# Thermal Modeling of GaAs/$Al_{0.45}Ga_{0.55}As$ Quantum Cascade Lasers

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## I. INTRODUCTION

In quantum cascade lasers (QCLs), the high active region temperature that stems from the high electrical power and poor heat extraction [1] becomes one of the key limiting factors for these structures' room-temperature continuous-wave (RT-cw) operations. 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 scatterings during the EMC simulation of electron transport.

## THERMAL MODEL

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

$$-\nabla\cdot\left(\kappa\nabla T\right)=Q \quad (1a)$$

$$Q=\frac{n}{N_{sim}t_{sim}}\sum\left(\hbar\omega_{ems}-\hbar\omega_{abs}\right) \quad (1b)$$

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. (1b). 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 the confinement dictates that only the probability density of finding an electron at a given position can be known from its wave function. To construct the distribution using Eq. (1b), the positions of the optical phonons must be translated. We introduce an additional random number $r$ (uniformly distributed between [0, 1]) in the EMC simulation to determine the electron's "position" in a subband [3]. The electron in subband $\alpha$ is considered to be within the i$^{th}$ grid $\left[z_i-\Delta z/2,\ z_i+\Delta z/2\right]$ if and only if

$$\int_0^{z_i-\Delta z/2}\left|\psi_\alpha(z)\right|^2 dz<r<\int_0^{z_i+\Delta z/2}\left|\psi_\alpha(z)\right|^2 dz \quad (2)$$

When an electron transitions from subband $\alpha$ to $\alpha'$ 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. (2) and the position where the phonon is emitted ( $z_{ph}$ ) 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 [4]. Temperature-dependent thermal conductivities of different layers in the device are taken into account using the analytical model [5]. The top panel of Fig. 1 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 number of optical phonons generated in 30 ps as obtained from the Monte Carlo simulation under 300 K.

Fig. 2 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 (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.

## CONCLUSION

We proposed 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 scatterings during the EMC simulation of electron transport.

## ACKNOWLEDGEMENT

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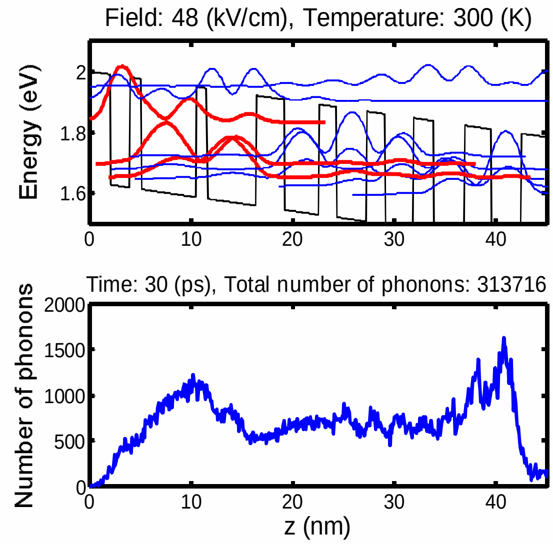


Fig. 1. A schematic conduction-band diagram of a QCL stage (top) and the real-space distribution of the generated optical phonons during the EMC simulation (bottom).

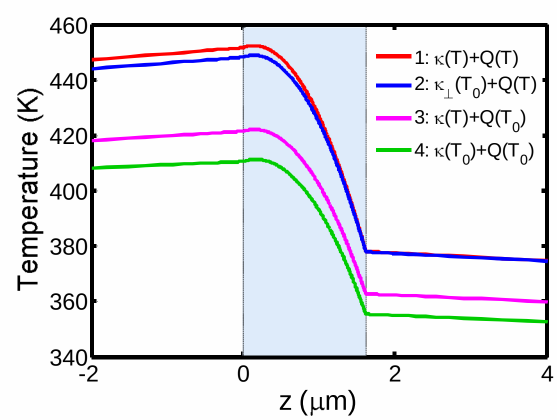


Fig. 2. Lattice temperature distribution of the QCL calculated based on (1) TD thermal conductivities and TD heat generation rate, (2) constant active region cross-plane thermal conductivity evaluated at the heat sink temperature $T_0$ = 300K, (3) constant heat generation rate at $T_0$, and (4) constant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