Nonequilibrium Green's function simulations of THz quantum cascade lasers

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We simulate THz quantum cascade lasers (QCLs) [1] with the nonequilibrium Green's function (NEGF) method [2][3], in which relevant observables, such as the energy resolved carrier density

$$\rho(z,E)=\sum_{\mathbf{k}}\sum_{\alpha,\beta}\Im\left\{G^{<}_{\alpha,\beta}(\mathbf{k},E)\phi^{*}_{\beta}(z)\phi_{\alpha}(z)\right\}$$

are expressed in terms of the Green's functions of the system, in this case the lesser Green's function $G^{<}$, and the basis wavefunctions with z-component $\phi_{\alpha}(z)$. The NEGF method allows for a detailed analysis of the transport, since the spatially and energy resolved carrier and current densities, as well as the density of states, can be obtained from the Green's functions.

Fig. 1 shows the conduction band edge, the Wannier-Stark states, and the carrier densities of the THz QCL from Ref. [4]. The simulated and measured current densities are shown in Fig. 2.

This phonon-photon-phonon (PPP) design [5] relies on two phonon resonances (with energy E_{LO}) occuring between the lower laser state (LLS) and the extraction state e (with splitting $\Delta E_{\mathrm{LLS,e}}$), as well as between the injection state i and the upper laser state (ULS) (with splitting $\Delta E_{\mathrm{i,ULS}}$) at a bias where i and e also align. These phonon and tunneling resonances create population inversion between the ULS and LLS, which allows for a lasing transition between those states.

The carrier densities in Fig. 1 show that carriers accumulate in the LLS due to the mis-match between $\Delta E_{\mathrm{LLS,e}}$ and E_{LO}, as well as in e, which is due to the thick injection barrier. Had this barrier been more narrow, the tunneling coupling at higher biases would be larger, meaning that biases where $\Delta E_{\mathrm{LLS,e}}$ and $\Delta E_{\mathrm{i,ULS}}$ are better aligned to E_{LO} could be reached.

The design in Fig. 3, described in Ref. [6], is an improvement of the one previously discussed, albeit $\Delta E_{\mathrm{LLS,e}}$ does not match E_{LO} either. The current density is peaked at a bias greater than the bias of the tunneling resonance i/e, since both $\Delta E_{\mathrm{LLS,e}}$ and $\Delta E_{\mathrm{i,ULS}}$ are better matched to E_{LO}. We identify the lack of mean field potential in the rate equation (RE) model used for design optimization as one of the causes for the mis-match of the resonances. In contrast, the NEGF model takes mean field and the real part of the self energies into account, which alters the energy levels and thus the bias at which different phonon and tunneling resonances occur.

As temperature increases, inversion decreases due to thermal backfilling from e to LLS as well as from ULS to i. A better matching of the biases giving tunneling and phonon resonances respectively, would reduce the backfilling and increase the population inversion.

The simulated gain profile and experimental laser spectra are shown in Fig. 4.

CONCLUSION

The experimental current densities as well as gain profiles of two THz QCLs have been reproduced with the NEGF model. The results for the gain spectra are significantly better than with a simple RE model. The energetically and spatially resolved transport dynamics suggest improvements of the design.

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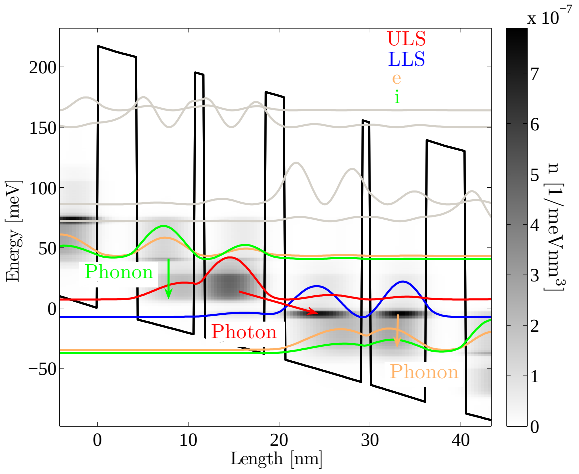

Fig. 1. Carrier densities and electronic states for the structure presented in Ref. [4], at operation bias. $T = 50$ K. The carriers accumulate in the LLS since the extraction energy does not match E_{LO}.

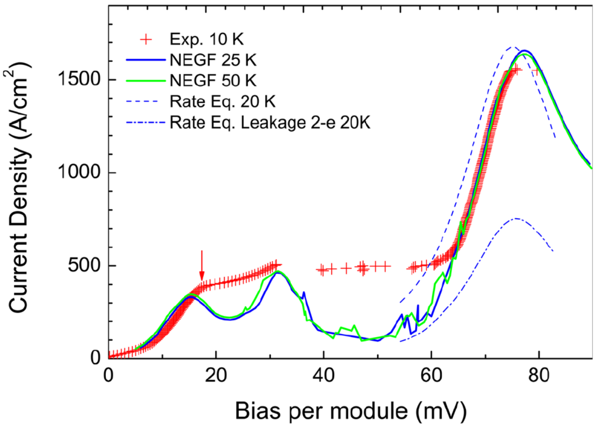

Fig. 2. Current density of the structure in Ref. [4] as a function of applied bias. Even though the rate equation model predicts the behaviour well, the NEGF is better in predicting the correct lasing frequency at different biases and identifying effects such as leakage currents and dispersive gain. Figure from Ref. [4].

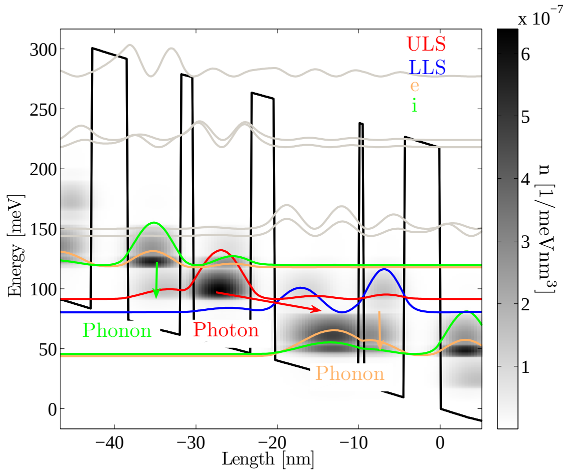

Fig. 3. Carrier densities and electronic states for the structure presented in Ref. [6] at operation bias. $T = 50$ K. Carriers accumulate in the injection and extraction states since the injection energy is not matched to E_{LO}, and the e/i states are not aligned to a high degree at this bias.

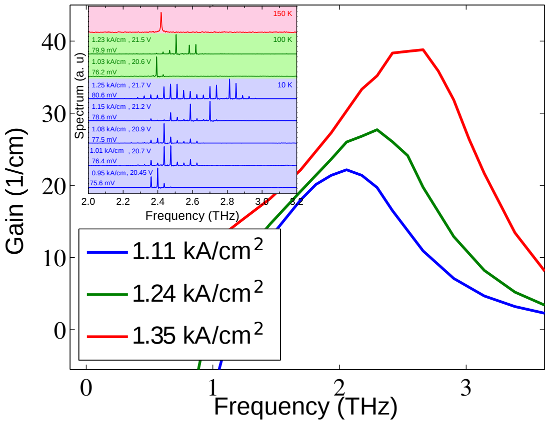

Fig. 4. NEGF simulated gain profile at T = 50 K of the structure presented in Ref. [6]. The inset shows experimental results. The qualitative agreement is good, showing a similar reduction of the laser frequency as bias is decreased from the bias of the maximum of the current density. The NEGF model also gives very similar lasing frequencies as seen experimentally.