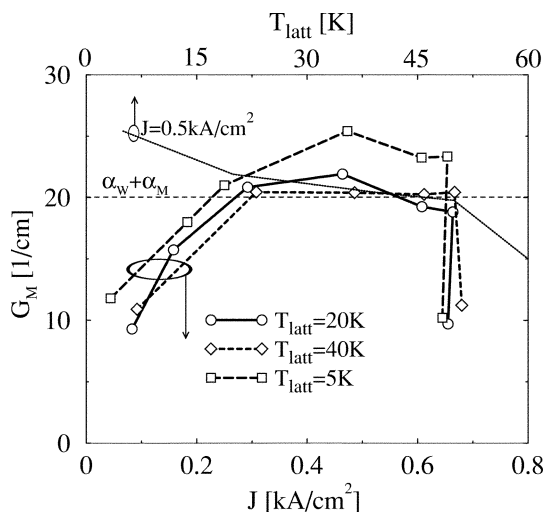


Fig. 3. Calculated modal gain versus current density dependence at cryogenic temperatures (bottom axis) and modal gain versus lattice temperature dependence for specific near optimal current density of  $J = 500$  A/cm<sup>2</sup> (top axis). The horizontal dashed line denotes the total losses ( $\alpha_M + \alpha_W \approx 20$  cm<sup>-1</sup>) [14].

also show that  $T_e$  has a prominent second-order dependence on current density, and can be written (up to the NDR feature) as  $T_e \approx T_{latt} + \alpha_1 J + \alpha_2 J^2$ , where  $\alpha_1 \sim 27$  K/(kAcm<sup>-2</sup>), and  $\alpha_2 \sim 35$  K/(kAcm<sup>-2</sup>)<sup>2</sup>.

In Fig. 3 the modal gain versus current density dependence (bottom axis) at lattice temperatures of 5 K, 20 K, and 40 K is calculated with  $\lambda = 70$   $\mu$ m,  $\underline{n} = 3.28$ ,  $\Gamma = 0.47$ ,  $L_p = 104.9$  nm, and  $2\gamma_{97} = 2-2.2$  meV [13]. In accordance with the experimentally obtained losses [14] from the intersection points of the total loss line  $\alpha_M + \alpha_W \approx 20$  cm<sup>-1</sup> and the  $G_M(J)$  lines, we obtain threshold currents  $J_{th} = 250-300$  A/cm<sup>2</sup>, in good agreement with experiment [14]. The structure starts to loose optical power quite abruptly at about  $\sim 650$  A/cm<sup>2</sup>, also in accordance with experimental findings, i.e., close to the saturation of the injected (nonparasitic) current. The modal gain versus lattice temperature for a near optimal current density  $J = 500$  A/cm<sup>2</sup> is also given in Fig. 3 (top axis). The model predicted that the laser is able to run up to  $\sim 50$  K which is close to the experimental maximum of  $\sim 55$  K [14].

In summary, we have used a fully self-consistent rate equation method for modeling carrier dynamics in terahertz QCLs. The results from the model are in very good agreement with experimental data. The calculations show large sensitivity of the electron temperature to the injection current, a fact that must be controlled through improved/optimized structure design to achieve high temperature operation of terahertz lasers.

#### ACKNOWLEDGMENT

The authors would like to thank A. Tredicucci and R. Köhler, from NEST-INFM and Scuola Normale Superiore in Pisa, Italy, for useful discussions and communicating their results before publication.

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