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Modeling and Optimization of Longwave Infrared Quantum Cascade Lasers

IRENA KNEZEVIC
UNIVERSITY OF WISCONSIN SYSTEM
21 N PARK ST STE 6301
MADISON, WI, 53715
USA

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14. ABSTRACT
AFOSR Award No. FA9550-18-1-0340 Modeling and Optimization of Longwave Infrared Quantum Cascade Lasers PI: Irena Knezevic, University of Wisconsin-Madison, iknezevic@wisc.edu The midinfrared (mid-IR) part of the electromagnetic spectrum, with wavelengths in the 3–20 Î¼m range, is of great industrial, medical, and military importance. The atmospheric low-absorption windows at 3–5 Î¼m and 8–13 Î¼m enable free-space applications, such as remote sensing of chemical and biological species, hard-target imaging, range finding, target illumination, and free-space communication. Quantum cascade lasers (QCLs) are the highest-power monolithic coherent light sources in the mid-IR. Today, room temperature (RT), continuous-wave (CW) lasing has been demonstrated throughout the mid-IR using QCLs based on the InGaAs/InAlAs material system on the InP substrate. Under high power, CW operation, the electron and phonon systems in QCLs are both very far from equilibrium and strongly coupled to one another. The problem of their coupled dynamics is both multi-physics (coupled electronic and thermal) and multiscale (bridging between a single stage and device level. Large amounts of energy are pumped into the electronic system, of which a small fraction is given back through the desired optical transitions, while the bulk of it is deposited into the optical-phonon system. The fast relaxation of electrons into optical phonons, followed by the optical-phonon slower decay into acoustic phonons, results in excess nonequilibrium phonons that can have appreciable feedback on electronic transport, population inversion, and the QCL figures of merit. To accurately describe QCL performance in the far-from-equilibrium conditions of CW operation, a multiscale electrothermal simulation is needed. We developed a multi-physics and multiscale simulation framework capable of capturing the highly nonequilibrium physics of the strongly coupled electron and phonon systems in QCLs [1-5]. The roles of nonequilibrium optical phonons in QCLs at the level of a single stage are accounted at the microscopic level. This microscopic level couples to device-level anisotropic thermal transport of acoustic phonons in QCLs in an efficient algorithm for multiscale electrothermal simulation that accounts for device heating and associated performance degradation [1-5]. Under this award, we achieved considerable progress [6] in the treatment of photon-assisted tunneling in mid-IR QCLs by developing a numerically efficient quantum-transport model [7] that is computationally inexpensive, requires no phenomenological parameters, and is conducive to intuition building [7]. We show that the inclusion of PA tunneling [6] leads to substantial changes in electron transport above the lasing threshold, and explain why those changes are pronounced in QCLs with a diagonal design. [1] Y. B. Shi and I. Knezevic, J. Appl. Phys. 116, 123105 (2014). [2] S. Mei and I. Knezevic, J. Appl. Phys. 118, 175101 (2015). [3] Y. B. Shi, S. Mei, O. Jonasson, and I. Knezevic, Fortschr.

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Final Report

FA9550-18-1-0340: Modeling and Optimization of Longwave Infrared Quantum Cascade Lasers

PI: Irena Knezevic, University of Wisconsin-Madison, iknezevic@wisc.edu

Abstract

The midinfrared (mid-IR) part of the electromagnetic spectrum, with wavelengths in the 3–20 μm range, is of great industrial, medical, and military importance. The atmospheric low-absorption windows at 3–5 μm and 8–13 μm enable free-space applications, such as remote sensing of chemical and biological species, hard-target imaging, range finding, target illumination, and free-space communication. Quantum cascade lasers (QCLs) are the highest-power monolithic coherent light sources in the mid-IR. Today, room-temperature (RT), continuous-wave (CW) lasing has been demonstrated throughout the mid-IR using QCLs based on the InGaAs/InAlAs material system on the InP substrate.

Under high-power, CW operation, the electron and phonon systems in QCLs are both very far from equilibrium and strongly coupled to one another. The problem of their coupled dynamics is both multiphysics (coupled electronic and thermal) and multiscale (bridging between a single stage and device level. Large amounts of energy are pumped into the electronic system, of which a small fraction is given back through the desired optical transitions, while the bulk of it is deposited into the optical-phonon system. The fast relaxation of electrons into optical phonons, followed by the optical-phonon slower decay into acoustic phonons, results in excess nonequilibrium phonons that can have appreciable feedback on electronic transport, population inversion, and the QCL figures of merit. To accurately describe QCL performance in the far-from-equilibrium conditions of CW operation, a multiscale electrothermal simulation is needed.

We present work on the development of a simulation framework capable of capturing the highly nonequilibrium physics of the strongly coupled electron and phonon systems in QCLs. We discuss the roles of nonequilibrium optical phonons in QCLs at the level of a single stage, anisotropic thermal transport of acoustic phonons in QCLs, outline the algorithm for multiscale electrothermal simulation, and present data for a mid-IR QCL based on this framework.

Furthermore, we showcase recent progress on the treatment of photon-assisted tunneling in mid-IR QCLs using a quantum-transport model that is computationally inexpensive, requires no phenomenological parameters, and is conducive to intuition building. We show that the inclusion of PA tunneling leads to substantial changes in electron transport above the lasing threshold, and explain why those changes are pronounced in QCLs with a diagonal design.

Background

The longwave infrared (LWIR) range (8-10 microns) within the second low-absorption atmospheric window is very important for free-space applications, such as long-range communication, remote sensing of chemical and biological species, and target search and imaging. These applications require portable sources of watt-level coherent optical power that operate reliably for many hours in continuous-wave (CW) mode at room temperature.

Quantum cascade lasers (QCLs) are high-power monolithic coherent light sources in the midinfrared. They are electrically driven, unipolar semiconductor devices that achieve population inversion based on quantum confinement and tunneling. Among the LWIR devices, the challenge is to achieve reliable CW room-temperature operation with high wallplug efficiency (WPE), watt-level high optical power, and high brightness. This mode of operation is challenging to model because electrons, lattice, and light are strongly coupled to one another and the problem bridges scales from a single stage to device level.

Objective

The objective of this project is to design and optimize quantum cascade lasers (QCLs) in the longwave infrared (LWIR) range (8-10 microns) so they would be long-term reliable and operate with high optical power (≥ 1 W), high wallplug efficiency (WPE), and high brightness in continuous-wave (CW) mode. To that end, the PI will develop a novel, comprehensive simulation tool for the modeling and design of these structures. The PI will work with experimental collaborators (separately funded) and employ the developed simulation tool to optimize the promising state-of-the-art step-taper active-region resonant-extraction (STA-RE) device that already shows 86% internal differential efficiency and 6% wallplug efficiency from single-facet emission at 8-9 microns, as is also temperature stable. The goal is to approach 20% wallplug efficiency and achieve $\geq$ 1 W CW operation.

Program Relevance

The LWIR range (8-10 microns) within the second low-absorption atmospheric window is very important for free-space applications, such as long-range communication, remote sensing of chemical and biological species, and target search and imaging. These applications require portable sources of watt-level coherent optical power that operate reliably for many hours in continuous-wave mode at room temperature. Quantum cascade lasers are the highest-power monolithic monolithic coherent light sources in the midinfrared. However, critical open problems currently limit the performance of LWIR devices. Remote communication and sensing require high brightness (single-mode lasing with high optical power) which requires good confinement (requiring buried ridges of width 8-10 microns with good current blocking), as well as high efficiency. Yet, the wallplug efficiency of top-performing devices is only ~6% even though the internal quantum efficiency is very high (86%). WPE of near 20% should be achievable in principle, but first the microscopic loss mechanisms have to be understood. This critical issue can be addressed by a careful optimization procedure that involves comprehensive modeling of LWIR QCLs operating at room temperature, which is what the PI proposes to do here.

Software and Shared Facilities

The PI's group develops their own computer programs to simulate relevant physics. Codes are written in Fortran (standard in scientific computing; we use a modern free compiler gfortran, which is supported by our main compute facilty CHTC, see below) and MATLAB (mostly smaller codes, data postprocessing, and visualization; these codes are generally run locally, on students' office workstations; user licenses are provided by the Univeristy).

The PI's group extensively uses the resources and assistance from UW Madison's Center for High Throughput Computing (CHTC). (Website: http://chtc.cs.wisc.edu/) CHTC resources are provided to all UW-Madison researchers, free of charge. For high-throughput computing (HTC) capability, UW-Madison maintains many compute clusters across campus, which are managed via software developed by the UW-Madison's HTCondor Project distributed computing research group; therefore, these clusters are linked together to share resources via widely adopted distributed computing technologies. Together these clusters represent roughly 25,000 CPU cores in support of research. Should these HTC resources not be sufficient for your project, the CHTC can also engage computing resources from the Open Science Grid (OSG), also at no cost. For high performance computing (HPC) capability, the CHTC maintains a shared-use cluster of approximately 4500 tightly coupled cores, with expansion room to increase cluster compute capacity as campus needs grow and as research groups contribute for dedicated access to a number of cores. Compute nodes have 16 or 20 cores, each, and 64 or 128 GB RAM, with access to a shared file system and resources managed via the open-source software, SLURM.

Technical Approach

The PI developed and validated a comprehensive simulation tool for predictive theoretical modeling and design of LWIR QCLs under CW, high-power operation. The simulation tool will be multiscale (bridging from a single stage to device level) and multiphysics (coupling electrons, lattice motion, and light). The simulation will rigorously incorporate the relevant loss mechanisms (such as intersubband absorption), rigorously account for the effects of all microscopic scattering mechanism on device performance (optical phonons, interface roughness, and alloy scattering), as well as analyze the role of strain on electronic, optical, and thermal parameters of the QCL. The quantum electronic transport simulation kernel will be based on the density matrix approach. It will be coupled with a finite-element global solver for the heat diffusion equation. Moreover, a full-wave electrodynamics solver based on the finite-difference time-domain technique will be coupled with the quantum-transport solver because high optical powers mean that the optical-system feedback on electron transport is strong.

The PI investigated the mechanisms of loss that limit both WPE and brightness, with particular emphasis on the poorly understood intersubband absorption and its interplay with strain, and on the microscopic scattering mechanisms that affect the various QCLS parameters (e.g., electroluminescence linewidth, loss, internal quantum efficiency). The mechanisms include electron scattering with optical phonons (commonly accounted for), but also elastic mechanisms, such as interface roughness and alloy scattering, which appear to have an important but underappreciated role on the LWIR QCL performance. The simulation will be accompanied by experimental validation by the PI's collaborators (separately funded). This predictive modeling tool has the potential to transform the design and analysis of QCLs.

This project produced an accurate and comprehensive simulator of mid-IR QCLs under high-power, continuous-wave operation. The tool does justice to the multiscale (from a single stage to device level) and multiphysics (coupled electrons, phonons, and photons) nature of the problem. The simulator will significantly advance our design capabilities for new structures, as it can easily incorporate new materials systems. This type of simulation will strongly affect the work on many experimental groups interested in mid-IR QCLs. The proposed tool can be readily adapted to QCLs and QCL arrays in other III-V materials.

This is a unique simulation tool that will couple quantum electronic transport, optical field, and thermal transport comprehensively in a single simulation. This enabled unprecedented accuracy in the simulation, design, and optimization of optoelectronic devices in general, and quantum cascade lasers in the midinfrared, in particular. The work will yield insight into the miscroscopic physics of loss during QCLs operation and remove barriers to further design optimization. This lack of microscopic insight is currently a roadblock for achieving high-brightness, high-wallplug-efficiency CW operation.

Project Participants

Principal Investigator

- Irena Knezevic (University of Wisconsin – Madison)

Postdoctoral Research Associates

- Laleh Avazpour

PhD Students

- Sina Soleimanikahnoj (graduation December 2021)
- Michelle King (graduation August 2021)

Collaborators (not funded under this award)

- Luke Mawst (University of Wisconsin – Madison)
- Sanjiv Sinha (University of Illinois at Urbana – Champaign)
- Brian Foley (Penn State)
- Mark Eriksson (University of Wisconsin – Madison)
- Sanjiv Sinha (University of Illinois at Urbana – Champaign)

Publications

PUBLICATIONS

1. L. Avazpour, M. L. King, S. Soleimanikahnoj, S. Schmidt, L. N. Maurer, and I. Knezevic, "Time-domain simulation technique for elastic-wave interactions with complex media and application to rough-interface scattering," in review (2022).
2. D. Gelda, L. Avazpour, M.G. Ghossoub, M.C. Rajagopal, I. Knezevic, and S. Sinha, "Spectroscopic Surface Scattering of Confined Acoustic Phonons in Thin Silicon Nanowires," in review (2022).
3. M. L. King, F. Karimi, S. Soleimanikahnoj, S. Suri, S. Mei, Y.B. Shi, O. Jonasson, and I. Knezevic, "Coupled simulation of quantum electronic transport and thermal transport in midinfrared quantum cascade lasers," in *Mid-Infrared and Terahertz Quantum Cascade Lasers*, edited by Dan Botez and Mikhail Belkin, Cambridge University Press, *in press* (2022).
4. S. Soleimanikahnoj, M. L. King, and I. Knezevic, "Density-Matrix Model for Photon-Driven Transport in Quantum Cascade Lasers," *Phys. Rev. Applied* 15, 034045 (2021).
5. S. Soleimanikahnoj, O. Jonasson, F. Karimi, I. Knezevic, "Numerically efficient density-matrix technique for modeling electronic transport in mid-infrared quantum cascade lasers," *J. Comput. Electron*. 20, 280-309 (2021).
6. G. R. Jaffe, S. Mei, C. Boyle, J. D. Kirch, D. E. Savage, D. Botez, L. J. Mawst, I. Knezevic, M. G. Lagally, and M. A. Eriksson, "Measurements of the thermal resistivity of InAlAs, InGaAs and InAlAs/InGaAs Superlattices," *ACS Appl. Mater. Interfaces* 11, 11970-11975 (2019).

Conference Presentations

Invited

1. I. Knezevic, "Coupled Simulation of Light, Charge, and Heat at the Nanoscale," Charles L. and Ann Brown Distinguished Colloquium, University of Virginia, March 18, 2022.
2. I. Knezevic, "Photon-Driven Transport in Quantum Cascade Lasers," SPIE Photonics West, San Francisco, CA, January 22-27, 2022. (unable to travel because of COVID surge)
3. I. Knezevic, "Quantum Transport Simulation for Predicting Optical and Plasmonic Properties of Low-Dimensional Nanomaterials," OSA Advanced Photonics Congress 2020 (NOMA Topical Meeting), virtual, July 13-16, 2020.
4. I. Knezevic, "Multiscale Electrothermal Simulation of Quantum Cascade Laser Operation," 19th Annual Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2019), Ottawa, Canada, July 2019.
5. I. Knezevic, "Phonon Dynamics in Disordered Nanostructures—A Chaos Perspective," 2019 MRS Spring Meeting, Phoenix, AZ, April 2019.

Contributed

1. S. Soleimanikahnoj, M. L. King, and I. Knezevic, "A density-matrix model for photon-assisted electron transport in quantum cascade lasers," International Workshop on Computational Nanotechnology (IWCN) 2021, Seoul, Korea, May 17-June 6, 2021. (virtual)
2. Laleh Avazpour, Michelle L. King, Sina Soleimanikahnoj, and Irena Knezevic, "Elastic-wave scattering from an object above a rough surface: A numerical time-domain technique," International Workshop on Computational Nanotechnology (IWCN) 2021, Seoul, Korea, May 17-June 6, 2021. (virtual)
3. M King, S Soleimanikahnoj, I Knezevic, "Multiscale electrothermal simulation of quantum cascade lasers," 2020 APS March Meeting, Denver (cancelled due to COVID) Abstract
4. S Soleimanikahnoj, M King, I Knezevic, "Photon Mediation of Electron Transitions in Quantum Cascade Lasers," 2020 APS March Meeting, Denver (cancelled due to COVID) Abstract
5. L. Avazpour, S. Soleimanikahnoj, S. Suri, and I. Knezevic, "Finite-Difference Time-Domain Study of Phonon Dynamics and Rough-Interface Scattering in Nanostructures," 20th International Workshop on Computational Nanotechnology (IWCN 20), Evanston, Illinois, USA, May 20-24, 2019.
6. M. King, F. Karimi, S. Schmidt, and I. Knezevic, "Simulation Tool for Coupled Quantum Transport and Electrodynamics," 20th International Workshop on Computational Nanotechnology (IWCN 20), Evanston, Illinois, USA, May 20-24, 2019.
7. L. Avazpour, S. Soleimanikahnoj, S. Suri, and I. Knezevic, "Thermal Transport Across Rough Interfaces—A Finite-Difference Time-Domain Study, 2019 MRS Spring Meeting, Phoenix, AZ, April 2019. (poster)

Highlights

- **<u>Highlight 1</u>: "Numerically efficient density-matrix technique for modeling electronic transport in midinfrared quantum cascade lasers,"** by S. Soleimanikahnoj, O. Jonasson, F. Karimi, I. Knezevic, *J. Comput. Electron.* 20, 280–309 (2021).

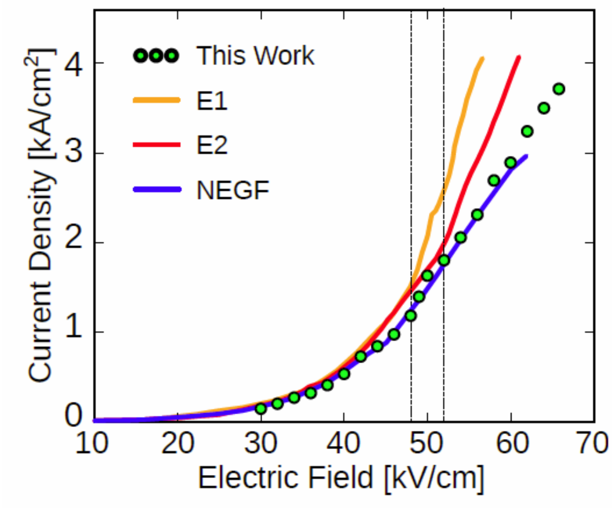

FIG. 2: Calculated current density vs field based on this work and comparison to results using nonequilibrium Green's functions (NEGF). Also shown are experimental results from Ref. [54] (E1) and a regrown device from [9], Lindskog et al. Appl. Phys. Lett. 105, 103106 (2014). (E2). Experimentally determined threshold fields of 48 kV/cm (E1) and 52 kV/cm (E2) are denoted by dashed vertical lines. Both theoretical results are given for a lattice temperature of 300 K. Experimental results are provided for pulsed operation, minimizing the effect of lattice heating above the heatsink temperature of 300 K.

We derived a Markovian master equation for the single-electron density matrix that conserves the positivity of the density matrix and is applicable to electron transport in both midinfrared and terahertz quantum cascade lasers. The master equation contains both the coherent (unitary) evolution of the density matrix as well as all relevant elastic and in-elastic scattering mechanism. Nonparabolicity in the band structure was accounted for by using a three-band **k.p** model, which includes the conduction band, light-hole band, and the spin-orbit split-off band. The model is an improvement of previous work employing density matrices because it does not rely on a phenomenological treatment of dephasing across thick injection barriers or a factorization of the density matrix into cross-plane and in-plane distribution. We demonstrated the validity of the model by simulating QCLs based in lattice-matched as well as strain-balanced heterostructures, with lasing wavelengths of 8.5 µm and 4.6 µm respectively. We compared our results to experiment as well as theoretical results based on nonequilobrium Green's functions (NEGF) and a semiclassical model.

For the 8.5-µm QCL, we calculated the current density vs electric field strength and obtained excellent agreement with experiments for electric fields below threshold, while current density was underestimated above threshold due to our omission of the laser electromagnetic field. We obtained a good agreement with NEGF for low field values (<42 kV/cm) and fair agreement for higher fields. At room temperature, we obtained a threshold electric field of E_{th}=48.0 kV/cm and threshold current density of J_{th}=1.55 kA/cm^2, in good agreement with experimental results of E_{th}=48.0 kV/cm and J_{th}=1.50 kA/cm^2 and in fair agreement with NEGF results of E_{th}=47.6 kV/cm and J_{th}=1.2 kA/cm^2. Comparison with a semiclassical model shows that off-diagonal matrix elements play a significant role. The semiclassical model (off-diagonal matrix elements are ignored) was found to overestimate current density by 29% around threshold and up to 60% for other electric field values. Our results for maximum gain vs field were in good agreement with NEGF except for very high (>70 kV/cm) field values. The semiclassical model was found to overestimate the peak gain above threshold, while giving fair agreement with DM and NEGF results below threshold. We predict significant electron heating, with in-plane distribution deviating strongly from a thermal distribution, especially the lower lasing state. We obtained an average electron temperature of 535 K around threshold, which is 235 K above the lattice temperature of 300 K. From a simple energy-balance equation, we obtained an energy-dissipation time of 0.79 ps for the considered device, which is similar to the scattering time due to polar-optical phonons.

For the 4.6-µm QCL, we calculated current density vs electric field strength at room temperature and obtained excellent agreement with experiment for fields up to 66 kV/cm, which is slightly above the experimentally determined threshold of 64 kV/cm. Above threshold, the calculated current density was below experimental results due to our omission of the laser electric field as well effects of lattice heating in continuous-wave operation. As in the case of the 8.5-µm QCL We found that a semiclassical model overestimates current density for all field values. The semiclassical model was found to overestimate current density by 40 % around threshold and up to 58% for other electric field values, demonstrating the need to include off-diagonal elements of the density matrix. Superlattices can be tuned by a factor of 2.5 by altering the lattice mismatch and thereby the phonon-mode mismatch at the interfaces, a principle that is commonly assumed for superlattices but has not been experimentally verified without adding new elements to the layers. We find that the additional resistance in superlattices does not increase significantly when the layer thickness is decreased from 4 to 2 nm. We also report measurements of 250–1000 nm thick films of undoped InGaAs and InAlAs lattice-matched to InP substrates, for there is no published thermal conductivity value for the latter, and we find it to be 2.24 ± 0.09 at 22 °C, which is 2.7 times smaller than the widely used estimates.

- **Highlight 2: "Density-Matrix Model for Photon-Driven Transport in Quantum Cascade Lasers,"** S. Soleimanikahnoj, M. L. King, I. Knezevic, Phys. Rev. Applied 15, 034045 (2021).

Quantum cascade lasers (QCLs) are unipolar sources of coherent radiation emitting in the terahertz and infrared portions of the electromagnetic spectrum. The gain medium of a QCL is a periodic stack of compound-semiconductor heterostructures. The resulting multi-quantum-well electron band structure in the growth direction has discrete energy levels, and the associated wave functions are quasibound. While lasing stems from radiative electron transitions between specific states, nonradiative transitions mediated by various scattering mechanisms also play important roles in device operation. In particular, photon-assisted (PA) transport in terahertz and midinfrared QCLs is significant at and above lasing threshold, and appears particularly prominent in devices with diagonal design. There is a need for a computationally efficient quantum-transport treatment of PA tunneling in QCLs that does not require phenomenological parameters and that employs broadly adopted intuitive concepts.

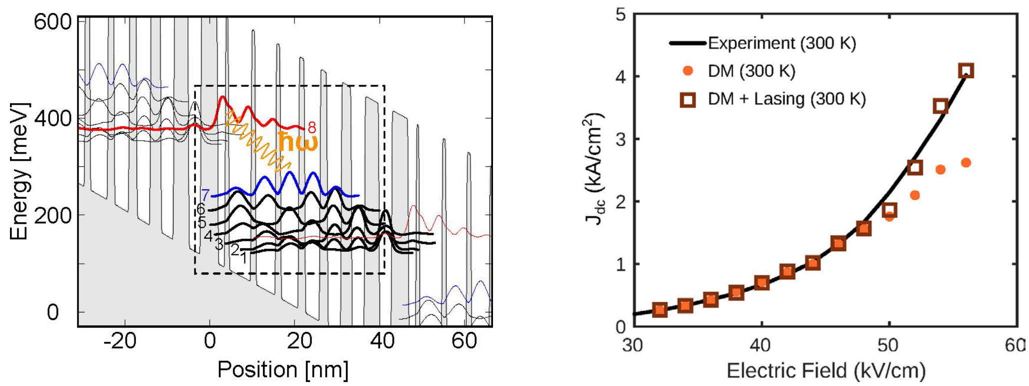

FIG. 2: (Left) Conduction-band edge and probability densities for the eight eigenstates used in calculations (bold curves) for the structure in [3]. The states that belong to neighboring periods are denoted by thin gray curves and the dashed box indicates a single stage, starting with the injection barrier. The bias electric field is 50 kV/cm. The states are numbered in the order of increasing energy, starting with the ground state. The radiative transition occurs from state 8 to state 7. **(Right)** Calculated *dc* current density as a function of the applied bias electric field at 300 K, with (open squares) and without (solid circles) the influence of photon-assisted tunneling. Experimental data from [3] is given by the solid black curve. Figure from [2].

During this project, the PI and team have developed and published a quantum-mechanical model for photon-driven transport in QCLs that is computationally inexpensive and conducive to intuition building [1,2]. The model stems from a rigorous theoretical framework with a positivity-preserving Markovian master equation of motion for the density matrix. The model was employed to characterize the steady-state and frequency response of a previously grown midinfrared QCL. Our results show that the inclusion of PA tunneling leads to substantial changes in electron transport around and above lasing threshold. Specifically, a significant increase in the current density is observed upon inclusion of PA tunneling, which allows for a significantly better agreement with experimental findings than the models that neglect this phenomenon. In particular, we show that, in quantum cascade lasers with diagonal design, photon resonances have a pronounced effect on electron dynamics around and above lasing threshold. This effect stems from a large spatial separation of the upper and lower lasing states.

- **Highlight 3**: **"A hybrid simulation technique for elastic wave scattering in CPML-truncated media: Application to rough interface scattering,"** L. Avazpour, M. L. King, S. Soleimanikahnoj, S. Schmidt, L. N. Maurer, and I. Knezevic, in review (2022); "Spectroscopic Surface Scattering of Confined Acoustic Phonons in Thin Silicon Nanowires," D. Gelda, L. Avazpour, M.G. Ghossoub, M.C. Rajagopal, I., Knezevic, S. Sinha, in review (2022).

The PI's group has developed a finite-difference time-domain (FDTD) numerical solver for the solution to the elastic-wave equation in the velocity-stress formulation [6]. Our velocity-stress formulation is fully capable of tracking mode conversion, and capturing phenomena such as

Rayleigh waves, which are critical near boundaries and interfaces and facets that are found in optoelectronic devices, and which strongly affect heat dissipation and device reliability.

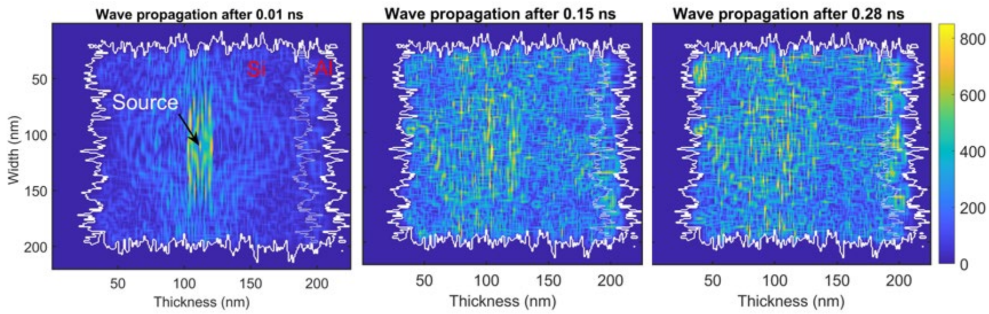

FIG. 3: A Gaussian wave packet launched from the center of a Si nanowire (170 nm width; 200 nm thickness) capped with Al (layer on the right). Snapshots taken 0.01 ns (left), 0.15 ns (center), and 0.28 ns (right) after launch. The rough surface is exponentially correlated with a correlation length of 1.7 nm (0.01 of the width) and rms roughness of 5 nm.

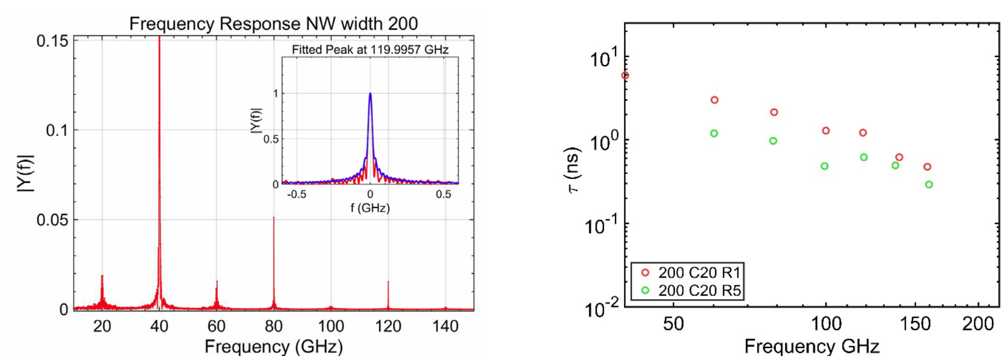

FIG. 4. (Left) Fourier transform of the time-resolved, spatially averaged velocity magnitude (divided by velocity magnitude of the launched Gaussian wave). Each prominent peak is fitted with a Lorentzian (see inset) whose width corresponds to the scattering rate, the inverse of lifetime due to roughness as averaged over the whole surface. (Right) Sample data presenting lifetime versus elastic-wave frequency for two different rms roughness (1 and 5 nm), but the same wire dimensions (200 nm x 200 nm) and correlation length (20 nm).

More recently, the PI's group has developed the capability to extract frequency-resolved scattering times for elastic waves interacting with rough interfaces directly from the simulation. Relevant data is shown in Figs. 3 and 4, and is accompanied by experimental work by Sanjiv Sinha (UIUC). In Fig. 3, we see a Gaussian longitudinal wave packet being launched in the center of a nanowire toward the rough interface formed between Si and Al (right boundary of the domain). The random roughness profile in these nanowires is generated based on a given correlation type, rms roughness and correlation length based on a stochastic algorithm. For a given rms roughness, correlation type and length, we generate many specific incarnations of a rough surface. The Gaussian pulse is centered around a certain frequency, typically one that coincides with a resonant mode. The time-resolved signal (velocity magnitude at different positions) is recorded over a long time, and its then Fourier transformed (Fig. 4). The simulations can be done for multiple frequencies and for various random-roughness incarnations for a given rms roughness and correlation length. As a result, the Fourier transform of this signal is peaked around the launch frequency and its harmonics, but there is a notable broadening to it that depends on roughness properties (see Fig. 4). Each prominent peak (i.e., a peak of sufficiently high intensity) is fitted with a Lorentzian to extract the line width, which corresponds to the scattering rate (inverse of scattering lifetime). An example of how the fit looks is given in the inset to Fig. 4 (left). In general, for a given nanostructure, waves of multiple frequencies are launched and their signals averaged using peak height squared (~ peak intensity) as weights.