Validating Simple Approaches for Quantum Cascade Laser Modeling

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The quantum cascade laser (QCL) is an intersubband-based light source operating in a wide range of wavelengths from the THz to mid-IR. In order to improve their performance and broaden their usage in general, much effort is put into simulating these devices. Recently, genetic algorithms have been employed for optimization[1], [2], [3]. As the number of parameters affecting the transport is large, an efficient model is necessary. At the same time, the model has to treat the complex many-body problem sufficiently detailed to avoid un-physical results.

Three classes of simulation models are mainly used for the simulation of QCLs. A rate equation (RE) model [4] uses scattering rates between subbands calculated via Fermi's golden rule, in order to give quick estimates of the level populations. Here, coherences between near-degenerate states have to be included as a tunneling rate. The transport problem is then solved via the Schrödinger equation. Density matrix (DM) approaches [5], [6], [7] in addition include coherences in the off-diagonal elements of the density matrix. Both RE and DM models assume thermalized sub-bands where the momentum-dependence is averaged out. In contrast, the non-equilibrium Green's function (NEGF) theory [8] includes inter-subband scattering and treats the many-body problem consistently. The Green's functions of the system are calculated via a set of self-consistent equations involving the scattering via self-energies. The theory is formulated as a perturbation expansion, where the expansion series is truncated at a suitable point. Thus, the NEGF is the most general of these models, and provides the most information.

We have performed NEGF simulations of a THz [4] and a mid-IR QCL [9], and compared our results to RE and DM simulations. The THz sample simulations are shown Fig. 1. For this structure with scattering injection, both the RE and NEGF models agree excellently with the experimental results. Similar results were also found for a similar structure [1].

A detailed comparison between NEGF and two DM models was performed in Ref. [10], where the main results are summarized in Fig. 2. Here it was found that in order for the DM model to produce reliable results, so-called second order currents have to be considered, which are naturally included in the NEGF model; for these tunneling injection designs, a higher sophistication is needed. Although the gain is quite different in the NEGF and DM models, they do predict very similar output powers and currents under irradiation so that they are indiscernible with the experimental data available.

Our findings show that simple approaches can be used if the relevant features are properly accounted for. In this context a fully self-consistent model like NEGF is a good tool for validating different approximations.

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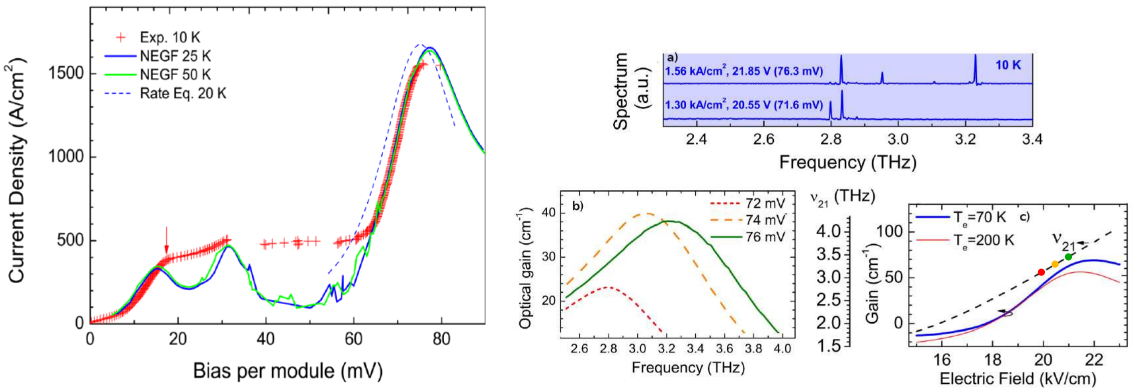

Fig. 1. Data taken from Ref. [4]. Left: Current density for the RE and NEGF models, as well as the experimental sample. Right: laser spectrum (a), NEGF gain simulations (b), and RE gain simulations (c). The colored circles in (c) indicate the points which correspond to the biases used in (a) and (b).

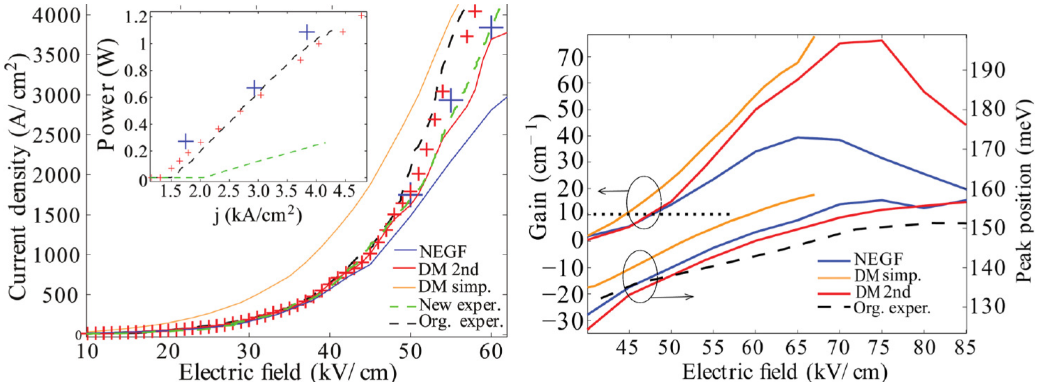

Fig. 2. Data taken from Ref. [10]. Left: Current density in the NEGF, two DM models, as well as experimental data, where crosses show current densities under irradiation. The inset shows the simulated and experimental radiated output power. Right: Gain and gain peak positions in the DM and NEGF models.