Density Matrix Simulations of Quantum Cascade Lasers: Optical and Microwave Dynamics

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***Abstract*—We discuss a self-consistent simulation approach for the dynamic modeling of quantum cascade lasers (QCLs). These feature a quantum-engineered active region, enabling unique functionalities such as frequency comb generation in the mid-infrared and terahertz range. The model combines a density matrix description of the active region with electromagnetic modeling of the microwave and optical propagation in the laser waveguide. Based on simulations of experimental QCL structures, we demonstrate the accuracy and numerical efficiency of the model. Due to its versatility, the approach can be adapted to different waveguide configurations and also to other quantum optoelectronic devices.**

***Index Terms*—Quantum cascade lasers, laser mode locking, microwave photonics**

I. Introduction

Quantum-engineered optoelectronic devices feature a nanostructured active region, offering unprecedented possibilities. The most prominent examples are the quantum dot, interband cascade and quantum cascade laser (QCL). The latter is a unipolar device, utilizing transitions between quantized states in the conduction band of a multi-quantum-well structure. In this way, the lasing wavelength becomes independent of the material band gap and can be custom-tailored over a wide range of the mid-infrared and terahertz region. Furthermore, the quantum active region exhibits unique dynamic gain properties and strong nonlinear effects such as four-wave mixing. These features can be exploited for the realization of compact, electrically pumped short-pulse and frequency comb sources at wavelengths hardly accessible to conventional diode lasers [1], [2]. More specifically, mode-locking techniques are utilized to generate periodic waveforms, including short-pulse trains and optical fields featuring broadband comb-like spectra. These laser sources open up a wide range of applications in fields such as sensing, metrology, imaging and communications. Recently, also more exotic optical waveforms have been realized, such as soliton crystals and other harmonic states featuring multiple optical waveform periods within a single roundtrip [3], [4].

Besides the quantum active region, also the optical waveguide plays an important role for dynamic operation, for example in the context of dispersion compensation [1]. Furthermore, adequately designed waveguides simultaneously act as microwave transmission lines, enabling propagation of microwave modulations in the pump bias along with the optical waveform. Recent research has started exploiting this design degree of freedom for the implementation of novel functionalities. For active mode-locking where waveform generation is triggered by external bias modulation, the optical and microwave co-propagation increases the modulation efficiency and has for example enabled the realization of quantum walk combs in QCLs, which are especially flat and broadband [5]. On the other hand, in free-running QCLs the optical dynamics leads to a modulation of the current along the waveguide, which has been exploited for photonics-based millimeter wave generation and can perspectively also be utilized for the self-stabilization of frequency combs [6], [7].

A targeted development of waveform-generating QCLs requires dynamic simulation models combining accuracy and versatility with numerical efficiency. In this context, semi-classical approaches employing a density matrix model for the quantum active region and a description of the optical waveguide field based on Maxwell's or related equations have proven particularly useful [8]. To incorporate above discussed microwave effects, the waveguide model has recently been adequately extended [9]. In the following, we describe the model and discuss simulation results of an experimental structure for photonics-based millimeter wave generation. Notably, by using a generalized multilevel Hamiltonian rather than the two-level model employed in Maxwell-Bloch equations, the electron dynamics in the active region due to light-matter and potentially also microwave-matter interaction can be self-consistently described.

II. Model

Our simulation approach combines a multi-level density matrix model of the quantum active region with optical and microwave propagation equations for the waveguide. The active region is at any spatial grid point modeled by a representative quantum system with the density operator $\hat{\rho}$. The time evolution is governed by a Lindblad-type equation

$$\mathrm{i}\hbar\partial_t\hat{\rho} = \left[\hat{H}_0 - \hat{d}E, \hat{\rho}\right] + \hat{D}\left(\hat{\rho}\right), \qquad (1)$$

with the Hamiltonian $\hat{H}_0$, optical dipole operator $\hat{d}$, and dissipator $\hat{D}\left(\hat{\rho}\right)$. For numerical efficiency, we introduce the widely used rotating-wave approximation. To this end, we write the optical field in terms of its forward and backward propagating envelopes $E^{\pm}(x,t)$ as

$$E = \Re\left\{\left[E^{+}\exp\left(\mathrm{i}\beta x\right) + E^{-}\exp\left(-\mathrm{i}\beta x\right)\right]\exp\left(-\mathrm{i}\omega_{\mathrm{c}}t\right)\right\}, \tag{2}$$

with the propagation constant β and center frequency ω_{c}, and discard the rapidly oscillating terms arising in (1). To further reduce the numerical effort, we assume that the waveguide geometry allows reduction of the model to a single spatial coordinate x along the optical propagation direction [8]. Within this framework, the optical propagation in the waveguide can be modeled by [8]

$$\partial_t E^{\pm} = \mp v_{\mathrm{g}}\partial_x E^{\pm} + f^{\pm} - v_{\mathrm{g}} a E^{\pm}/2 - \mathrm{i} v_{\mathrm{g}}\beta_2\partial_t^2 E^{\pm}/2, \tag{3}$$

with the power loss coefficient a, group velocity v_{g} and group velocity dispersion coefficient β_2. The polarization contribution of the quantum system $f^{\pm}(x,t)$ is computed from (1). By adding the transmission line equations

$$\begin{aligned}\partial_x u &= -L'\partial_t i - R'i\,,\\ \partial_x i &= -C'\partial_t u - Jw\end{aligned} \tag{4}$$

to the model, microwave propagation along the waveguide can be described in terms of the voltage $u(x,t)$ and current $i(x,t)$. Here, the microwave properties of the waveguide are characterized via the distributed inductance L', capacitance C' and resistance R'. For realistic simulation results, especially the frequency dependence of R' must be accounted for in the numerical scheme [9]. The current density $J(x,t)$ through the quantum active region of width w is again computed from (1). On the other hand, $\hat{H}_0$, $\hat{d}$ and $\hat{D}$ in (1) generally depend on u obtained from (4). A coupled simulation of (1), (3) and (4) provides a closed model for the quantum, optical and microwave dynamics in the device.

III. Simulation Results

We apply above simulation approach to an experimental QCL structure for photonics-based millimeter wave generation [6]. The Hamiltonian, optical dipole moments and dissipation rates in (1) are extracted from carrier transport simulations [10]. Furthermore, the optical waveguide parameters are obtained from literature, and the microwave model is taken from [9]. The setup is simulated over 10,000 roundtrips to ensure convergence. The results depend on the exact choice of transmission line parameters, demonstrating the influence of the waveguide microwave characteristics on the overall dynamic QCL operation. In Fig. 1, the simulated instantaneous intensity and bias at the right facet are displayed for an exemplary waveguide, along with the associated power spectral densities. Overall, the results show good agreement with experimental data [6].

In conclusion, the presented simulation approach enables the targeted design of QCL devices for the generation of optical waveforms and microwave fields. Furthermore, since the model employs a multi-level density matrix description of the active region, it is quite versatile and may be adapted to other quantum optoelectronic devices, such as interband cascade and quantum dot lasers.

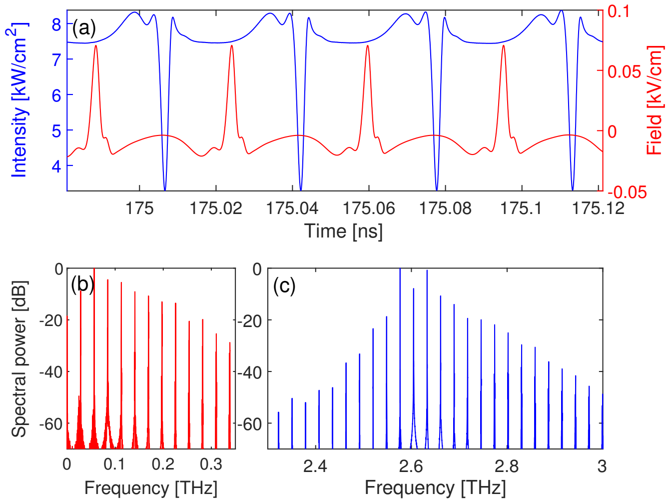

Fig. 1. (a) Outcoupled optical intensity and AC bias field at the right facet. (b) Power spectral density of the microwave signal. (c) Optical power spectrum.

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