Numerical Optimization of Quantum Cascade Detector Heterostructures

Johannes Popp[1], Michael Haider[*1], Martin Franckié[2], Jérôme Faist[2], and Christian Jirauschek[1]
[1]Department of Electrical and Computer Engineering, Technical University of Munich, 80333 Munich, Germany
[2]Department of Physics, ETH Zurich, Auguste-Piccard-Hof 1, 8093 Zurich, Switzerland
[*]michael.haider@tum.de

***Abstract*—We demonstrate a Bayesian optimization framework for quantum cascade (QC) devices in the mid-infrared (mid-IR) and terahertz (THz) regime. The optimization algorithm is based on Gaussian process regression (GPR) and the devices are evaluated using a perturbed rate equation approach based on scattering rates calculated self-consistently by Fermi's golden rule or alternatively extracted from an Ensemble Monte Carlo (EMC) simulation tool. Here, we focus on the optimization of a mid-IR quantum cascade detector (QCD) at a wavelength of $4.7\,\mu\mathrm{m}$ with respect to the specific detectivity as a measure for the signal to noise ratio. At a temperature of $220\,\mathrm{K}$ we obtain an improvement in specific detectivity by a factor ~ 2.6 to a value of 2.6×10^8 Jones.**

I. Introduction

The detection of light in the mid-IR and THz regime can be accomplished by optical intersubband transitions (ISB) between quantized levels in the conduction band of semiconductor heterostructures. There exist different working principles for ISB photodetectors which are divided mostly into two subtypes consisting of photoconductive quantum well infrared photodetectors (QWIPs) and photovoltaic QCDs. The focus of this work lies on the optimization of quantum cascade detectors [1] [2], which are commonly based on the design of quantum cascade lasers (QCLs). By utilizing the asymmetric conduction band potential in quantum cascade structures a net photocurrent due to photon assisted excitation of electrons is measurable without applying an external bias. Due to the absence of bias, dark current noise in QCDs is negligible and the dominating noise contribution is thus given by Johnson noise.

The well-established simulation models for QCLs (e.g., EMC and rate equations [3]) can be adapted to QCDs [4]–[7]. The fast and low-noise operation of QCDs utilizes them for applications such as spectroscopy in combination with QCL frequency combs. Thus, the systematic design optimization of QCDs is an essential task for obtaining highly sensitive detectors. In terms of QCLs genetic [8] as well as Bayesian [9] optimization algorithms have been used. The latter has been shown to be much faster in terms of convergence and robustness [10]. A Bayesian optimization algorithm was used for the optimization of the operation temperature in THz QCLs [11]. For the optimization we focus on the well-established mid-IR QCD design N1022 with a detection wavelength of $4.7\,\mu\mathrm{m}$ [12]. The bandstructure and calculated wavefunctions are presented in Fig. 1. We use an one-dimensional GPR algorithm [13] for the optimization of the specific detectivity simulated by a perturbed rate equation approach based on scattering rates between the quantized levels. We present the method of GPR optimization utilizing carrier transport simulations of mid-IR QCDs and discuss the obtained results of improved spectral dectectivity.

This work was supported by Qombs Project, EU-H2020-FET Flagship on Quantum Technologies (Grant No. 820419), and by the German Research Foundation (DFG JI 115/4-2).

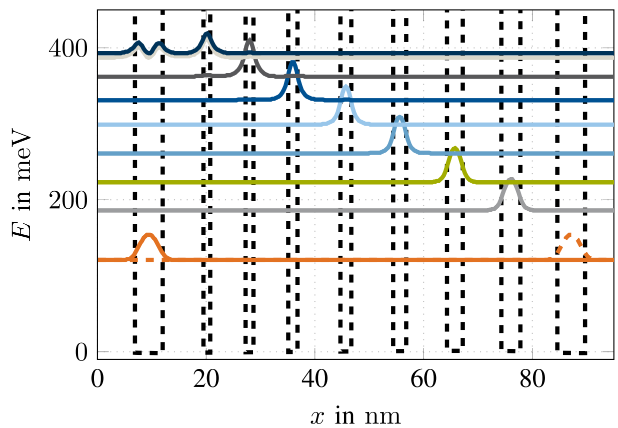

Fig. 1. Calculated conduction band profile and probability densities of the investigated mid-IR QCD structure N1022 [12] detecting at $4.7\,\mu\mathrm{m}$. Space charge effects are included by solving self-consistently the Schrödinger and Poisson equation. The electron densities in each state are modeled accounting for thermal equilibrium under zero external bias and no incident light.

II. Method

For the characterization of photodetector performance a key figure of merit is the specific detectivity D^*. The Johnson noise limited detectivity for QCDs can be expressed as [12]

$$D^* = R_\mathrm{p}\sqrt{\frac{AR_0}{4k_\mathrm{B}T}}, \tag{1}$$

where R_p is the peak responsivity, R_0 the detector resistance, T the temperature and k_B the Boltzmann constant. We have developed a robust method calculating R_p by solving perturbed rate equations in analogy to [7], [14] and calculating the absorption efficiency using transition rates calculated by Fermi's golden rule [3].

Our goal is to enhance the absorption efficiency, while keeping the Johnson noise low. Therefore, we decided to

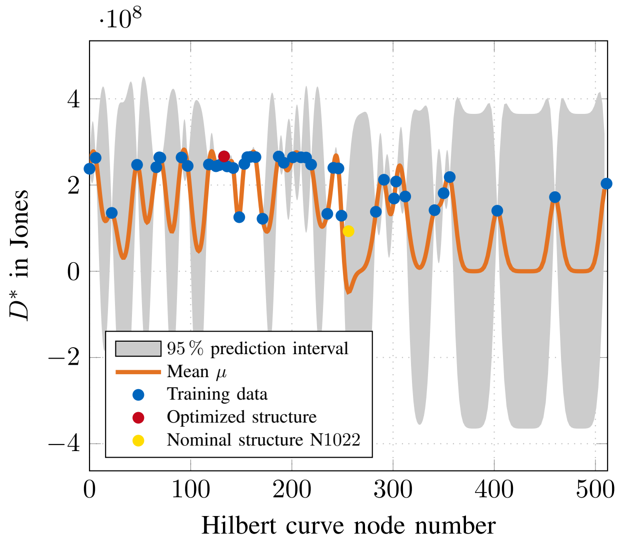

Fig. 2. Simulated specific detectivities of test structures (blue dots) and of the nominal structure N1022 (yellow dot) at the temperature of 220 K. For the used squared exponential covariance function K we obtain the optimized hyperparameters $\sigma_f = 1.83 \cdot 10^8$, $\sigma_l = 5.66$ and $\sigma_{\text{noise}} = 0$.

evaluate changes in the two barriers and the small well next to the active well. The variation width is set to 0.5 Å. To visualize the three-dimensional optimization problem we use the third-order space-filling Hilbert curve obtaining 512 input points. This can then be fed into the optimization algorithm. Therefore, we have used the one-dimensional GPR algorithm given in the aftershoq [13] environment. A Gaussian process is a generalization of the Gaussian distribution, and can be described as a distribution over functions [15], [16]. The Gaussian predictive distribution is described by a normal distribution:

$$p(y^*|x^*, \mathbf{x}, \mathbf{y}, \theta) \sim \mathcal{N}(\mu, K), \tag{2}$$

with mean μ, covariance matrix K and hyperparameters θ. The training data from all previous iterations are summarized in $(\mathbf{x}, \mathbf{y})$. New function values y^* can thus be drawn for the test inputs x^*. By optimizing the marginal likelihood $p(\mathbf{y}|\mathbf{x}, \theta)$ the optimal values of hyperparameters θ for an efficient optimization can be found.

III. Results

The simulation tool was evaluated by comparing the simulated detectivity with the measured results of the QCD teststructure N1022 given by Giorgetta *et al.* [12] at a temperature of 300 K. The simulated specific detectivity $D^* = 0.85 \times 10^7$ Jones is in good agreement with the measured value. With regard to future commercial applications, we consecutively focus on an elevated temperature of 220 K for optimization which is accessible by thermoelectric cooling. The simulated detectivity values D^* are given in Fig. 2. The different test structures are here illustrated over the Hilbert curve node number, i.e. the respective index number on the Hilbert curve. For the training of the GPR algorithm, we have evaluated 42 test inputs $\mathbf{x}$. We obtain an optimized structure with a simulated specific detectivity $D^* = 2.6 \times 10^8$ Jones, which is ~ 2.6 times higher than the simulated detectivity of the teststructure N1022.

IV. Conclusion

In summary, a sensitive and precise optimization algorithm for QCD structure designs is introduced. We applied our modeling approach to an existing mid-IR design and could tremendeously improve the specific detectivity of our test design. Further extensions of our optimization framework utilizing EMC simulations of QC devices are in progress. GPR is suitable for EMC, since it can directly deal with the inherently noisy outputs that are obtained from the EMC simulations due to the stochastic sampling.

References

[1] D. Hofstetter, M. Beck, and J. Faist, “Quantum-cascade-laser structures as photodetectors,” *Appl. Phys. Lett.*, vol. 81, no. 15, pp. 2683–2685, 2002.

[2] L. Gendron, M. Carras, A. Huynh, V. Ortiz, C. Koeniguer, and V. Berger, “Quantum cascade photodetector,” *Appl. Phys. Lett.*, vol. 85, no. 14, pp. 2824–2826, 2004.

[3] C. Jirauschek and T. Kubis, “Modeling techniques for quantum cascade lasers,” *Appl. Phys. Rev.*, vol. 1, no. 1, p. 011307, 2014.

[4] O. Baumgartner, Z. Stanojevic, K. Schnass, M. Karner, and H. Kosina, “VSP–A quantum-electronic simulation framework,” *J. Comput. Electron.*, vol. 12, no. 4, pp. 701–721, 2013.

[5] A. Harrer, B. Schwarz, S. Schuler, P. Reininger, A. Wirthmüller, H. Detz, D. MacFarland, T. Zederbauer, A. M. Andrews, M. Rothermund, H. Oppermann, W. Schrenk, and G. Strasser, “4.3 μm quantum cascade detector in pixel configuration,” *Opt. Express*, vol. 24, no. 15, pp. 17 041–17 049, 2016.

[6] C. Koeniguer, G. Dubois, A. Gomez, and V. Berger, “Electronic transport in quantum cascade structures at equilibrium,” *Phys. Rev. B*, vol. 74, p. 235325, 2006.

[7] J. Popp, M. Haider, M. Franckié, J. Faist, and C. Jirauschek, “Monte carlo modeling of terahertz quantum cascade detectors,” arXiv preprint arXiv:2004.05891, 2020.

[8] A. Bismuto, R. Terazzi, B. Hinkov, M. Beck, and J. Faist, “Fully automatized quantum cascade laser design by genetic optimization,” *Appl. Phys. Lett.*, vol. 101, no. 2, p. 021103, 2012.

[9] M. Franckié, L. Bosco, M. Beck, C. Bonzon, E. Mavrona, G. Scalari, A. Wacker, and J. Faist, “Two-well quantum cascade laser optimization by non-equilibrium green’s function modelling,” *Appl. Phys. Lett.*, vol. 112, no. 2, p. 021104, 2018.

[10] M. Franckié and J. Faist, “Bayesian optimization of terahertz quantum cascade lasers,” *Phys. Rev. Appl.*, vol. 13, p. 034025, 2020.

[11] L. Bosco, M. Franckié, G. Scalari, M. Beck, A. Wacker, and J. Faist, “Thermoelectrically cooled THz quantum cascade laser operating up to 210 K,” *Appl. Phys. Lett.*, vol. 115, no. 1, p. 010601, 2019.

[12] F. R. Giorgetta, E. Baumann, M. Graf, Q. Yang, C. Manz, K. Kohler, H. E. Beere, D. A. Ritchie, E. Linfield, A. G. Davies, Y. Fedoryshyn, H. Jackel, M. Fischer, J. Faist, and D. Hofstetter, “Quantum cascade detectors,” *IEEE J. Quantum Electron.*, vol. 45, no. 8, pp. 1039–1052, 2009.

[13] M. Franckié, “[aftershoq]: A flexible tool for em-radiation-emitting semiconductor heterostructure optimization using quantum models,” 2018.

[14] C. Jirauschek, “Universal quasi-level parameter for the characterization of laser operation,” *IEEE Photonics J.*, vol. 10, no. 4, p. 1503209, 2018.

[15] C. E. Rasmussen, “Gaussian processes in machine learning,” in *Advanced Lectures on Machine Learning*, O. Bousquet, U. von Luxburg, and G. Rätsch, Eds. Berlin, Heidelberg: Springer Berlin Heidelberg, 2004, pp. 63–71.

[16] C. K. Williams and C. E. Rasmussen, *Gaussian processes for machine learning*. MIT press Cambridge, MA, 2006, vol. 2, no. 3.