Thermal Simulation of GaAs-Based Midinfrared Quantum Cascade Lasers

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

I. INTRODUCTION

One of the limiting factors for the room-temperature continuous-wave (RT-cw) operation of quantum cascade lasers (QCLs) is the high temperature in the active region that stems from the high electrical power and poor heat extraction [1]. In order to simulate the thermal behavior of QCLs, the heat diffusion equation with appropriate source and boundary conditions needs to be solved. However, the heat generation rate of the active region under a given bias is both space- and temperature-dependent. In this paper, we present a method of extracting the heat generation rate by recording the electron-optical phonon scattering during the ensemble Monte Carlo (EMC) simulation of electron transport under different temperatures. The extracted nonlinear heat source together with appropriate thermal conductivity models enable self-consistent calculation of temperature distribution throughout QCLs. We apply the thermal model to investigate the cross-plane temperature distribution of a 9.4 μm infrared GaAs-based QCL [2]. The nonlinear effects stemming from the temperature dependence of thermal conductivity and the heat generation rate are studied.

II. THERMAL MODEL

The heat generation in the active region of QCLs originates from the optical phonons emitted due to phonon-assisted intra- and intersubband electronic transitions. These optical phonons with negligible group velocities then decay into acoustic phonons that are efficient at diffusing heat [3], [4]. The EMC simulation of electron transport provides statistic information on the scattering processes, from which the heat generation rate term Q in the heat diffusion equation (1) can be derived by Eq. (2) [5]:

$$-\nabla\cdot(\kappa\nabla T)=Q, \tag{1}$$

$$Q=\frac{n}{N_{sim}t_{sim}}\sum(\hbar\omega_{ems}-\hbar\omega_{abs}), \tag{2}$$

where n is the electron density. N_{sim} and t_{sim} are the number of particles and the simulation time, respectively. $\hbar\omega_{ems}$ and $\hbar\omega_{abs}$ are the energies of the emitted and absorbed optical phonons. Each emitted (absorbed) phonon is recorded and its energy added to (subtracted from) the sum on the right-hand side of Eq. (2). In addition, the temperature dependence of the heat generation rate can be captured by interpolating the results of a set of EMC simulation runs under different temperatures.

In QCLs, the wavelike behavior of electrons in the cross-plane direction due to confinement dictates that only a probability density of finding an electron at a given position can be known from its wave function. After the interaction with an optical phonon, an electron may end up in another subband with a completely different probability distribution. On the other hand, embedding the information on the optical phonon generation into the heat source term using Eq. (2), an exact position of each optical phonon is required. We propose a method to translate the space distribution of the optical phonons by introducing an additional random number r (uniformly distributed between [0, 1]) in the EMC simulation to determine the electron's "position" in a subband [6]. The electron in subband α is considered to be within the i^{th} grid cell of width Δz, i.e. it is considered to be within the spatial interval $[z_i-\Delta z/2,\, z_i+\Delta z/2]$ if and only if

$$\int_0^{z_i-\Delta z/2}|\Psi_\alpha(z)|^2dz<r<\int_0^{z_i+\Delta z/2}|\Psi_\alpha(z)|^2dz. \tag{3}$$

When an electron transitions from subband α to α' by scattering with an optical phonon, two random numbers are used to find the electron's position in the initial and final subband, respectively, according to Eq. (3) and the position where the phonon is emitted or absorbed (z_{ph}) is found as their average.

We apply the thermal model to a GaAs/Al$_{0.45}$Ga$_{0.55}$As mid-infrared QCL designed for emission at 9.4 μm [2]. Temperature-dependent thermal conductivities of different layers in the device are taken into account by using an analytical model [7]. Fig. 1 shows the temperature dependence of the thermal conductivites of different layers, together with the average heat generation rate in a stage as extracted from EMC simulation. The top panel of Fig. 2 shows the subband energy levels and wavefunction moduli squared in a single stage at the threshold field (48 kV/cm) at 300 K. The three bold red lines, from top to bottom, denote the upper lasing level, the lower lasing level, and the ground level, respectively. The bottom panel shows the space distribution of the net generated optical phonons (in 30 ps) as obtained using the proposed method.

Fig. 3 shows the temperature distribution of the GaAs/Al$_{0.45}$Ga$_{0.55}$As QCL mounted epitaxial-side onto a copper heat sink at $T_0 = 300$ K calculated using (1) temperature-dependent (TD) heat generation rate and TD thermal conductivities, (2) constant active region thermal conductivity evaluated at T_0, (3) constant heat generation rate at T_0, and

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(4) both constant thermal conductivities and constant heat generation rate at T_0. The results show that nonlinearity of the heat generation rate plays an important role in the accuracy of the calculated lattice temperature, while the temperature dependence of thermal conductivity of the active region should not be neglected in a rigorous calculation.

III. CONCLUSION

We presented a self-consistent thermal model for QCLs that extracts the nonuniform and temperature-dependent heat generation rate in the active region through recording the electron-optical phonon scattering events during the EMC simulation of electron transport. A GaAs/Al0.45Ga0.55As mid-IR QCL was investigated using the model. The results show that nonlinearity of the heat generation rate plays an important role in the accuracy of the calculated temperature, while the temperature-dependence of thermal conductivity of the active region cannot be neglected in a rigorous calculation.

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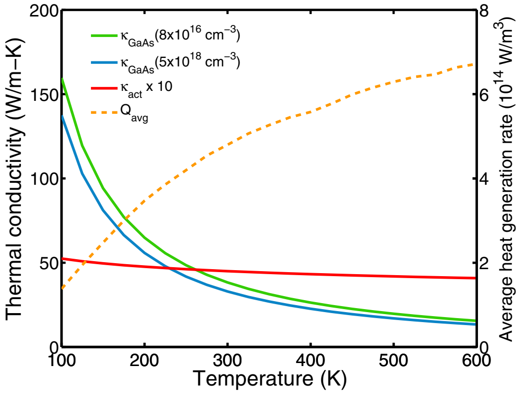

Fig. 1. Thermal conductivities of the active region and the GaAs cladding layers and the average heat generation rate in a stage as a function of temperature.

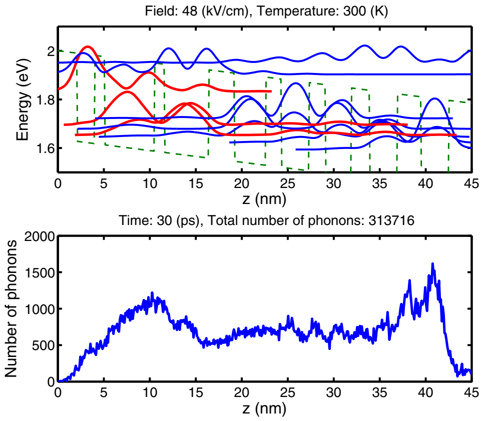

Fig. 2. A schematic conduction-band diagram of a QCL stage (top) and the real-space distribution of the generated optical phonons during the EMC simulation (bottom).

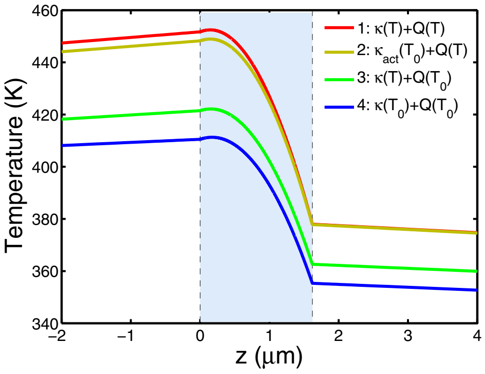

Fig. 3. Lattice temperature distribution of the QCL calculated based on (1) TD thermal conductivities and TD heat generation rate, (2) constant active region cross-plane thermal conductivity evaluated at the heat sink temperature $T_0 = 300$ K, (3) constant heat generation rate at T_0, and (4) constant thermal conductivities and heat generation rate at T_0. The shaded area marks the active region, while the white regions are the cladding layers.