Journal of Physics: Conference Series **193** (2009) 012062 doi:10.1088/1742-6596/193/1/012062

Importance of Coulomb interactions in bound-to-continuum THz quantum cascade lasers

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Abstract. We demonstrate the importance of Coulomb interactions in bound-to-continuum THz quantum cascade lasers, employing an ensemble Monte-Carlo analysis. In such structures, the electron-electron interactions between the closely spaced energy levels in the minibands tend to play a more important role than in resonant-phonon depopulation designs, where the energy levels are more energetically separated and LO phonon scattering prevails. Also a significant conduction band bending due to space charge effects is observed. Thus, especially for bound-to-continuum structures careful modelling of Coulomb interactions is crucial to obtain good agreement with experiment.

1. Introduction

THz quantum cascade lasers (QCLs) are commonly based either on the bound-to-continuum (BTC) or the resonant-phonon (RP) design. BTC structures feature closely spaced energy levels forming so-called minibands. In RP designs, the depletion transition is tuned to the longitudinal-optical (LO) energy to achieve efficient depletion of the lower laser level, and also the other energy levels tend to be more energetically separated. While the transport in such structures is (at least for elevated temperatures) governed by LO phonon scattering, Coulomb interactions play a pronounced role for the carrier transport in BTC designs and also lead to significant conduction band bending [1, 2, 3]. Thus, a careful modeling of Coulomb interactions is crucial especially for BTC devices. In the following, we focus on investigating the influence of Coulomb interactions in THz BTC QCLs, using an ensemble Monte-Carlo (EMC) transport simulation. Some widely-used approximations and assumptions which work fine for THz RP structures are shown to lead to erroneous results for THz BTC QCLs.

2. Method

Coulomb interactions in QCLs are due to the attraction or repulsion of charges in the structure, i.e., the interaction of electrons with other electrons and ionized impurities. In our simulation, this effect is considered in two ways [3, 4]: The quantized energy levels and wavefunctions are determined by solving the coupled Schrödinger-Poisson (SP) system to account for mean field effects. Here, the Coulomb interactions manifest themselves as space charge effects, leading to a conduction band bending. Furthermore, the electron-electron (e-e) and electron-impurity (e-i) interactions enter the

EMC transport simulation in the form of corresponding scattering events, which are evaluated based on Fermi's golden rule.

The EMC method allows for a self-consistent carrier transport and optical gain analysis [3]. As discussed above, the coupled Schrödinger-Poisson system is solved to obtain the quantized energy levels, based on which the carrier transport simulation is self-consistently performed. All essential scattering mechanisms (acoustic and LO phonons, e-e and e-i scattering, interface roughness) are included, and the Pauli exclusion principle is accounted for, as well as hot phonon effects [3, 4]. For e-e scattering, screening and spin effects are taken into account [5]. The evaluation of e-e scattering is much more computationally demanding than single-electron processes like electron-phonon interactions and thus has, up to now, not been included in comparable quantum mechanical simulations of QCLs [6, 7]. Since the quantized energy levels obtained by the SP solver depend on the space charges (i.e., the electron distributions obtained from EMC) and the EMC simulation is in turn based on these quantized energy levels, both simulations have to be performed iteratively until convergence of the carrier distribution as well as the conduction band bending is obtained, yielding so-called self-self-consistent solutions [1].

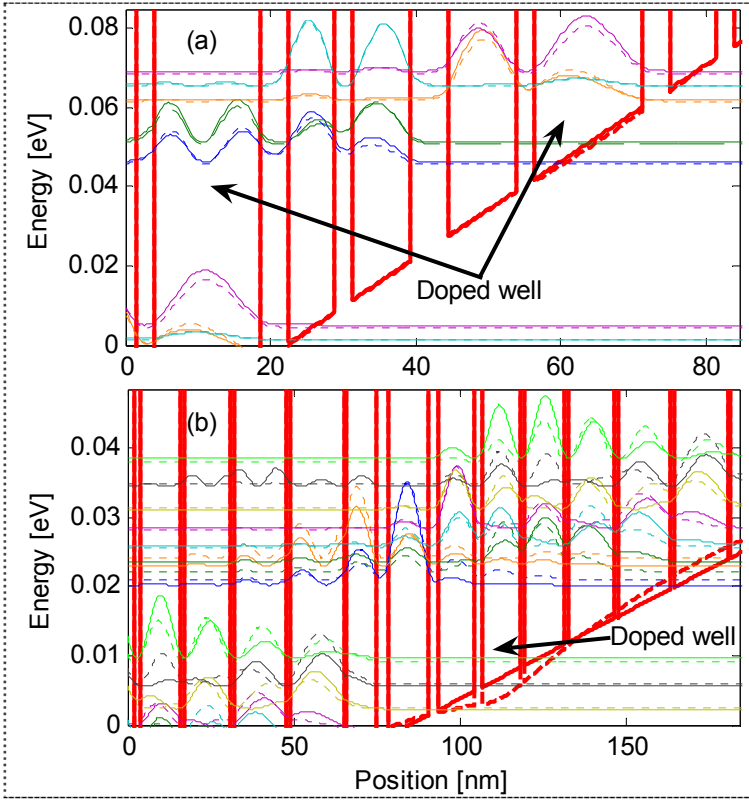

Figure 1. Conduction band profile and probability densities for space charge effects neglected (i.e., disabled Poisson solver) (solid lines) and a self-self-consistent simulation (dashed lines). (a) RP structure at 12.25 kV/cm and 30 K. (b) BTC structure at 2.5 kV/cm and 30 K.

3. Results

3.1. Influence of space charges

In figure 1, the conduction band profile and the probability densities of the quantized energy levels are displayed for the two investigated QCLs, a 3.4 THz RP design (figure 1(a)) [8] and a 3.5 THz BTC design (figure 1(b)) [9]. We see that the conduction band bending due to space charge effects plays a secondary role in the investigated RP structure, while this effect is quite pronounced in the BTC design, although the doping level is comparable in both structures. Here, multiple iterations of SP and EMC simulation are necessary to obtain self-self-consistent solutions.

In the following, we investigate to what degree these space charge effects, leading to modified energy levels and wavefunctions in the SP solver, influence the outcome of the carrier transport

analysis. Figure 2 shows the simulation results for the spectral gain profile of both the RP and BTC design. Here, a full EMC simulation is performed including all the scattering mechanisms, but space charge effects are considered with a varying degree of complexity. Shown are the results as obtained by completely neglecting space charge effects, i.e., disabling the Poisson solver, running the SP solver once in the beginning (assuming a thermal carrier distribution [2]) and then carrying out the EMC simulation, and iteratively performing the SP and EMC simulations until convergence is obtained. For the RP structure (figure 2(a)), the simulation results are relatively insensitive to space charge effects. In contrast, for the BTC structure (figure 2(b)), disabling the Poisson solver (dotted line) produces an almost vanishing gain, which is in clear contrast to the experimentally observed lasing of the structure [9]. This reflects the influence of space charge effects on the energy level alignment and the wave function shapes. Accounting for these effects (dashed and solid lines) produces realistic gain profiles centered around approximately 3.5 THz, in agreement with experiment. However, the exact shape of the gain profile is somewhat different for the non-iterative (dashed line) and iterative (solid line) approach, demonstrating the need of iterative SP and EMC simulations to obtain the self-self-consistent solution for such structures. The significant conduction band bending for the investigated BTC structure, shown in figure 1(b), is attributed to the fact that the positive charges due to the ionized dopants are concentrated in a single well per period, while the negative charges due to the electrons in the minibands are distributed across the whole period, leading to a pronounced net charge profile.

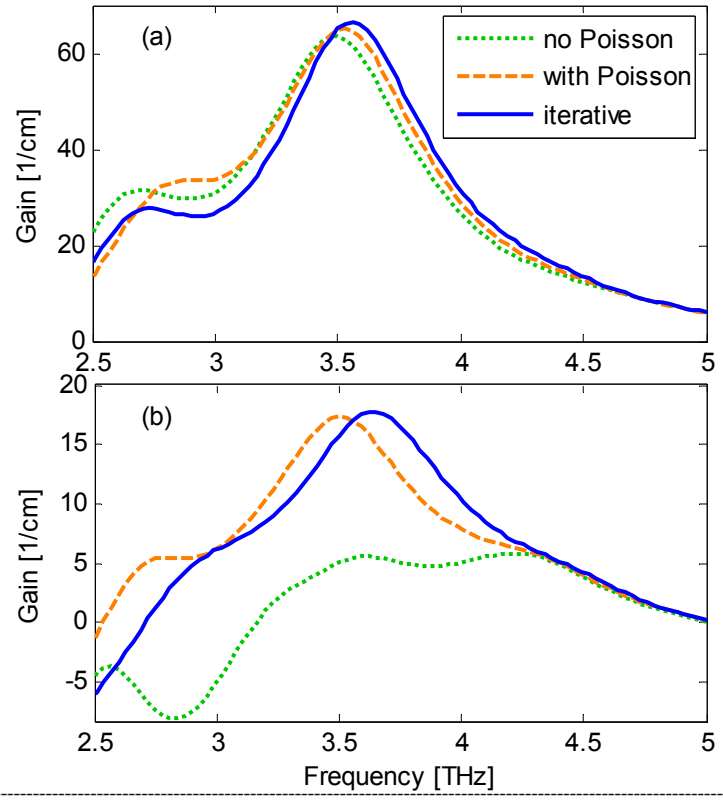

Figure 2. Simulated spectral gain versus frequency with disabled Poisson solver (dotted lines), running the Poisson solver once assuming a thermal carrier distribution (dashed lines), and a self-self-consistent solution obtained by iteratively running the SP and EMC simulations (solid lines). (a) RP structure at 12.25 kV/cm and 30 K. (b) BTC structure at 2.5 kV/cm and 30 K.

3.2. Influence of electron-electron scattering

As we have seen in the previous section, space charge effects have a quite strong influence on the investigated BTC structure. In the following, we investigate if e-e scattering, i.e., the inclusion of Coulomb interactions beyond the mean field approximation, also plays an important role for the simulation of such devices. This question is especially interesting from a simulation point of view: Since the evaluation of e-e scattering is by far the most computationally demanding scattering process,

it is usually neglected in quantum mechanical transport simulations of QCLs. This works well for RP structures, where good agreement with experiment is obtained [6,7]. Figure 3 shows the self-self-consistent EMC result for the BTC gain structure, now with e-e scattering taken into account as in figure 2 (solid line), and with e-e scattering neglected (dashed line). Omission of e-e scattering yields an unrealistic gain profile featuring two excessively narrowed spikes, demonstrating the significant role of this scattering process. Only the full simulation yields reasonable results. Specifically, the obtained gain bandwidth (full width at half-maximum) of 0.85 THz agrees very well with the experimental value of around 0.9 THz, deduced from electroluminescence measurements [9]. This shows that electron-electron scattering between the closely spaced energy levels in the minibands plays a pronounced role for the carrier transport in BTC designs.

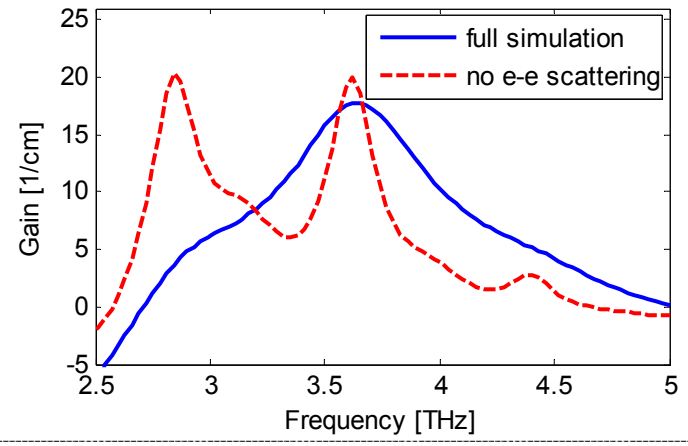

Figure 3. Simulated spectral gain versus frequency with (solid line) and without (dashed line) e-e scattering.

4. Conclusion

Employing an EMC analysis, we have investigated the importance of Coulomb interactions in THz quantum cascade lasers, and specifically THz BTC structures. Here, conduction band bending has a significant influence on the level alignment, calling for a self-self-consistent SP and EMC simulation. Also e-e scattering between the closely spaced energy levels in the minibands plays an important role and is the dominant gain broadening mechanism. The EMC analysis, where both effects can be adequately accounted for, is shown to yield meaningful results for the investigated BTC structure, which are in good agreement with experiment.

Acknowledgments

C.J. and A.M. acknowledge support from the Emmy Noether program of the German Research Foundation (DFG, JI115/1-1).

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