Numerical Simulations of Terahertz Quantum Cascade Laser Electronic Structure and Dynamics

Nikola Vuković
School of Electrical Engineering
University of Belgrade
Belgrade, Serbia
nvukovic@etf.bg.ac.rs

Milan Ignjatović
School of Electrical Engineering
University of Belgrade
Belgrade, Serbia
ignjatovic@etf.bg.ac.rs

Novak Stanojević
School of Electrical Engineering
University of Belgrade
Vlatacom Institute of High Technologies
Belgrade, Serbia
novak.stanojevic@vlatacom.com

Aleksandar Demić
School of Electronic and Electrical Engineering
University of Leeds
Leeds, United Kingdom
A.Demic@leeds.ac.uk

Mihailo Stojković
School of Electrical Engineering
University of Belgrade
Belgrade, Serbia
sm180469d@student.etf.bg.ac.rs

Filip Perišić
School of Electrical Engineering
University of Belgrade
Belgrade, Serbia
fperisic12@gmail.com

Dragan Indjin
School of Electronic and Electrical Engineering
University of Leeds
Leeds, United Kingdom
D.Indjin@leeds.ac.uk

Jelena Radovanović
School of Electrical Engineering
University of Belgrade
Belgrade, Serbia
radovanovic@etf.bg.ac.rs

***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, bio-medical 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 .

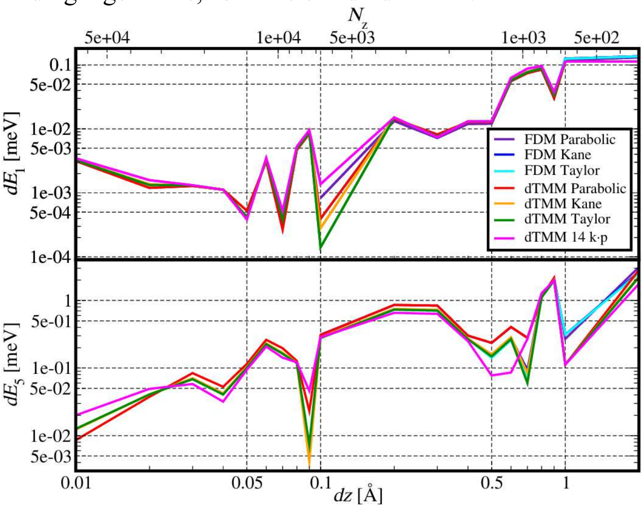

Fig. 1. Convergence of calculated first and fifth energy states vs spatial step size (bottom x-axis) and spatial resolution (top x-axis) for two-well record high-temperature THz QCL from [4]. The convergence is calculated as the energy difference between consecutive solutions as the spatial resolution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

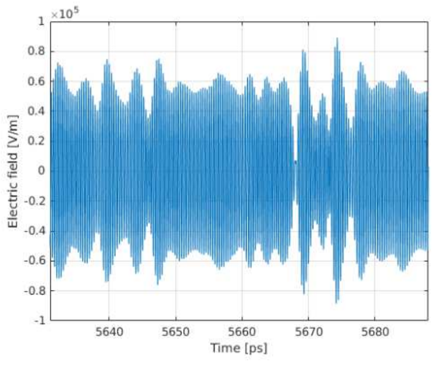

Fig. 2. Electric field waveform at the right mirror for the duration of one roundtrip without SA.

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.

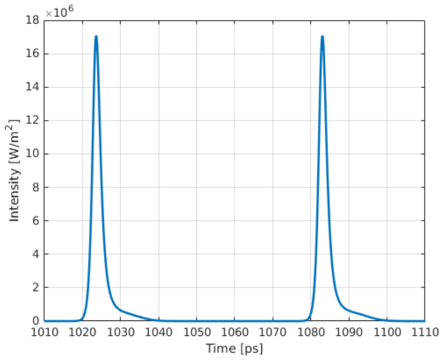

Fig. 3. The intensity at the right mirror when graphene SA is included.

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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