Modeling of THz Comb Emission in Difference-Frequency Quantum Cascade Lasers

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***Abstract*—The generation of terahertz (THz) frequency comb emission by intracavity difference frequency generation (DFG) in a mid-infrared (mid-IR) quantum cascade laser (QCL) is a promising alternative to direct THz QCL frequency comb generation. Concerning their room temperature operation capabilities, these devices are well suited for applications in rotational molecular spectroscopy and sensing. In order to better understand the second-order nonlinear mixing process required for the THz frequency comb generation, we present an extensive analysis of such THz DFG-QCL comb devices using a full-wave Maxwell-Bloch equation solver. All input parameters for the Maxwell-Bloch simulations, e.g. scattering rates or dephasing rates, are calculated self-consistently using an ensemble Monte Carlo simulation toolbox.**

I. Introduction

In quantum cascade lasers the desired transition frequency and other optical and electrical properties such as the electron transport are selected by quantum engineering. QCL laser sources in the mid-IR or THz regime can be composed by a suitable choice of the well-established material systems. Hence, this kind of semiconductor laser is favorable for closing the THz gap between microwaves and optics. In recent years the generation of QCL frequency combs both in the mid-IR and THz regime was demonstrated [1]. Unfortunately, the direct THz QCL operation at room temperature is quite difficult to achieve, as the THz photon energy is well below the thermal energy of $26\,\mathrm{meV}$, resulting in thermal carrier redistribution, which is detrimental for the buildup of population inversion [2]. However, a new THz QCL design with a maximum operating temperature of $250\,\mathrm{K}$ has recently been published opening up the door to temperature regions accessible by thermoelectric Peltier cooling [3].

As direct THz QCL devices still have problems with the continuous-wave (CW) operation at elevated temperatures, an alternative approach based on intracavity difference frequency generation in dual-wavelength mid-IR QCL sources is favorable to overcome the limitations of operation temperature and frequency tunability. A major advantage of THz DFG-QCLs is the stable THz operation at room temperature, without requiring population inversion between upper and lower laser level. The first THz DFG-QCL device was introduced in 2007 [4] and since then great effort has been put into the engineering and development of such devices [5]. QCL active regions with a large second-order nonlinear susceptibility were designed, to obtain an efficient DFG THz process. Here, the two mid-IR pump frequencies in the QCL cavity interact with each other via a nonlinear mixing process and generate the favored THz radiation in the active region by downconversion. The first THz DFG-QCL designs with modal phase matching of both THz and mid-IR modes in a single waveguide suffered from excessive THz absorption [4]. Implementing a new waveguide concept utilizing a Cherenkov phase-matching scheme greatly improved the performance by emitting the THz radiation into the substrate [6]. The THz radiation can now be efficiently extracted over the full device length. Furthermore, the replacement of stacked bound-to-continuum active regions by dual-upper-state (DAU) active regions resulted in a stronger nonlinearity due to additional DFG triplet states while keeping the gain curve comparably broad [7]. With DAU designs broadband THz frequency combs were generated [8]. By mixing a single mid-IR mode selected by an integrated largely frequency detuned distributed feedback (DFB) grating with a frequency comb centered at a second mid-IR pump frequency in the Fabry-Perot (FP) cavity, a broadband THz frequency comb can be generated.

The open-source solver tool mbsolve for the full-wave generalized Maxwell-Bloch equations is used to model such a broadband THz DFG-QCL frequency comb devices [9], [10]. The evolution of the QCL quantum system is described by the optical Bloch equations coupled to Maxwell's equations, which capture the optical field description. The generalized one-dimensional Maxwell-Bloch equations are treated here without invoking the rotating wave approximation (RWA). This is especially important for DFG-QCL devices, as they cover a broadband spectrum extending from the THz to the mid-IR regime. For the Maxwell-Bloch simulations all necessary parameters to describe the QCL quantum system are calculated self-consistently with our in-house Monaco framework, a quantum cascade device simulation tool consisting of a Schrödinger-Poisson solver and an ensemble Monte Carlo (EMC) simulation tool [11].

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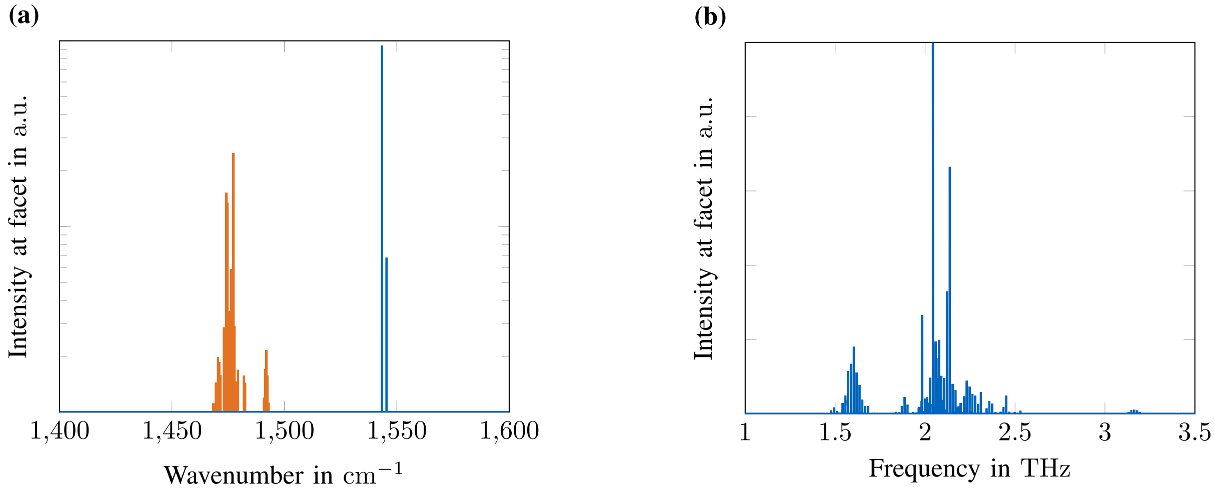

Fig. 1: Simulated mid-IR (a) and THz (b) spectra of the DFG-QCL at a temperature of $78\,\mathrm{K}$. The simulation parameters are determined from EMC simulations for an applied voltage of $13.5\,\mathrm{V}$.

II. Simulation

The modeled THz DFG-QCL design consists of a DAU active region, which is based on strain-compensated InGaAs/InAlAs [7], [8]. A single period DFB grating defined by nanoimprint lithography is used for single mode DFB lasing at $\lambda_{\mathrm{DFB}} = 6.5\,\mathrm{\mu m}$ and FP frequency comb emission is achieved around $\lambda_{\mathrm{FP}} \sim 6.9\,\mathrm{\mu m}$. By mixing the broadband FP emission with the single DFB mode, a THz comb spectrum extending from $1.5\,\mathrm{THz}$ to $3.3\,\mathrm{THz}$ is obtained. Here, it is crucial to mention, that the DFG mode has to be largely detuned from the gain maximum to avoid the suppression of the broadband FP emission.

For the spatiotemporal simulation of the THz DFG-QCL device, we consider optical transitions between two upper laser levels and three lower laser levels (miniband). The injection of charge carriers into the upper laser levels is here modeled by resonant tunneling from two injector states of the adjacent period. The corresponding dipole moments and anticrossing energies are added to the quantum mechanical description of the DFG-QCL system. To simulate the nonlinearities in the active gain medium thoroughly, we add three triplets of states responsible for the resonant DFG process. Using our EMC input parameters, a total second-order nonlinear susceptibility $\left|\chi^{(2)}\right| \approx 12\,\mathrm{nm\,V^{-1}}$ at a DFG frequency of around $2.5\,\mathrm{THz}$ is calculated. The obtained DFG-QCL simulation results are depicted in Fig. 1(a) for the mid-IR spectrum and in Fig. 1(b) for the THz frequency comb. Both spectra compare reasonably well with the experimentally measured results [8]. As our simulated gain curve exhibits a slight blue shift in comparison to experimental results, the THz frequency gap between the FP comb and the two reference modes is slightly smaller as compared to the experiment.

III. Conclusion

In this paper, Maxwell-Bloch simulation results of a broadband THz DFG-QCL frequency comb approach are presented. The simulation results are in good agreement with the experimental measurements. In comparison to the experiment, the simulated mid-IR FP frequency comb is slightly shifted towards higher frequencies resulting in a small red-shift of the THz frequency comb. We obtain a THz spectrum extending from $1.4\,\mathrm{THz}$ to $2.6\,\mathrm{THz}$, which reproduces the measured ultra-broadband THz emission.

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