Modeling of the Effects of Band Structure and Transport in Quantum Cascade Detectors

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One of the essential technologies in modern photonic systems are semiconductor heterostructures. The first use of a QCL as a photo-detector has been reported by [1] and was since then refined for infrared and terahertz wavelengths [2] leading to the current quantum cascade detectors (QCD).

The operating principle of a QCD is outlined in Fig. 1. A ground level electron is excited to a higher state by absorbing a photon. Due to the asymmetric design, the electron relaxes in a preferred direction into the quantum well of the next cascade. This concept reduces dark current and dark current noise.

We use the semi-classical Pauli master equation (PME) [3], [4] to model current transport through the multi-layer semiconductor heterostructure. We developed an efficient Monte Carlo (MC) simulator in C++ as part of the Vienna-Schrödinger-Poisson (VSP) simulation framework [5]. The versatility of the simulator was successfully demonstrated by the design and automatized optimization of a bi-functional QCL and QCD device [6]. The Hamiltonian includes the band edge formed by the heterostructure, and thus, coherent tunneling is accounted for through the delocalized eigenstates. Transport occurs via scattering between the subbands. Due to the periodicity of the device, periodic boundaries are imposed on the PME. As scattering sources, we currently consider non-polar acoustic and optical phonons, and polar optical phonons as well as alloy disorder, intervalley processes and interface roughness. The incorporated model for stimulated emission and absorption of photons is essential for the description of a QCD. For the calculation of the rates the effect of in-plane nonparabolicity can be included.

Band nonparabolicity in cross-plane direction is essential to determine the subbands in QCDs. We employed a two-band $\mathbf{k}\cdot\mathbf{p}$ [7] and a four-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. The periodic wavefunctions (Fig. 1) are picked automatically by a reliable algorithm. For the in-plane transport treatment we investigated three approaches: (I) parabolic effective (density of states) mass as input parameter; (II) parabolic effective mass measured by $\langle\psi_i|m(z)|\psi_i\rangle$ for each subband, (III) non-parabolic dispersion $\mathcal{E}(1+\alpha\mathcal{E}) = \frac{\hbar^2 k^2}{2m}$ fitting the mass m and nonparabolicity coefficient α to the numerical subband structure determined by the Schrödinger equation.

As a test device we use a mid-infrared QCD operating at a wavelength of $4.7\,\mu$m. The design of the InGaAs/InAlAs QCD is taken from [2] (device N1022) and all simulation results are compared to the measurements therein. We calculate the responsivity, which relates the incoming photon flux to the detected current, for each combination of band structure model (2-band/4-band $\mathbf{k}\cdot\mathbf{p}$) and in-plane dispersion of the transport model (parabolic, nonparabolic, parameters obtained using methods (I)-(III) as outlined above). Each simulation takes about ten minutes. Fig. 2 and Fig. 3 depict the responsivity for parabolic transport with the well mass as input parameter. The 4-band $\mathbf{k}\cdot\mathbf{p}$ model shows a considerably better agreement with measurement. Using method (II) instead of (I) to determine the subband mass does not influence the result (Fig. 4). Finally, Fig. 5 shows the results for method (III), which show the best agreement with measurements.

In conclusion, we presented a versatile simulator, that allows quick simulation studies of QCLs and QCDs, while still accurately capturing the relevant physics. The importance of nonparabolicity to correctly describe the behavior of QCDs is shown.

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References

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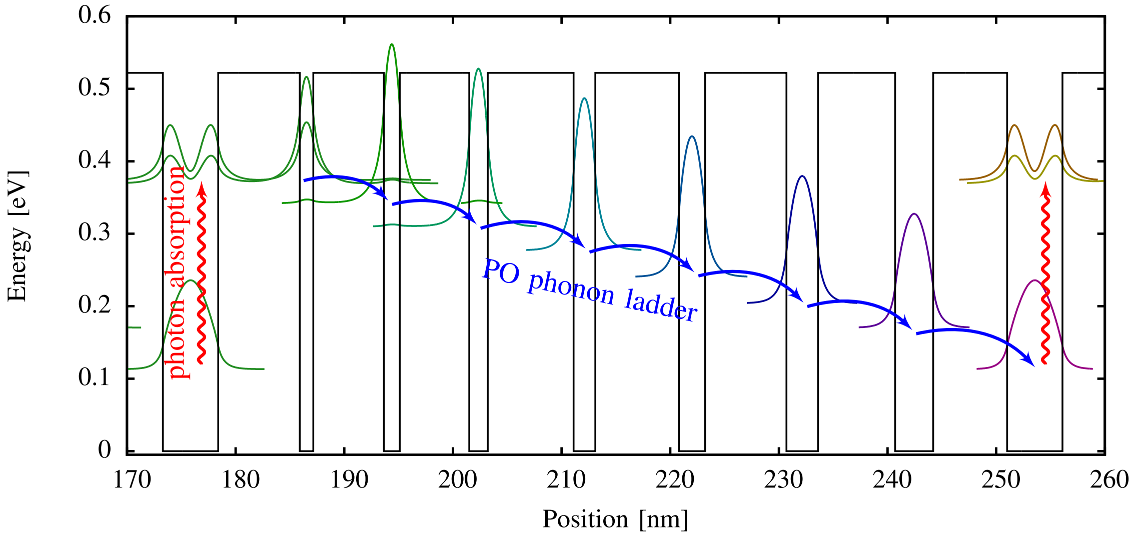

Fig. 1. Calculated wave functions of the QCD from [2] using a four-band **k·p** model; electrons are excited to higher states by absorbing photons. The polar optical phonon ladder causes the electron to preferably relax towards the next cascade.

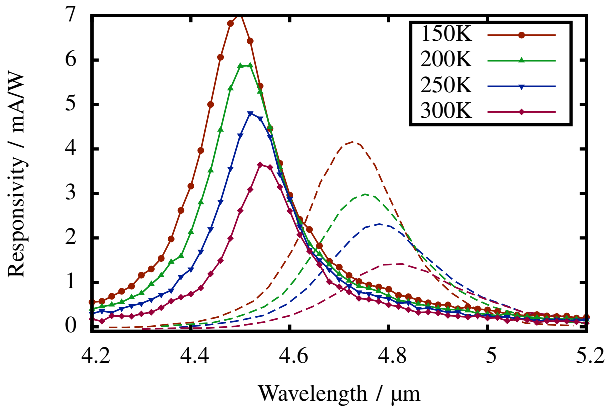

Fig. 2. Calculated responsivity (solid) of the QCD compared to measurements of [2] (dashed); cross-plane band structure modeled with a two-band **k·p** Hamiltonian. In-plane dispersion in the transport model is assumed parabolic with the effective mass set to the well material effective mass.

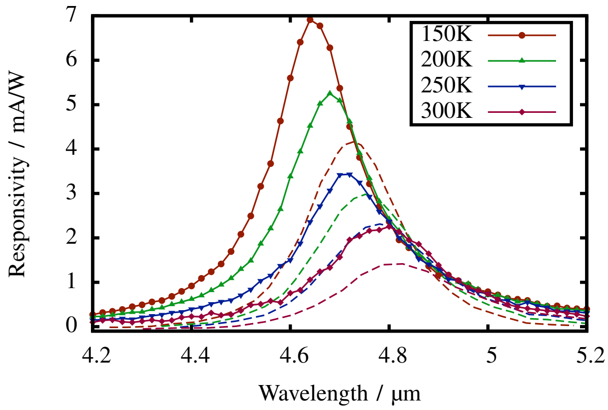

Fig. 3. Same as Fig. 2, but with a four-band **k·p** Hamiltonian; the wavelengths of the peak responsivity agree closer with measurements than for the two-band **k·p** Hamiltonian.

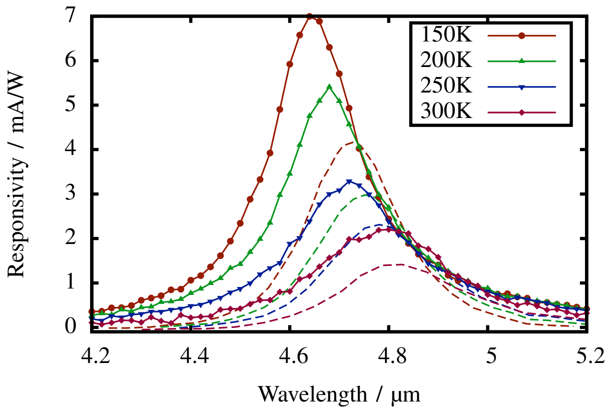

Fig. 4. Same as Fig. 3 but the mass for the parabolic in-plane dispersion in the transport model has been averaged for each subband; no visible improvement is observerd using this model.

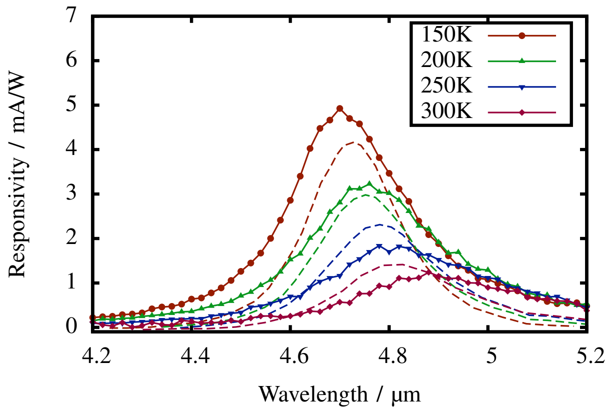

Fig. 5. Same as Fig. 3 but the in-plane dispersion in the transport model is assumed non-parabolic with the effective mass and non-parabolicity coefficient fitted to the subband structure; inclusion of nonparabolicity has substantial effects on the responsivity.