# Efficient method for the calculation of dissipative quantum transport in quantum cascade lasers

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We present a novel and very efficient method for calculating inelastic electron transport in quantum cascade lasers (QCLs). It follows the nonequilibrium Green's function (NEGF) framework but sidesteps the calculation of lesser self-energies by replacing them by a quasi-equilibrium expression. This method generalizes the phenomenological Büttiker probe model by taking into account individual scattering mechanisms.

## 1. Details

This newly developed multi-scattering Büttiker probe (MSB) model [1] offers the numerical efficiency of the simple Büttiker probe model but more importantly, it extends it by using realistic self-energies derived from the NEGF method for the probes. It is therefore orders of magnitude more efficient than a fully self-consistent NEGF calculation for realistic devices. We propose a new THz QCL design which works up to 250 K. It is based on a two quantum well design with alternating barrier heights where the threshold voltage is designed to match the energy of a LO phonon (36 meV). The widths of the layers as well as the heights of the barriers were optimized with a genetic algorithm based on this new MSB model. The MSB method has been implemented into the next**nano**.MSB software (`http://www.nextnano.com`) and allows finding an optimal QCL layout very quickly, as variations in alloy concentration, barrier thickness, and further parameters can be calculated in parallel.

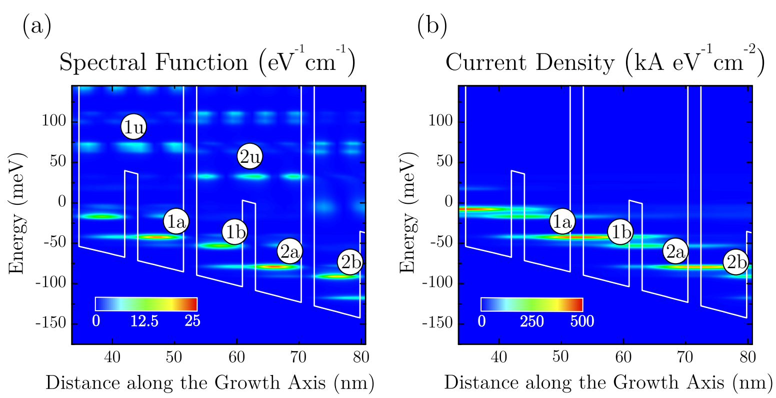


FIGURE 1. (a) Calculated conduction band profile (white line) and contour plot of the energy and position resolved spectral function $\mathbf{A}(z = z', E_z)$ at vanishing in-plane momentum $k_\parallel = 0$ for the proposed THz QCL at the threshold bias voltage of 36 mV per period and a lattice temperature of 100 K. (b) Corresponding contour plot of the energy and position resolved current density.

## References

[1] P. Greck, S. Birner, B. Huber, and P. Vogl, Efficient method for the calculation of dissipative quantum transport in quantum cascade lasers, accepted for publication in *Optics Express* (2015).