User-friendly Software for the Simulation of Quantum Cascade Lasers with the NEGF Method

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Abstract

In this contribution, we present a new software for simulating the operation of quantum cascade lasers (QCLs) [1]. We have implemented an advanced nonequilibrium Green's functions (NEGF) algorithm [2] into the nextnano software package. Experimentalists can use this software in a straightforward way to understand, design and optimize QCL active regions.

1. Introduction

A detailed understanding of carrier dynamics is crucial for the design and improvement of complex semiconductor heterostructures such as QCLs. A powerful method for simulating nanoelectronic devices is provided by the NEGF formalism [3]. It captures the tight interplay between incoherent relaxation processes and quantum interference effects and has been applied very successfully to QCLs [4, 5]. Yet, up to now, the complexity of the underlying NEGF formalism has prevented its broad application in the QCL community. Here, we present a software with a user-friendly interface and without any needed prerequisite in the underlying NEGF formalism.

2. Results

Our accurate implementation of the NEGF method involves the self-consistent solution of the charge carrier quantum dynamics, scattering processes, and electrostatic effects (Poisson equation). Scattering processes are calculated based on accurate microscopic modeling, including optical and acoustic phonons, charged impurities, interface roughness, and alloy disorder. From the steady-state Green's functions, the software outputs the local density of states $\rho(x,E)$ (Fig. 1), the energy-resolved charge density $n(x,E)$ (Fig. 1) and current density $j(x,E)$ (Fig. 2). Finally, the gain spectrum, as well as energy and position resolved optical gain

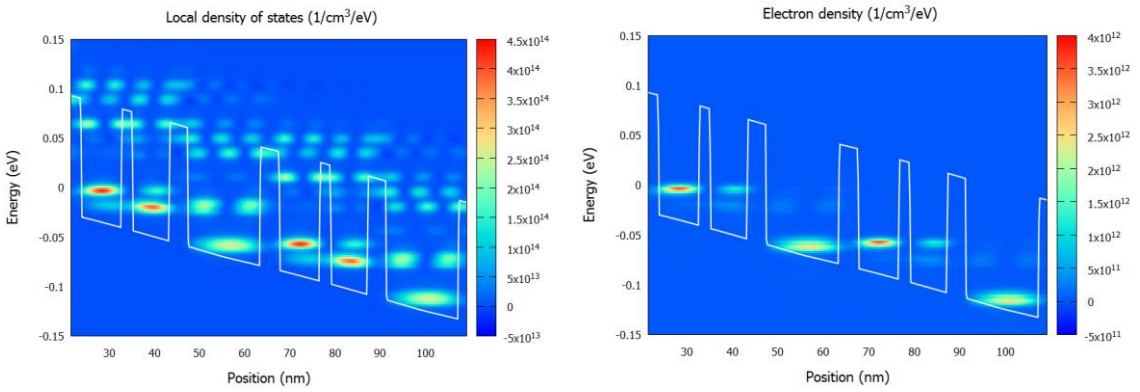

Fig. 1: Local density of states $\rho(x,E)$ (left), and energy resolved electron density $n(x,E)$ (right)

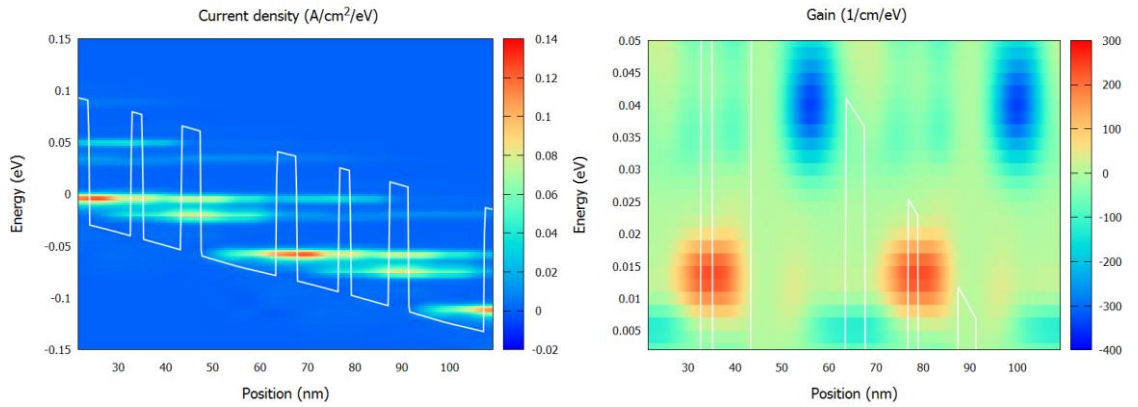

Fig. 2: Energy resolved current density $j(x,E)$ (left), and energy resolved optical gain $\alpha(x,E)$ (right)

$\alpha(x,E)$ are calculated (Fig. 2) in a self-consistent way. The figures show screenshots of the software package for an AlGaAs/GaAs THz QCL design [6] at an applied electric field of 12.3 kV/cm, i.e. under lasing conditions.

By visualizing the local density of states (LDOS) $\rho(x,E)$, the QCL designer can see where, and at which energy, electron states are available. The electron density is obtained by occupying this LDOS with charge carriers using a nonequilibrium distribution. The energy and position resolved electron density $n(x,E)$ then reveals where, and at which energy, the electrons are located, i.e. which of the states are populated. One can then directly see if the condition of population inversion is fulfilled which is necessary for a laser to operate. The energy and position resolved current density $j(x,E)$ allows to visualize the interplay between coherent transport and scattering processes. In particular, it shows at which position and energy electrons are scattered, e.g. by LO phonon scattering processes. Finally, the position and energy resolved gain $\alpha(x,E)$ shows where, and at which photon energy, absorption and gain occur. For instance, one can easily identify parasitic absorption processes.

By making efficient use of these plots it becomes possible – even for nonexperts – to design and optimize QCLs by varying e.g. doping concentration and doping profiles, alloy concentrations, barrier and well thicknesses, materials and further parameters such as strain.

References

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