

# Dynamic Simulation of Quantum Cascade Laser Structures with Optical Nonlinearities

Christian Jirauschek

Institute for Nanoelectronics  
Technische Universität München  
Arcisstr. 21, D-80333 München, Germany  
Email: jirauschek@tum.de

**Abstract**— A dynamic modeling approach for quantum cascade lasers (QCLs) with optical nonlinearities is presented. To describe the coherent nonlinear interaction between the optical cavity field and the electrons, we use an extended Maxwell-Bloch equation model, coupled to hybrid density matrix/ensemble Monte Carlo carrier transport simulations. The resulting multi-domain approach offers high numerical efficiency as required for spatiotemporally resolved simulations, and is self-consistent, avoiding the use of empirical input parameters. Numerical results are shown for a QCL-based frequency comb source, and validated against experimental data.

**Keywords**— *Quantum cascade lasers; nonlinear optical devices; optical mixing; laser mode locking*

## I. INTRODUCTION

— The quantum cascade laser (QCL) is a unipolar semiconductor-based light source, operating in the mid-infrared (MIR) or terahertz (THz) portions of the spectral region. For a given material system, the lasing wavelength can be adjusted over a broad spectral range by adequately designing the quantum well active region. The optical field dynamics in QCLs is greatly influenced by resonant optical nonlinearities arising in the quantum well structure. The coherent nonlinear light-matter interaction can lead to the formation of optical instabilities affecting the emitted spectrum [1], and is increasingly exploited in a targeted manner to implement innovative functionalities into QCL devices. In particular, four-wave mixing plays a crucial role for the generation of QCL-based frequency combs [2]. Furthermore, the coherent nonlinear light-matter interaction greatly affects ultrashort pulse generation by active mode-locking [3], [4], and is speculated to enable self-induced transparency mode-locking in QCLs [5].

The targeted development of QCL sources exploiting coherent nonlinear light-matter interaction effects requires careful design based on sophisticated modeling approaches. These have to consider the time-dependent coupled electron and optical field dynamics along the propagation axis, which requires a numerically efficient model. The widely used Maxwell-Bloch (MB) equations depend however on empirical input parameters [1], [6], affecting the versatility of the

approach. Here, we present a numerically efficient extended MB description of the coherent light-matter interaction [7], coupled to an advanced hybrid density matrix/ensemble Monte Carlo (EMC) carrier transport model which provides the electron lifetimes and dephasing rates.

## II. SIMULATION APPROACH

In [7], an extended MB model coupled to EMC carrier transport simulations has been introduced. Instead of EMC, we here employ a hybrid density matrix/EMC approach, which can adequately treat incoherent tunneling transport, forming a bottleneck for thick barriers [8].

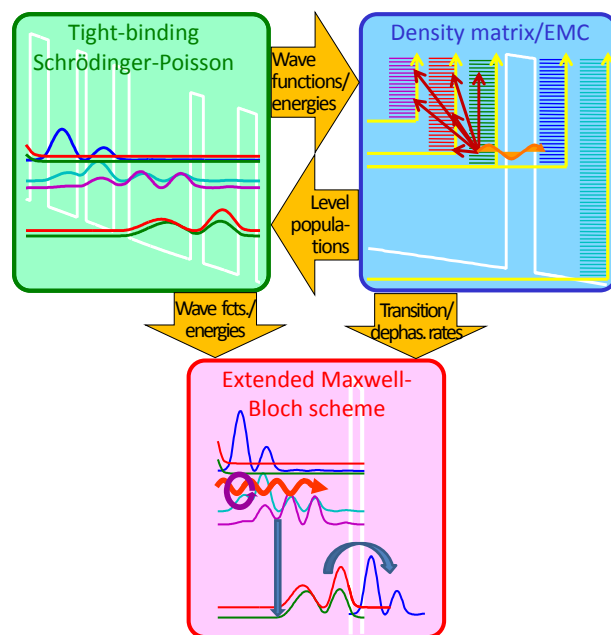


Fig. 1. Schematic illustration of our multi-domain modeling approach for the dynamic simulation of QCL structures with optical nonlinearities.

In our implementation, the phase relaxation rates, which determine the tunneling dephasing as well as the optical transition linewidths, are self-consistently extracted, considering lifetime broadening [9] as well as pure dephasing based on Ando's model [10]. This completely eliminates the need for empirical input parameters. The resulting multi-

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domain simulation scheme is illustrated in Fig. 1. The Schrödinger-Poisson solver delivers the electron wavefunctions and eigenenergies of the quantum well structure in a tight-binding approximation, which is advantageous for the evaluation of tunneling transport in the hybrid density matrix/EMC approach [8]. The calculated scattering and dephasing rates, along with the wavefunctions and eigenenergies, serve as an input for the MB model, which describes the coherent nonlinear light-matter interaction between the laser levels as well as the tunneling dynamics between the injector and upper laser level. The MB equations have been extended to account for further important effects, such as chromatic dispersion and spatial hole burning [7].

### III. SIMULATION OF QCL-BASED FREQUENCY COMBS

The nonlinear light-matter interaction in the QCL active region induces a coupling between the longitudinal cavity modes, which is utilized for the generation of frequency combs [2], [11] and picosecond pulses [3]. We have applied our simulation approach, described in Section II, to an experimental THz frequency comb QCL structure [11].

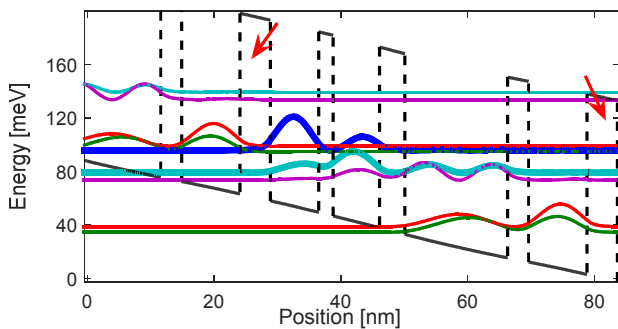


Fig. 2. Conduction band profile and probability densities of the tight-binding states for the investigated frequency comb QCL structure.

In Fig. 2, the conduction band profile of the active region is displayed. In our extended MB model, the coherent nonlinear interaction between the electrons in the laser levels (marked by thick lines in Fig. 2) and the optical field is considered. Furthermore, tunneling across the thick injection barriers,

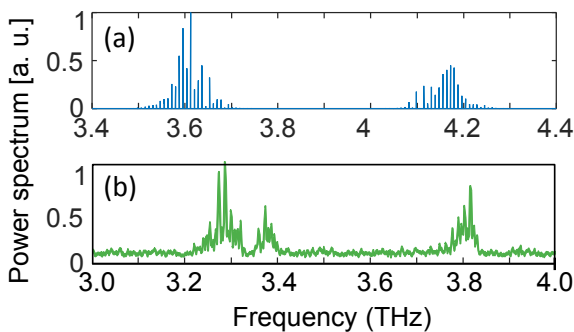


Fig. 3. Simulated (a) and experimental (b) optical power spectrum of the QCL frequency comb source in [11].

marked by arrows, is accounted for. The scattering transitions between the levels are modeled using the scattering rates extracted from the density matrix/EMC approach. Figure 3 contains a comparison between the self-consistently simulated and the experimentally measured frequency comb spectrum. Good agreement is found; in particular, splitting into a high and a low frequency lobe is observed both in theory and experiment.

### IV. CONCLUSION

In conclusion, by combining an extended MB model with a density matrix/EMC approach, we have developed a self-consistent, numerically efficient tool for the dynamic simulation of QCL structures with optical nonlinearities. Comparison of numerical and experimental data for a QCL-based frequency comb source yields good agreement, confirming the validity of our approach.

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