# Modelling of THz quantum cascade lasers for imaging, sensing, and biomedical applications

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## ABSTRACT

THz frequency quantum cascade lasers (QCL) have remarkably developed during the last two decades and represent a promising solution for bridging the dead zone between electronics and optics, the so-called THz technology gap. THz radiation is safe to use on humans and animals since it is non-ionizing, it interacts strongly with water but passes through a few millimeters of biological tissue, which makes it suitable for medical imaging and studying cellular and molecular biology. What is needed to reduce the cost and complexity of THz spectroscopy and imaging systems are higher-power sources that work at higher temperatures where cryogenic cooling is not necessary, being able to generate a series of ultra-short and high-intensity THz pulses, as well as more sensitive detectors. Another interesting field of study with application in spectroscopy is a combination of laser feedback interferometry with the optical frequency comb QCL. This method of self-detection does not require fast detectors and provides possibilities for the investigation of many new phenomena and the development of new methodologies.

In this contribution we present various modeling results of THz QCLs, devices that can be used for imaging, sensing, and biomedical applications. These results include numerical simulations of different GaAs/AlGaAs designs, consideration of new material platforms based on wide-bandgap semiconductors, exploration of the possibilities for ultra-short pulsing using the passive mode-locking technique, and investigation of the THz QCL dynamics arising from self-mixing. Methods consist of Schrodinger-Poisson solver, density matrix formalism for transport, and Maxwell-Bloch equations for modeling electron dynamics and optical field.

**Keywords:** Terahertz quantum cascade laser, Schrodinger-Poisson equations, density matrix formalism, Maxwell-Bloch equations, self-mixing

## 1. INTRODUCTION

Quantum cascade lasers (QCLs) are superlattice-based optical sources operating in MIR and THz spectral range which is enabled by engineering of quantum wells and barriers and adjusting the voltage across the device so that quantum tunnelling effects can be exploited [1], [2]. While MIR QCLs are commercially available, THz QCLs are still largely in the research phase. THz QCL represents a promising solution for bridging the dead zone between electronics and optics, the so-called THz technology gap. They play a central role as local oscillators for heterodyne spectroscopy in astronomical observations, real-time THz imaging, bio-medical imaging etc. [3]. Currently, the recently reached record temperature performance in pulsed operation is up to 261 K [4] for a two-well design which has enabled the use of Peltier-coolers instead of the costly cryogenic equipment such as Sterling coolers or liquid Helium cryostats, which drastically reduces the system cost and opens commercial prospects for the THz field. Although researchers in THz field often report their access to sources across 1.2 to 5.7 THz, the reality is that operation frequency is unevenly distributed. Furthermore, laser applications predominantly require continuous wave (CW) operation which in the THz field is limited since CW THz QCLs have low power levels and operating temperatures up to 129 K and ~6-10 mostly hybrid designs are used. In this theoretical contribution we will we present our recent modelling results of THz QCLs, in particular numerical simulations of different GaAs/AlGaAs designs, and we will also consider alternative material platforms based on wide-bandgap semiconductors which offer new possibilities in terms of operating frequency range and temperature performance. Furthermore, we are interested in dynamics modelling of compact and inexpensive THz short pulse

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emitters beneficial for applications in sensing and spectroscopy, and investigation of the THz QCL dynamics arising from self-mixing, a fast and sensitive technique that removes the need for an external THz detector that is important for emerging applications ranging from imaging of human skin pathologies [5] to hidration sensing in agriculture [6].

## 2. METHODOLOGY

**Density matrix transport model**

Carrier transport simulations are used for the extraction of parameters for the dynamical simulations. Localized wavefunctions are calculated by solving the Schrödinger-Poisson equation system for a tight-binding potential, the transport of electrons through the quantum well heterostructure is modeled by a density matrix model developed at University of Leeds [7]–[10] where relevant scattering rates are calculated from Fermi's golden rule using the wavefunctions and material parameters as inputs. It is a versatile quantum transport model with low numerical complexity which generates material gain, current density and emission frequency as functions of the applied external electric bias. Model performance is illustrated in Fig.1. The model has ~5% tolerance for cut-off temperature prediction making it ideal for high-temperature optimisation. This model also has state-of-the-art numerical efficiency, a two-well structure I-V characteristic (Fig. 1c) can be computed in less than 5 minutes. This is a significant advantage over commercial modelling package that employs non-equilibrium-Green-function approach which would require several hours of computations.

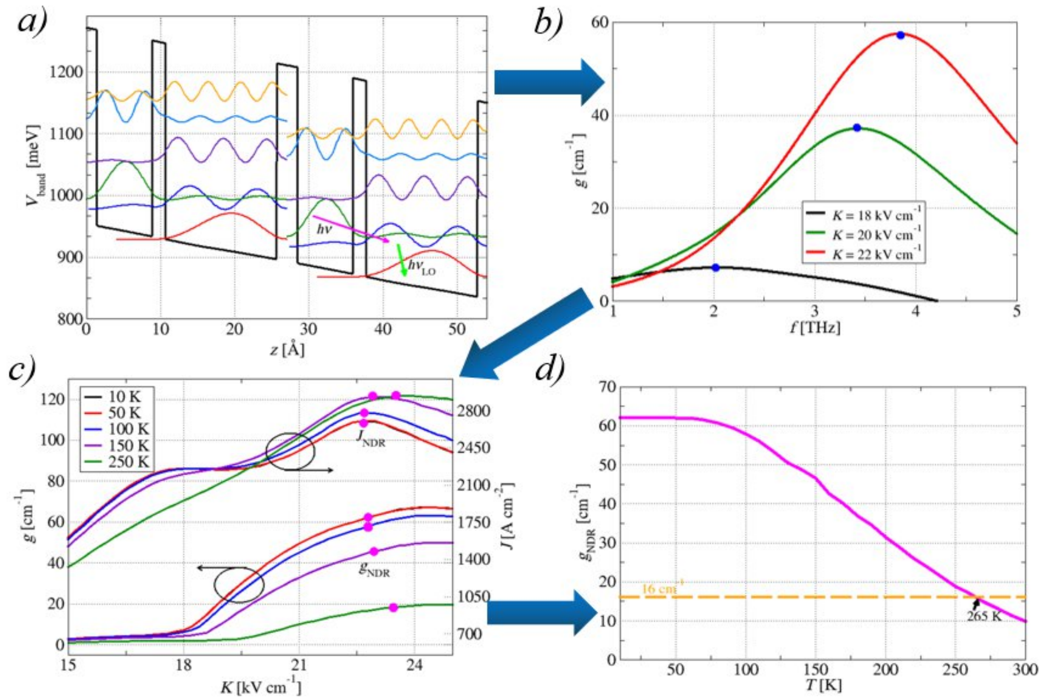


Figure 1. Illustration of simulation procedure on exemplary two-well LO-phonon 261 K structure. *a)* Electronic structure at resonant bias at 10 K, *b)* Material gain dependence on frequency at 10 K for various values of external bias. Blue circles illustrate the most likely lasing frequency. *c)* Profile of current density, material gain and frequency on applied bias at different temperatures, the material gain traces are selected as peaks of profiles in *b)*, the pink circles indicate the NDR values. *d)* Profile of material gain versus temperature, values are taken from pink circles in *c)*, orange line indicates the estimated waveguide loss, predicted cut-off temperature is 265 K.

## 3. MODELLING RESULTS

**High temperature optimization**

However, although efficient, the parameter space required for designing novel THz QCLs has big-data scale and more advanced techniques that employ high performance computing (HPC) and machine learning are required. Namely, if we wanted to explore the full range of layers thicknesses with half a monolayer resolution, the parameter space ends up being too large for brute-force exploration. Novel schemes with paradigm shift enable high-temperature performance >250 K. Taller barriers and higher LO–phonon depopulation energies (> 45 meV) are beneficial for high temperature performance. The model has yielded several 3-well and 4-well prospective active region designs that could outperform the 2-well 261 K record structure.

**MBE growth effects**

THz QCLs are typically grown by molecular beam epitaxy (MBE) due to its high growth quality. THz QCLs consist of >100 periods of multiple-quantum-well heterostructures and are greatly affected by MBE process and fluctuations of growth parameters. In our recent publication [11] we have developed and implemented a computational procedure to study three effects associated with MBE growth that may have a prominent impact on THz QCL performances: background doping, interface composition diffusion (interdiffusion) and layer thickness fluctuations. These effects have been numerically tested on the four exemplary designs: 200 K LO-phonon THz QCL, 2 THz bound to continuum (BTC) QCL, Hybrid and 261K MIT two-well LO-phonon [11].

**New material platforms based on wide-bandgap semiconductors**

The model from Fig. 1 was tested on $ZnO/Mg_xZn_{1-x}O$ material system in which large ZnO LO-phonon energy (~70 meV) reduces the thermally activated LO-phonon scattering which promises better temperature performance of THz QCLs. Furthermore, this alternative material system provides access to frequencies not accessible to GaAs-based QCLs because of the reststrahlen band absorption from 8-9 THz. However, no successful laser action from ZnO-based THz QCL was reported so far in the literature, only electroluminescence [12]. There were some issues reported in [12] a very high doping; design predicted a gain peak at ~24 meV, while the observed emission energy was ~35 meV which was atributed to the uncertainties in the material parameters; negative differential resistance (NDR) was not observed. It is our belief that with a good transport model, together with HPC optimization, it is possible to design a device which will provide successful lasing action.

In our recent publication [13] we have considered an alternative material system, $Ga_2O_3/(Al_xGa_{1-x})_2O_3$ and analysed double barrier resonant tunnelling diode (RTD) as a promising step towards THz QCL. We have optimised barrier thickness and doping level for maximum peak-to-valley ratio (PVR) at NDR.

**Ultrashort pulses modelling**

Ultrafast and intense THz light pulses represents key enabling technology for time-resolved measurements, nonlinear photonics, coherent control of matter and frequency comb synthesis for high-precision metrology and spectroscopy. Nevertheless, compact and inexpensive short pulse emitters are deficient. Passive mode-locking in THz QCL with distributed saturable absorber was only recently demonstrated (2023) [14]. In order to model the underlying dynamics, it is necessary to solve Maxwell-Bloch (MB) equations [15] either using computationally intensive full-wave treatment [16] or invoking the rotating wave approximation (RWA) in combination with the slowly varying envelope approximation (SVEA) [17]. We have explored both approaches and included graphene saturable absorber as an intensity-dependent loss.

**Model for THz QCLs with optical feedback**

THz standoff imaging using using laser feedback interferometry (LFI) with THz QCLs is a fast and sensitive technique that removes the need for an external THz detector. It was demonstrated for a wide range of applications, including the measurement of internal laser characteristics, trace gas detection, materials analysis, biomedical imaging, and near-field imaging [18], early detection of skin cancer using laser feedback interferometry [5], and hydration sensing in leaves [6]. One can model the dynamic effects of optical feedback by using reduced rate equation models and Lang–Kobayashi formalism[18]. However, in this contribution our modelling results are based on effective semiconductor MB equations (ESMBE) for the FP cavity with optical feedback, similar to [19]. We have considered 2 THz BTC QCL design and simulated output power waveform, and optical power spectrum for various values of current, external cavity length and target reflectivity.

## 4. CONCLUSIONS

Growing effects such as background doping, interdiffusion of the barrier material and layer thickness fluctuations need to be taken into account for successful realization of THz QCLs in $GaAs/Al_xGa_{1-x}As$ as well as other material systems.

High performance computing and AI schemes are necessary for prediction of new THz QCL designs optimized for room temperature operation. Investigation of alternative material platforms based on wide-bandgap semiconductors offers new possibilities in terms of operating frequency range and temperature performance. Dynamics of compact and inexpensive THz short pulse emitters is beneficial for applications in sensing and spectroscopy and modelling of these peculiarities need to be better understood. Modelling dynamics of LFI with THz QCLs is important for emerging applications and among various existing models our model of choice was based on ESMBE with external feedback.

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## REFERENCES

[1] J. Faist, F. Capasso, D. L. Sivco, C. Sirtori, A. L. Hutchinson, and A. Y. Cho, “Quantum Cascade Laser,” *Science (80-. ).*, vol. 264, no. 5158, pp. 553–556, Apr. 1994, doi: 10.1126/science.264.5158.553.

[2] R. Köhler *et al.*, “Terahertz semiconductor-heterostructure laser,” *Nature*, vol. 417, no. 6885, pp. 156–159, May 2002, doi: 10.1038/417156a.

[3] G. Scalari and J. Faist, “30 years of the quantum cascade laser,” *Commun. Phys.*, vol. 7, no. 1, p. 394, Dec. 2024, doi: 10.1038/s42005-024-01888-z.

[4] A. Khalatpour, M. C. Tam, S. J. Addamane, J. Reno, Z. Wasilewski, and Q. Hu, “Enhanced operating temperature in terahertz quantum cascade lasers based on direct phonon depopulation,” *Appl. Phys. Lett.*, vol. 122, no. 16, Apr. 2023, doi: 10.1063/5.0144705.

[5] X. Qi *et al.*, “Terahertz imaging of human skin pathologies using laser feedback interferometry with quantum cascade lasers,” *Biomed. Opt. Express*, vol. 14, no. 4, p. 1393, Apr. 2023, doi: 10.1364/BOE.480615.

[6] K. Singh *et al.*, “Comparison of Physical and System Factors Impacting Hydration Sensing in Leaves Using Terahertz Time-Domain and Quantum Cascade Laser Feedback Interferometry Imaging,” *Sensors*, vol. 23, no. 5, p. 2721, Mar. 2023, doi: 10.3390/s23052721.

[7] A. Demic *et al.*, “Infinite-Period Density-Matrix Model for Terahertz-Frequency Quantum Cascade Lasers,” *IEEE Trans. Terahertz Sci. Technol.*, vol. 7, no. 4, pp. 368–377, Jul. 2017, doi: 10.1109/TTHZ.2017.2705481.

[8] A. Demić, Z. Ikonić, P. Dean, and D. Indjin, “Dual resonance phonon–photon–phonon terahertz quantum-cascade laser: physics of the electron transport and temperature performance optimization,” *Opt. Express*, vol. 28, no. 26, p. 38788, Dec. 2020, doi: 10.1364/OE.410014.

[9] A. Demić, Z. Ikonić, R. W. Kelsall, and D. Indjin, “Density matrix superoperator for periodic quantum systems and its application to quantum cascade laser structures,” *AIP Adv.*, vol. 9, no. 9, Sep. 2019, doi: 10.1063/1.5095246.

[10] A. Demić, Z. Ikonić, P. Dean, and D. Indjin, “Prospects of temperature performance enhancement through higher resonant phonon transition designs in GaAs-based terahertz quantum-cascade lasers,” *New J. Phys.*, vol. 24, no. 3, p. 033047, Mar. 2022, doi: 10.1088/1367-2630/ac5b41.

[11] N. Stanojević *et al.*, “Effects of background doping, interdiffusion and layer thickness fluctuation on the transport characteristics of THz quantum cascade lasers,” *Sci. Rep.*, vol. 14, no. 1, p. 5641, Mar. 2024, doi: 10.1038/s41598-024-55700-7.

[12] B. Meng *et al.*, “Terahertz Intersubband Electroluminescence from Nonpolar m-Plane ZnO Quantum Cascade

Structures," *ACS Photonics*, vol. 8, no. 1, pp. 343–349, Jan. 2021, doi: 10.1021/acsphotonics.0c01641.

[13] N. Stanoiević, A. Demić, X. Wang, N. Vuković, D. Indjin, and J. Radovanović, "Design of Ga 2 O 3 /(AlGa) 2 O 3 Double-Barrier Resonant Tunnelling Diode," in *2024 11th International Conference on Electrical, Electronic and Computing Engineering (IcETRAN)*, Jun. 2024, pp. 1–4. doi: 10.1109/IcETRAN62308.2024.10645113.

[14] E. Riccardi *et al.*, "Short pulse generation from a graphene-coupled passively mode-locked terahertz laser," *Nat. Photonics*, vol. 17, no. 7, pp. 607–614, Jul. 2023, doi: 10.1038/s41566-023-01195-z.

[15] C. Jirauschek, M. Riesch, and P. Tzenov, "Optoelectronic Device Simulations Based on Macroscopic Maxwell–Bloch Equations," *Adv. Theory Simulations*, vol. 2, no. 8, Aug. 2019, doi: 10.1002/adts.201900018.

[16] M. Riesch and C. Jirauschek, "mbsolve: An open-source solver tool for the Maxwell-Bloch equations," *Comput. Phys. Commun.*, vol. 268, p. 108097, Nov. 2021, doi: 10.1016/j.cpc.2021.108097.

[17] L. Seitner, J. Popp, M. Haider, S. S. Dhillon, M. S. Vitiello, and C. Jirauschek, "Theoretical model of passive mode-locking in terahertz quantum cascade lasers with distributed saturable absorbers," *Nanophotonics*, vol. 13, no. 10, pp. 1823–1834, Apr. 2024, doi: 10.1515/nanoph-2023-0657.

[18] A. D. Rakić *et al.*, "Sensing and imaging using laser feedback interferometry with quantum cascade lasers," *Appl. Phys. Rev.*, vol. 6, no. 2, p. 021320, Jun. 2019, doi: 10.1063/1.5094674.

[19] C. Silvestri, X. Qi, T. Taimre, and A. D. Rakić, "Frequency combs induced by optical feedback and harmonic order tunability in quantum cascade lasers," *APL Photonics*, vol. 8, no. 11, Nov. 2023, doi: 10.1063/5.0164597.