# Modeling of THz Difference-Frequency Comb Generation in Mid-Infrared Quantum Cascade Lasers

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**Short Abstract:** Portable terahertz (THz) frequency comb emission sources are highly desired for applications in rotational molecular spectroscopy and sensing. As direct THz quantum cascade laser (QCL) frequency comb generation is not achievable at room temperature, THz comb generation based on intracavity difference frequency generation (DFG) in mid-infrared (mid-IR) QCLs is a promising alternative. Here, we present a numerical study of THz DFG-QCL comb generation in mid-IR QCLs using a full-wave Maxwell-Bloch equation solver.

#### 1. Introduction

The quantum cascade laser is one of the leading laser sources for THz and mid-IR emission, besides continous-wave operation, the formation of QCL frequency combs based on four-wave mixing processes is practicable [1]. Apart from direct THz QCL operation, the generation of THz radiation is also possible by intracavity difference frequency generation in dual-wavelength mid-IR QCL sources, having the advantages of room temperature operation and wide frequency tunability. Here, a nonlinear mixing process of two mid-IR pump modes results in the downconversion to the desired THz frequency. By implementing a new waveguide concept based on a Cherenkov phase-matching scheme for efficient THz outcoupling and introducing a dual-upperstate (DAU) active region providing strong second-order nonlinearity, the performance of THz DFG-QCL devices could be improved significantly within the last two decades [2]. The generation of broadband THz frequency combs can be accomplished by mixing a single mid-IR mode in a frequency detuned distributed feedback (DFB) grating with a Fabry-Perot (FP) frequency comb centered at a second mid-IR pump frequency [3]. To model such a broadband THz DFG-QCL frequency comb, we use the open-source solver tool mbsolve for the full-wave generalized Maxwell-Bloch equations [4]. Here, the optical Bloch equations for the evolution of the quantum system are coupled to Maxwell's equations for the classical description of the optical field. With our in-house Monaco framework, a quantum cascade device simulation tool consisting of a Schrödinger-Poisson and an ensemble Monte Carlo (EMC) solver, we can calculate all necessary parameters to describe the QCL quantum system considered in the open-source tool mbsolve for the Maxwell-Bloch simulations [5].

#### 2. Simulation

The modeled THz DFG-QCL design consists of a single-phonon resonance depopulation structure based on strain-balanced InGaAs/InAlAs [6, 3]. Here, a 4 mm-long waveguide is patterned with a 1.5 mm DFB grating and finished with a high-reflection (HR) coated back facet. A single period DFB grating defined by e-beam lithography and dry etching is used for single mode DFB lasing at  $\lambda_{\text{DFB}} = 7.25 \,\mu\text{m}$ , which is detuned by  $80 \,\text{cm}^{-1}$  from the gain maximum. In Fig. 1 (a), the gain curve obtained with EMC and the experimentally measured curve are illustrated and match well. The DFB grating is defined by a period length  $\Lambda = 1.15 \,\mu\text{m}$  with a coupling constant  $\kappa =$  $35 \,\text{cm}^{-1}$ . Broadband FP frequency comb emission is obtained at a wavelength of around  $\lambda_{\text{FP}} \sim$  $7.81 \,\mu\text{m}$ . For the spatiotemporal simulation of the THz DFG-QCL device, we use a tight-binding



**Fig. 1:** (a) Comparison of EMC simulated and experimental results for the normalized gain curve of the THz DFG-QCL structure. Simulated mid-IR (b) and THz (c) spectra of the DFG-QCL at a temperature of 293 K. The simulation parameters are determined from EMC simulations for an applied voltage of 10.46 V.

solution for the wavefunctions giving rise to one upper laser level and three lower laser levels. Here, the injection of charge carriers into the upper laser level is modeled by resonant tunneling from two injector states of the adjacent period. All necessary mechanisms, e.g. DFG, incoherent tunneling and optical transitions are fully taken into account by adding the corresponding dipole moments and anticrossing energies to the system Hamiltonian. Using our EMC input parameters and considering three DFG triplets of states, a second order nonlinear susceptibility of  $|\chi^{(2)}| \approx 3.52 \text{ nm/V}$  at a DFG frequency of around 3 THz is calculated. The obtained DFG-QCL simulation results are depicted in Fig. 1 (b) for the mid-IR spectrum and in Fig. 1 (c) for the THz frequency comb. By mixing the mid-IR FP comb with the DFB reference mode, a THz comb extending from 2.5 THz to 4.3 THz is generated.

## 3. Conclusion

In summary, we performed full-wave Maxwell-Bloch simulations of THz frequency comb emission in a DFG-QCL device. The room temperature THz spectrum around 3 THz is in good agreement with experimental measurements. Here, the obtained results are based on broadband FP frequency comb lasing states. The experimentally documented FP multimode harmonic state at lower currents is also intriguing, and will be investigated in more detail in the future.

### References

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