Design and Simulation of THz Quantum Cascade Lasers

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Strategies and concepts for the design of THz emitters based on the quantum cascade scheme are analyzed and modeled in terms of a fully three-dimensional Monte Carlo approach; this allows for a proper inclusion of both carrier-carrier and carrier-phonon scattering mechanisms. Starting from the simulation of previously published far-infrared emitters, where no population inversion is achieved, two innovative designs are proposed. The first one follows the well-established chirped-superlattice scheme whereas the second one employs a double-quantum well superlattice to allow energy relaxation through optical phonon emission. For both cases a significant population inversion is predicted at temperatures up to 80 K.

Since the first demonstration of the Quantum Cascade (QC) laser in 1994, its performance has experienced tremendous improvement, and the range of emission has been continuously extended. At present, the longest wavelength QC lasers operate at \( \lambda \sim 21.5 \mu m \) and 24 \( \mu m \), still above the LO-phonon energy threshold of the host material \( \hbar \omega_{LO} \sim 34 \text{ meV} \) in InGaAs, \( \hbar \omega_{LO} \sim 36 \text{ meV} \) in GaAs). Although lasing at longer wavelength has not been observed yet, electroluminescence in the THz region of the spectrum has already been detected from a variety of QC structures as well as from other quantum well devices, stimulating a number of theoretical proposals. These strong efforts aimed at fabricating a THz semiconductor laser are mainly driven by the lack of compact, convenient solid-state sources operating at THz frequencies, despite the many possible applications in wireless communications, medical imaging, security screening, etc.

As prototypical design for THz emitters, we shall consider the GaAs/AlGaAs QC structure proposed by Rochat et al. This can be regarded as a scaled down version of the conventional mid-infrared QC design, based on a vertical optical transition (see Fig. 1 in Ref. 3 for its band diagram). This implementation is characterized by a narrow injector miniband, chosen to avoid scattering of electrons from the upper state through LO-phonon emission and cross-absorption of the emitted light. Moreover, it features a relatively small electron tunneling between the states in the active region and in the injector. As stressed before, while electroluminescent devices were reported by several groups, to date no population inversion could be achieved. In fact, several problems inherent to this design undermine the functionality of the structure. First, the width of the miniband forbids the use of LO-phonon emission as the main mechanism to deplete the lower state of the lasing transition. Second, the small miniband dispersion and low tunneling probability also restrict efficient electrical transport to a narrow range of currents and voltages, limited by the onset of negative differential resistance. Third, the small energy separation between the levels in the active region and the quasi-Fermi level of the injector electrons makes the device very sensitive to hot-carrier effects (‘backfilling’ of the upstream active region).

In order to gain a better understanding of these limiting factors, we have applied a global simulation scheme, recently proposed in Refs. 14, 15, to the prototypical structure of Rochat et al. Such a technique consists of a Monte Carlo sampling of a coupled set of fully three dimensional (3D) Boltzmann-like equations. To properly model energy relaxation as well as carrier thermalization, we included both carrier-phonon \( (c-p) \) and carrier-carrier \( (c-c) \) interaction mechanisms. Thanks to periodic boundary conditions, we are able to get the device current-voltage characteristics as well as its gain spectrum without resorting to phenomenological parameters.

At 80 K, under the design electric field of 2.7 kV/cm and assuming a sheet density of 1.2 \( \times 10^{10} \text{ cm}^{-2} \), our simulated experiments give an electron density in the upper laser level 2 of about 8 \( \times 10^{9} \text{ cm}^{-2} \), compared to the 3.5 \( \times 10^{9} \text{ cm}^{-2} \) in the lower state 1. These values are far from the transparency condition of the intersubband transition, as already inferred from experimental data. This is not a consequence of rapid non-radiative depopulation of state 2 but rather of a slow extraction of electrons from level 1 into the downstream injector region. Indeed our simulation shows rather a long lifetime \( \tau_2 = 2.2 \text{ ps} \), mainly determined by \( c-p \) interactions.
scattering of electrons with high in-plane momentum to subband 1 ($\tau_{21} = 2.7$ ps). On the other hand for level 1 we compute a significantly longer lifetime $\tau_1 = 14.5$ ps resulting from almost comparable $c$-$c$ and $c$-$p$ contributions. In reality, the electron dynamics is dominated by very fast $c$-$c$ scattering with a quasi-resonant level (1’ in Ref. 7). However, such a process acts in both directions ($1 \rightarrow 1'$ and $1' \rightarrow 1$) with nearly equal rates, thus giving only a marginal contribution to the electron depletion of state 1. From the simulation we also obtain the value of the operational current density, 500 A/cm$^2$, in very good agreement with the measured one at this bias field.

Starting from these considerations we have designed two structures tuned for emission at $\lambda \sim 69$ μm that can overcome the limitations associated with the above prototypical design. Both structures are based on a vertical-transition configuration, which is known to lead to larger dipole matrix elements and narrower linewidths. The first scheme employs a conventional chirped-superlattice design[7], which allows flat minibands in the active region without requiring large concentrations of dopants. The band diagram under an average applied electric field of 3.5 kV/cm is shown in Fig. 1. Its operating strategy is based on the same concepts successfully implemented for $\lambda \sim 17 - 24$ μm QC lasers[6, 8, 7]. In order to minimize the density of electrons in the lower laser subband 1 we employ a dense miniband with seven subbands, which provides a large phase space where electrons scattered either from subband 2 or directly from the injector can spread. The miniband dispersion is chosen as large as possible compatibly with the need of avoiding cross-absorption. This suppresses thermal backfilling, and provides a large operating range of currents and voltages. Also in this structure, however, energy relaxation within the first miniband appears to be hindered by the lack of final states with appropriate energy to allow for LO-phonon emission. Nevertheless, carrier-carrier interactions may beneficially operate as an activation mechanism, which can provide sufficient in-plane momentum for the electrons to open a scattering path via optical phonon emission at THz frequencies[21].

Considering the dipole matrix element of 7.8 nm and 4.5 nm computed for the optical transitions in the two structures, respectively, and assuming a linewidth of 2 meV as experimentally detected at similar wavelengths[6], we estimate, on the basis of the above populations, gain coefficients of about 31 cm$^{-1}$ and 110 cm$^{-1}$. These values compare favorably to the optical losses (approximately 50 cm$^{-1}$) measured in double-surface plasmon waveguides at THz frequencies[21], and indicate that laser action with such active region designs is a realistic goal.

In summary, we have proposed two QC structures designed for THz lasing. Our theoretical analysis of their performance is based on a global simulation scheme
which allows for a proper inclusion of the most relevant scattering mechanisms. The proposed designs both exhibit significant population inversion up to 80 K. This, together with the large transition dipoles, is expected to lead to high optical gain. Finally, it should be noted that our simulation predicts current densities of more than 1 kA/cm\(^2\) which is roughly one order of magnitude higher than the current density measured in the prototypical design of Ref. 8 before the onset of negative differential resistance. We attribute this effect to the improved carrier relaxation and higher tunneling efficiency of our structures.

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[1] J. Faist, F. Capasso, D. L. Sivco, C. Sirtori, A. L. Hutchinson, A. Y. Cho, Science 264, 553 (1994).
[2] F. Capasso, C. Gmachl, R. Paiella, A. Tredicucci, A. L. Hutchinson, D. L. Sivco, J. N. Baillargeon, A. Y. Cho, H. C. Liu, IEEE J. Select. Topics Quantum Electron. 6, 931 (2000).
[3] D. Hofstaetter, M. Beck, T. Aellen, J. Faist, U. Oesterle, M. Illegems, E. Gini, H. Melchior, Appl. Phys. Lett. 78, 1964 (2001).
[4] J. Faist, F. Capasso, D. L. Sivco, S. N. G. Chu, A. Y. Cho, Appl. Phys. Lett. 72, 680 (1998).
[5] A. Tredicucci, C. Gmachl, F. Capasso, D. L. Sivco, A. L. Hutchinson, A. Y. Cho, Appl. Phys. Lett. 74, 638 (1999).
[6] A. Tredicucci, C. Gmachl, M. C. Wanke, F. Capasso, A. L. Hutchinson, D. L. Sivco, S. N. G. Chu, A. Y. Cho, Appl. Phys. Lett. 77, 2286 (2000).
[7] R. Colombelli, F. Capasso, C. Gmachl, A. L. Hutchinson, D. L. Sivco, A. Tredicucci, M. C. Wanke, A. M. Sergent, A. Y. Cho, Appl. Phys. Lett. 78, 2620 (2001).

TABLE I: Population of the individual levels in the 'chirped' SL, calculated at 80 K with only carrier-phonon (c-p) scattering and with both c-p and carrier-carrier (c-c) scattering. Letters refer to the injector states comprising the first miniband in Fig. 1. g represents the injector ground state while capital letters label the other levels in ascending order.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Subband & Energy & Pop. (c-p only) & Pop. (c-p & c-c) \\
index & (meV) & \text{\times 10^{9} \text{cm}^{-2}} & \text{\times 10^{10} \text{cm}^{-2}} \\
\hline
3 & 51.7 & 0.02 & 0.06 \\
2 & 36.1 & 0.94 & 3.99 \\
1 & 17.9 & 4.72 & 2.83 \\
F & 14.1 & 7.13 & 4.72 \\
E & 11.0 & 8.08 & 6.08 \\
D & 7.7 & 7.34 & 5.45 \\
C & 4.5 & 5.14 & 5.98 \\
B & 3.2 & 1.99 & 4.62 \\
g & 0 & 6.19 & 7.87 \\
\hline
\end{tabular}
\end{table}

TABLE II: Population of the individual levels in the DQW SL, calculated at 80 K with only carrier-phonon (c-p) scattering and with both c-p and carrier-carrier (c-c) scattering. Subbands are named with the same convention as in table I.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
Subband & Energy & Pop. (c-p only) & Pop. (c-p & c-c) \\
index & (meV) & \text{\times 10^{9} \text{cm}^{-2}} & \text{\times 10^{10} \text{cm}^{-2}} \\
\hline
2 & 63.4 & 0.27 & 1.22 \\
1 & 45.5 & 0.07 & 0.46 \\
E & 42.6 & 0.02 & 0.27 \\
D & 37.1 & 0.05 & 0.27 \\
C & 28.7 & 0.27 & 0.27 \\
B & 9.2 & 1.22 & 1.16 \\
A & 5.9 & 0.82 & 1.43 \\
g & 0 & 5.24 & 2.99 \\
\hline
\end{tabular}
\end{table}

[19] M. C. Wanke, F. Capasso, C. Gmachl, A. Tredicucci, D. L. Sivco, A. L. Hutchinson, S. N. G. Chu, A. Y. Cho, IEEE Photon. Technol. Lett. 13, 278 (2001).
FIG. 1: Conduction band energy diagram of the 'chirped' superlattice under an average electric field of 3.5 kV/cm. The layer thickness (in nm) are, from left to right, starting from the injection barrier 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, where Al$_{0.15}$Ga$_{0.85}$As layers are in bold face and the 10.2 nm wide GaAs well is doped $4 \times 10^{16}$ cm$^{-3}$. Also shown are the moduli squared of the wavefunctions; the optical transition occurs between states 2 and 1.

FIG. 2: Conduction band energy diagram of the DQW-SL under an average electric field of 8.7 kV/cm. The layer thickness (in nm) are, from left to right, starting from the injection barrier 3.5/6.8/1.7/6.4/2.5/7.9/0.6/7.5/2.0/6.8/1.0/6.5/2.0/5.9, 1.4/5.5, where Al$_{0.3}$Ga$_{0.7}$As layers are in bold face and doped ($6 \times 10^{16}$ cm$^{-3}$) GaAs layers are underlined. The Al concentration in this design, and thus the barrier height, is raised compared to the previous design in order to better accommodate the split miniband.