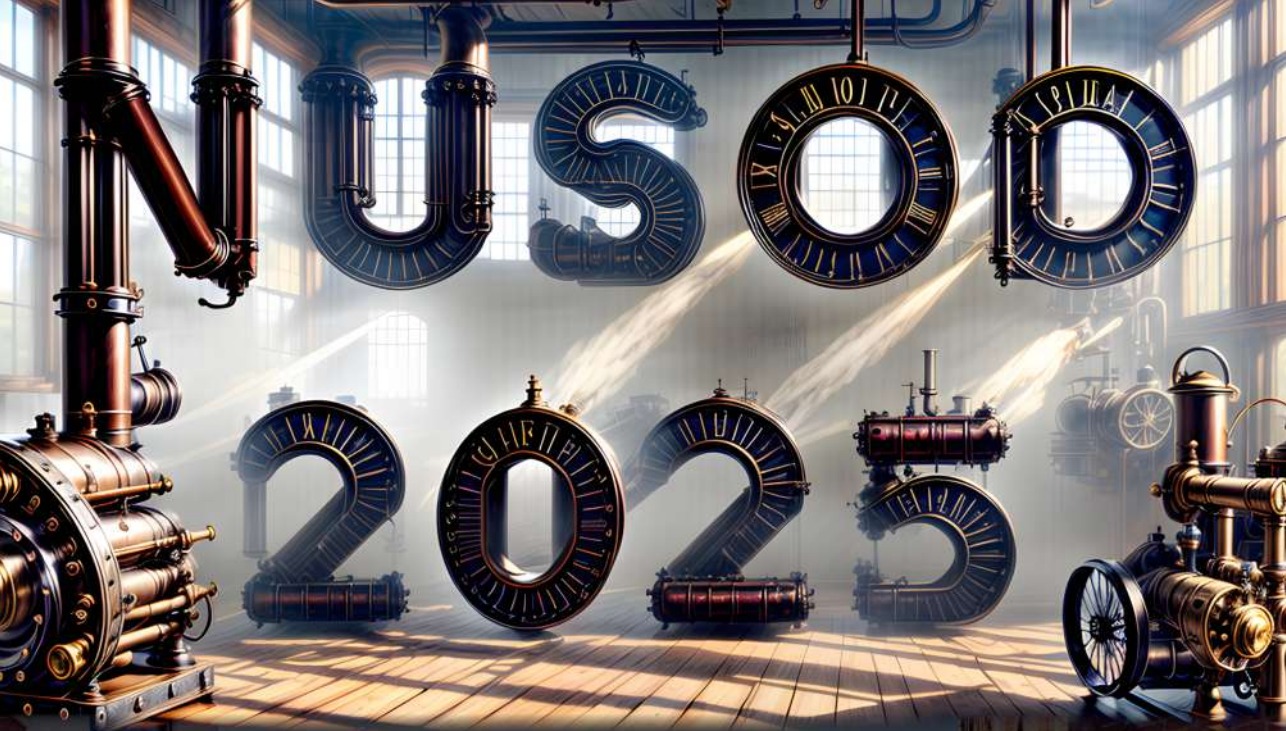




25th Anniversary Conference on
Numerical Simulation of
Optoelectronic Devices

BOOK OF ABSTRACTS

14–18 September 2025, Łódź, Poland

25th Anniversary Conference on

**Numerical Simulation
of Optoelectronic Devices**

14 – 18 September 2025
Łódź, Poland

Editors / Chairs:
Paolo Bardella and Maciej Dems

Invited Speakers

Nicola Vukovic, *School of Electrical Engineering, University of Belgrade, Serbia*, Numerical Simulations of Terahertz Quantum Cascade Laser Electronic Structure and Dynamics [MA02]

Lucio Andreani, *University of Pavia, Italy*, Bound States in the Continuum Empowering Maximum Chirality and Strong Coupling Regime in Plasmonic Metasurfaces [MB01]

Kamil Postava, *Technical University of Ostrava, Czech Republic*, Coherent and incoherent phenomena in anisotropic periodic gratings [TuA01]

David Childs, *Huawei R&D UK Ltd, Ipswich, UK*, Sooner and Better, Perfection in Compromise and Getting it Right First Time: Some Hopes and Realities of Simulation in Industry [TuA02]

Michał Matuszewski, *Institute of Physics Polish Academy of Sciences, Poland*, Strong light-matter coupling in nanostructures and quantum neural networks [TuA03]

Christian Jirauschek, *Technical University of Munich, Germany*, Density Matrix Simulations of Quantum Cascade Lasers: Optical and Microwave Dynamics [WB02]

Runzhang Xie, *Shanghai Institute of Technical Physics, Chinese Academy of Sciences, China*, Renormalization Theory and Monte Carlo Simulation of HgCdTe Single Carrier Avalanche Process [ThA01]

Lilli Kuen, *Weierstrass Institute, Germany*, Numerical study of spatio-temporal dynamics in all semiconductor PCSELs [ThB02]

Lin Zschiedrich, *JCMwave GmbH, Germany*, Efficient Photonic Component Analysis via AAA Rational Approximation [ThC01]

Thomas Christensen, *Technical University of Denmark, Denmark*, Tight-binding models for 3D photonic crystals [ThC02]

Monday, 15

Novel Materials and Devices I

8:45–10:35

chair: Prof. Franco Prati

- MA01** Extreme light control with structured nanophotonics; A. Alù; Advanced Science Research Center, City University of New York (USA) – **(KEYNOTE)**
- MA02** Numerical Simulations of Terahertz Quantum Cascade Laser Electronic Structure and Dynamics; N. Vukovic (1), M. Ignjatovic (1), N. Stanojevic (1),(2), A. Demic (3), M. Stojkovic (1), F. Perisic (1), D. Indjin (3), J. Radovanovic (1); (1) School of Electrical Engineering, University of Belgrade (SRB); (2) Vlatacom Institute of High Technologies, Belgrade (SRB); (3) School of Electronic and Electrical Engineering, University of Leeds (UK) – **(INVITED)**
- MA03** Solution-Processed Heterojunction Oxide Thin-Film Transistors for Displays; W. Cai; Chongqing University (CHN)
- MA04** Solvent-free Synthesis of Hybrid Copper Halides for High-performance White Emission and X-ray Imaging; S. Zhao; Chongqing University (CHN)

Photonics I

11:05–13:10

chair: Prof. Andrea Alù

- MB01** Bound States in the Continuum Empowering Maximum Chirality and Strong Coupling Regime in Plasmonic Metasurfaces; L. Andreani (1), H. Ali (1), G. Pellegrini (1), E. Petronijevic (2); (1) University of Pavia (ITA); (2) Sapienza University of Rome (ITA) – **(INVITED)**
- MB02** Investigation on digital twin model of 3×3 Mach-Zehnder Interferometer mesh; T. Ma (1), A. Marchisio (1), F. Da Ros (2), V. Curri (1), A. Carena (1), P. Bardella (1); (1) Politecnico di Torino (ITA); (2) Danmarks Tekniske Universitet (DEN)
- MB03** Novel Variable Confinement SOAs Modelling; C. Cruz (1), C. Calò (1), H. Carrere (2); (1) III-V Lab, a joint laboratory between Nokia Bell Labs, Thales Research & Technology and CEA-LETI, Palaiseau (FRA); (2) Laboratoire de Physique et Chimie des Nano-Objets, Université de Toulouse, Toulouse (FRA)
- MB04** On-chip Rewritable Phase-change Metasurfaces for Programmable Optical Routing; S. Zarei; Department of Electrical Engineering, Sharif University of Technology, Tehran, Iran
- MB05** Graphics Processor Unit Accelerated Design of Multimode Interference Reflectors; G. M. Jandu, P. M. Smowton; The school of physics and astronomy, Cardiff University, Cardiff (UK)
- MB06** A Tunable MOEMS Open Microring Resonator for the Detection of Water Concentration in Ethanol Solutions; N. Hanine (1), A. Buzzin (1), L. Giannini (1), A. Alaeddini (1), N. P. Belfiore (2), R. Asquini (1); (1) Sapienza University of Rome (ITA); (2) Roma Tre University (ITA)

Abstracts

Numerical Simulations of Terahertz Quantum Cascade Laser Electronic Structure and Dynamics

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Abstract—In this work, we present our recent numerical modelling results of the terahertz frequency quantum cascade laser active region. Electronic structure calculations are performed using the derivative transfer matrix method, while dynamics simulations are based on the Maxwell-Bloch formalism in various QCL configurations and model complexities.

Keywords— terahertz quantum cascade laser, transfer matrix method, density matrix, Maxwell-Bloch equations, passive mode-locking

I. INTRODUCTION

Terahertz quantum cascade lasers (THz QCLs) [1], [2] applications span from local oscillators for heterodyne spectroscopy in astronomy, to real-time THz imaging, biomedical imaging, dual-comb spectroscopy with QCL frequency combs, [3], etc. Recent thermoelectric cooling [4] and remarkable bandwidth coverage will drive this technology to new fields of research. In this contribution, we present our recent numerical modelling results of these devices in a Fabry-Perot (FP) configuration. In particular, the electronic structure is obtained using the derivative transfer matrix method, while the laser dynamics is modelled using macroscopic Maxwell-Bloch (MB) equations, owing to their intuitiveness, flexibility, and numerical efficiency. One of the major disadvantages of transfer matrix approaches is the necessity of sweeping parameters in a shooting-like manner, which results in lower precision in comparison to

finite difference methods (FDM). The recently developed machine precision derivative transfer matrix method [5] outperforms FDM by handling higher spatial resolution and having better time performance while computing eigenvalues with high precision and linear numerical complexity. The main idea of the derivative transfer matrix method (dTMM) is solving the eigenvalue problem by numerically finding the zeroes of the analytically calculated first derivative of the transfer matrix using numerically efficient zero finding algorithms, instead of using the numerically complex minima finding algorithms, as in the standard TMM.

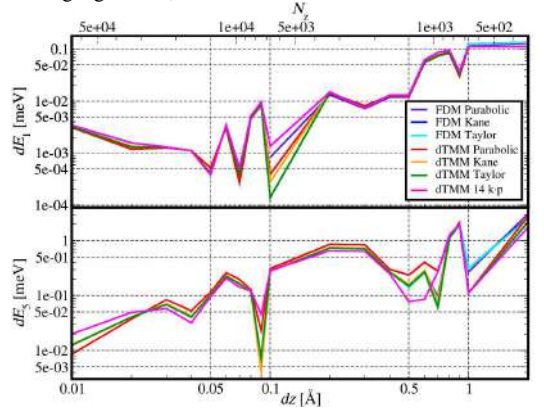


Fig. 1. Convergence of calculated first and fifth energy states vs spatial step size (bottom x-axis) and spatial resolution (top x-axis) for two-well record high-temperature THz QCL from [4]. The convergence is calculated as the energy difference between consecutive solutions as the spatial resolution is varied. The range of spatial step size was an array between 0.01 and 2 Å.

Fig. 1 shows dTMM versus FDM tested on the standard Schrödinger equation under effective mass approximation

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with parabolic subbands, on two-band Kane nonparabolicity model and its Taylor approximation, and finally on a 4th-order Schrödinger equation that accounts for nonparabolic subbands using the 14-band $\mathbf{k}\cdot\mathbf{p}$ approach, which takes into account the interaction of the lowest conduction band with the light-hole and heavy-hole valence bands, split-off band, and three higher conduction bands.

Investigation of light-matter interactions with applications in metrology and ultrahigh-speed communications requires ultrashort terahertz pulses with large intensities, only recently achieved using passively mode-locked bound-to-continuum THz QCL [6]. Mode-locking operation with 4-ps-long pulses was realized using graphene-based saturable absorber (SA) stripes distributed along the laser cavity. Here, we perform self-consistent carrier transport density matrix simulations [7] of the QCL active region and extract the eigenenergies, optical dipole moments, scattering and dephasing rates, material gain, current density, and frequency using laser parameters from [8] for the structure operating at 3 THz. The active region dynamics is modelled using MB equations, with and without graphene saturable absorber, using full-wave treatment and also employing rotating wave approximation (RWA) and slowly varying envelope approximation (SVEA) to reduce the numerical load. We try a two-level model for mode-locking described in [9], but we are also interested in simulations with an arbitrary number of laser levels [10], [11]. Interesting dynamics arise when effective semiconductor MB equations are applied in modelling QCL in a self-mixing configuration, which was investigated in [12].

II. RESULTS AND DISCUSSION

Time evolution and spatial distribution of the electric field inside the resonator of length 2.37 mm are calculated by solving MB equations and adopting SVEA and RWA. Nine quantized levels per period in the active region were considered. Fig. 2 shows the electric field waveform on the right mirror without a saturable absorber. The electric field oscillates rapidly and the dominant frequency is around 3 THz. The simulation takes into account the attenuation at the mirrors, GVD and charge carrier diffusion.

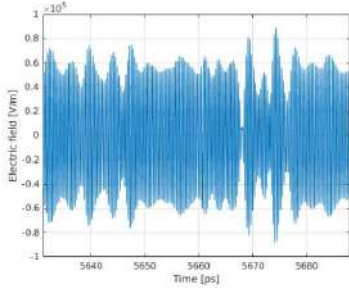


Fig. 2. Electric field waveform at the right mirror for the duration of one roundtrip without SA.

Simulation results when the effect of the SA is taken into account using the equation for slow absorber are shown in Fig. 3, where pulses with distinct intensity peaks can be seen occurring at time intervals of one roundtrip. Intensity waveform on the right mirror is a consequence of the movement of the pulse inside the resonator, where it is reflected alternately between the left and right mirrors.

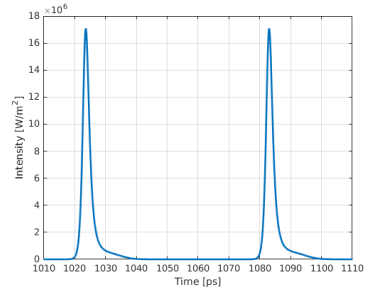


Fig. 3. The intensity at the right mirror when graphene SA is included.

III. CONCLUSION

In this paper, we present the results of our numerical simulations of the THz QCL active region, where we use a novel numerical method for electronic structure calculation and Maxwell-Bloch equations for modelling dynamics.

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