From single-stage to device-level simulation of coupled electron and phonon transport in quantum cascade lasers

Y.-B. Shi, S. Mei, and I. Knezevic
Department of Electrical and Computer Engineering, University of Wisconsin - Madison
1415 Engineering Dr, Madison, WI 53706-1691, USA
Email: yshi9@wisc.edu, knezevic@engr.wisc.edu

A critical challenge for quantum cascade lasers (QCLs) is achieving reliable room–temperature continuous–wave (RT-cw) operation at high powers required by many applications. However, the high operating lattice temperature, accompanied by the high electronic temperature, has a detrimental impact on the threshold current density, wall plug efficiency (WPE), and device reliability [1]. Therefore, fully understanding the coupled transport of electrons and phonons and connecting the insights to device performance metrics is critical for further developments of QCLs.

In QCLs, the high electric field and current density required for lasing pump considerable energy into the electronic system. The accelerated electrons can scatter with each other, with phonons, with layer interfaces, imperfections, or impurities. Among these possible scattering mechanisms, the electronic system relaxes its energy mainly through the emission of longitudinal optical (LO) phonons [3]. Owing to the low group velocities, LO phonons are not efficient at carrying the heat away, and act as a temporary energy storage system. The main lattice cooling mechanism is the anharmonic decay of LO phonons into acoustic (LA) phonons [4], and the high group velocities of LA phonons make them the primary heat carriers to transfer the energy, through the waveguide and substrate, to the heat sink. The electron–LO phonon interaction is fast process, with a time scale on the order of 0.1 ps, while the anharmonic decay of LO phonons into LA phonons is much slower and typically takes several ps [5]. As a result, the population of LO phonons is built up over time in the active core and their distribution is driven far from equilibrium [3], [5]. The abundance of nonequilibrium LO phonons will also feed back to the electronic transport by affecting LO phonon scattering rates. Therefore, both the electron and phonon subsystems are essential to laser characteristics.

Simulation of coupled electron and phonon transport in QCLs is a multiscale problem. The electron transport is confined in the active core consisting of many repeated stages, typically with a total thickness of several microns. In contrast, the only constraints for thermal transport are the thermal boundary conditions, as specified by the waveguide and mounting configurations, in a much larger spatial scale, typically several hundreds of microns. The large-scale thermal transport causes the lattice temperature in the active core to become stage dependent. Consequently, the periodic electron transport feature in the active core is no longer justified, since the electron-phonon scattering rate varies from stage to stage. The scale difference and the coupling between electron and phonon transport makes the simulation challenging, and a single-stage simulation, which most existing studies adopt, is not sufficient to accurately describe these processes.

Here, we present a multiscale simulation technique for coupled electron and phonon transport on the example of a 9 μm GaAs-based midinfrared (mid-IR) QCL [2]. The core of the simulator is a very detailed "table" of electronic current densities J and the corresponding heat generation rates Q obtained for a large range of assumed effective lattice temperatures T_L and given electric fields F; the table is calculated using a single-stage coupled ensemble Monte Carlo (EMC) simulator for electron and phonon transport within a single stage, developed previously [6]. The table essentially provides a generic and compact representation of the J–F and heat generation characteristics of a single stage under a wide range of possible operation conditions.

Next, based on the charge-current continuity equation and solving the global heat diffusion equation, we obtain the temperature and field profiles. Namely, we start from an assumed current density J and assumed tempera-

ISBN 978-0-692-50554-0

ture profile, with each stage becoming a temperature-dependent source for the heat diffusion equation. We iterate the temperature profile until the required thermal boundary conditions are satisfied, updating the field and heat generation rate profiles as we go. Once we have the final temperature profile, we also have the appropriate field profile for the given current and temperature, and we can calculate the total voltage drop V over the whole structure. As a result, we will get a realistic temperature profile and $I-V$ curves, directly relatable to experiment.

The simulated device is a GaAs-based mid-infrared QCL designed for emission at 9 μm [2]. Figure 1 shows the lattice temperature over the entire active core of the QCL for the heat sink temperature (T_0 = 77 K). A maximum temperature of 160 K indicates strong self heating. The stage-dependent electric field is plotted in Fig. 2, which shows the electric field difference among all the stages can be as large as 2.7 kV/cm at J = 10 kA/cm^2. The integration of the stage-dependent electric field gives the voltage across the active core, and Fig. 3 shows the calculated current density–voltage characteristics along with experiment results. The discrepancy between simulation and experiment likely results from the simplified cross-plane thermal conductivity model of the active core used in the simulation; we are presently working on an improved microscopic calculation [7].

This work was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, Physical Behavior of Materials Program, award DE-SC0008712.

References

[1] M. S. Vitiello, G. Scalari, B. Williams, and P. D. Natale, "Quantum cascade lasers: 20 years of challenges," *Opt. Express* 23, 5167 (2015).

[2] H. Page, C. Becker, A. Robertson, G. Glastre, V. Ortiz, and C. Sirtori, "300 K operation of a GaAs-based quantum-cascade laser at $\lambda \approx 9$ μm," *Appl. Phys. Lett.* 78, 3529 (2001).

[3] G. Paulavicius, V. Mitin, and M. A. Stroscio, "Hot-optical-phonon effects on electron relaxation in an AlGaAs/GaAs quantum cascade laser structure," *J. Appl. Phys.* 84, 3459 (1998).

[4] S. Usher and G. P. Srivastava, "Theoretical study of the anharmonic decay of nonequilibrium LO phonons in semiconductor structures," *Phys. Rev. B* 50, 14179 (1994).

[5] R. C. Iotti, F. Rossi, M. S. Vitiello, G. Scamarcio, L. Mahler, and A. Tredicucci, "Impact of nonequilibrium phonons on the electron dynamics in terahertz quantum cascade lasers," *Appl. Phys. Lett.* 97, 033110 (2010).

[6] Y. B. Shi and I. Knezevic, "Nonequilibrium phonon effects in midinfrared quantum cascade lasers," *J. Appl. Phys.* 116, 123105 (2014).

[7] Y. B. Shi, S. Mei, and I. Knezevic, "Multiscale simulation of coupled electron and phonon transport in quantum cascade lasers," *in preparation* (2015).

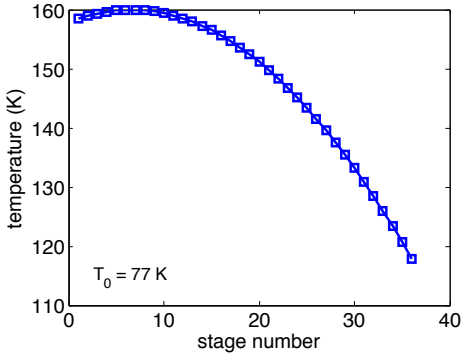

Fig. 1: Lattice temperature distribution in the active core of the QCL (heat sink is at 77 K).

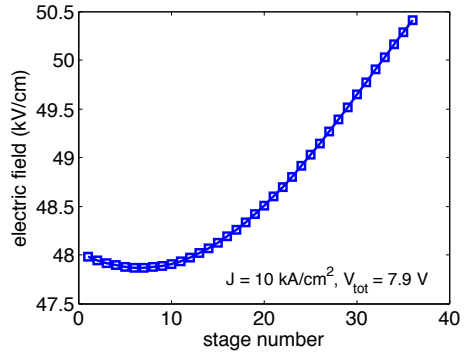

Fig. 2: Electric field distribution in the active core of the QCL.

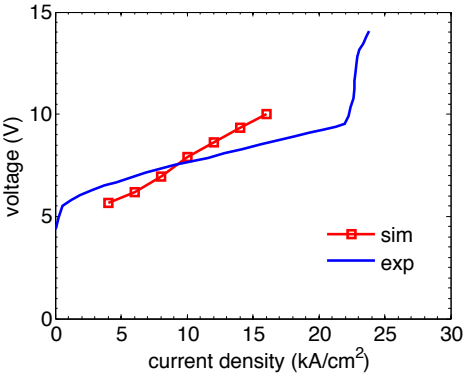

Fig. 3: A comparison between the current density–voltage characteristics obtained in the simulation and measurement [2]. Correction of the slope requires an accurate microscopic model for the thermal conductivity tensor, which we are currently developing [7].