Simulation of a midinfrared quantum cascade laser using a density-matrix formalism

O Jonasson and I Knezevic

University of Wisconsin-Madison, USA

Quantum cascade lasers (QCLs) are intra- subband light-emitting sources in the midinfrared and THz parts of the electromagnetic spectrum. The core of the QCL (the gain medium) is a vertically grown semiconductor heterostructure consisting of an alternating arrangement of quantum wells and barriers with a typical layer width of a few nanome- ters [1]. In this work, we propose a computationally efficient density-matrix model capable of describing quantum transport in QCLs. The model is based on a Markovian master equation for the single-electron density matrix that conserves the positivity of the density matrix and includes full in-plane dynamics.

Existing simulation methods for electron trans- port in QCLs in include semiclassical methods (rate equations [2] and Monte Carlo [3]) and quan- tum techniques (density matrix [4], [5], [6] and nonequilibrium Green's functions (NEGF) [7], [8]). Semiclassical methods are advantageous because of their low computational cost, but can fail when off-diagonal density-matrix (DM) elements (coher- ences) are similar in size to the diagonal ones [9]. While NEGF simulation can capture quantum trans- port in QCLs, they are computationally intensive, especially for short-wavelength devices, where a large range of energies are involved. Density-matrix models offer a compromise, as they can describe coherent-transport features with lower computa- tional overhead than NEGF.

Previously proposed density-matrix models have drawbacks that are avoided in this work. One draw- back is the assumption of thermalized subbands with electron temperature as an input parameter [6], [10]. This approximation is not warranted far from equilibrium, when the in-plane energy distribution deviates far from a heated thermal distribution. A second drawback with existing DM models is the phenomenological treatment of dephasing across thick potential barriers, where transport is treated semiclassically within a subregion of a QCL (typically a single stage) and coupling between stages is treated using phenomenological dephas- ing times [6], [10]. We present a computationally tractable density-matrix model that makes neither of the aforementioned simplification.

In order to verify our model, we simulated QCL based on the InGaAs/InAlAs material system emit- ting around 8.5 μm [11]. We chose this specific device because it has previously been successfully modeled using the NEGF formalism [10], enabling us to compare our results to both both experimental and theory. Figure 1 shows the bandstructure at a field strength of 52 kV/cm, which is slightly above threshold. The bandstructure is calculated using a 3-band $\mathbf{k} \cdot \mathbf{p}$ model that includes the conduction band, light-hole band and the spin split-off band. The upper (lower) lasing level is labeled as 8 (7) and the lowest-energy injector state is 1.

Figure 2 shows the current density vs electric field calculated using our density-matrix model, along with comparison with experiment and the- oretical results using the NEGF formalism. Our results are in excellent agreement with NEGF for all considered fields. Our results are also in good agreement with experiment up to threshold (denoted by vertical dashed lines). Note that our model does not include the laser electromagnetic field, so we do not expect to reproduce current density far above threshold.

Figure 3 shows our theoretical results for the peak optical gain, as well as a comparison with NEGF [10]. The estimated threshold gain from experiment E1 is denoted by a horizontal dashed line. We see that our results are in fairly good agreement with NEGF for fields up to 60 kV/cm, while for higher fields, we predict higher gain. From

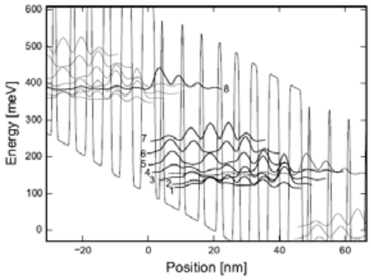

Fig. 1. Conduction-band edge (thin black curve) and probability densities for the 8 eigenstates used in calculations (bold curves). States belonging to neighboring periods are denoted by thin gray curves. States are numbered in increasing order of energy, starting with the ground state in the injector. The length of one period is 44.9 nm, with a layer structure (in nanometers), starting with the injector barrier (centered at the origin) **4.0**/1.8/**0.8**/5.3/**1.0**/4.8/**1.1**/4.3/**1.4**/3.6/**1.7**/3.3/**2.4**/3.1/**3.4**/2.9, with barriers denoted bold. Underlined layers are doped to 1.2×10^{17} cm^{-3}.

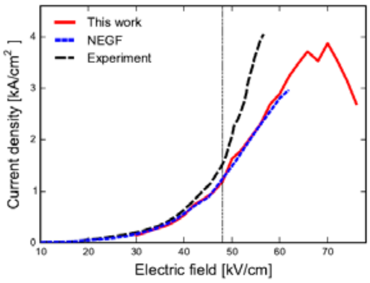

Fig. 2. Current density vs electric field. Shown are theoretical results based on this work, as well as results based on NEGF [10]. Experimental results from Ref. [11] are aslo shown. Experimentally determined threshold field of 48 kV/cm is denoted by the dashed vertical line.

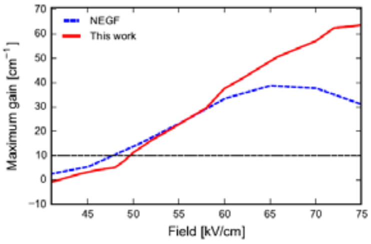

Fig. 3. Peak gain vs electric field, based on this work (solid red) and NEGF (dashed blue). The dashed horizontal line denotes the estimated threshold gain of 10 cm^{-1}.

the data presented in Figs. 2 and 3 we geta threshold field of E_{th} = 49.5 kV/cm and threshold current density of J_{th} = 1.53 kA/cm^2, which is close to the experimentally determined values of E_{th} = 48.0 kV/cm and J_{th} = 1.50 kA/cm^2. The results are also in fairly good agreement with the NEGF results (E_{th} = 47.6 kV/cm and J_{th} = 1.20 kA/cm^2).

In conclusion, we have proposed a density-matrix model based on a Markovian master equation that preserves positivity and includes full in-plane dy- namics. We compared our results with experiment, as well as a theoretical results based on the more computationally demanding NEGF formalism. We obtained excellent agreement with experiment and NEGF for the current density and fair agreement with the calculated optical gain.

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