

# Simulation of electron transport in mid-infrared QCLs using non-equilibrium Green's functions

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Electron transport in the active region of mid-infrared QCLs relies on a subtle interplay between quantum tunneling processes and scattering processes. The use of non-equilibrium Green's functions (NEGF) constitutes an advanced method for modeling electronic quantum transport in presence of energy and phase dissipation. The nextnano.NEGF software is based on such formalism, and was previously successfully applied to the simulation of terahertz (THz) QCLs [1]. More recently, we have extended this tool to the simulation of mid-IR QCL active regions using an effective 3-band approach. The relevant scattering mechanisms are modeled on a microscopic basis, in particular optical phonon emission/absorption, interface roughness, alloy disorder [2]. The grading of interfaces is included and combined with the description of interface roughness [3]. In addition, we have included photon-induced transport above lasing threshold, enabling to simulate and optimize the light-current characteristics and wall-plug efficiencies in mid-infrared QCLs.

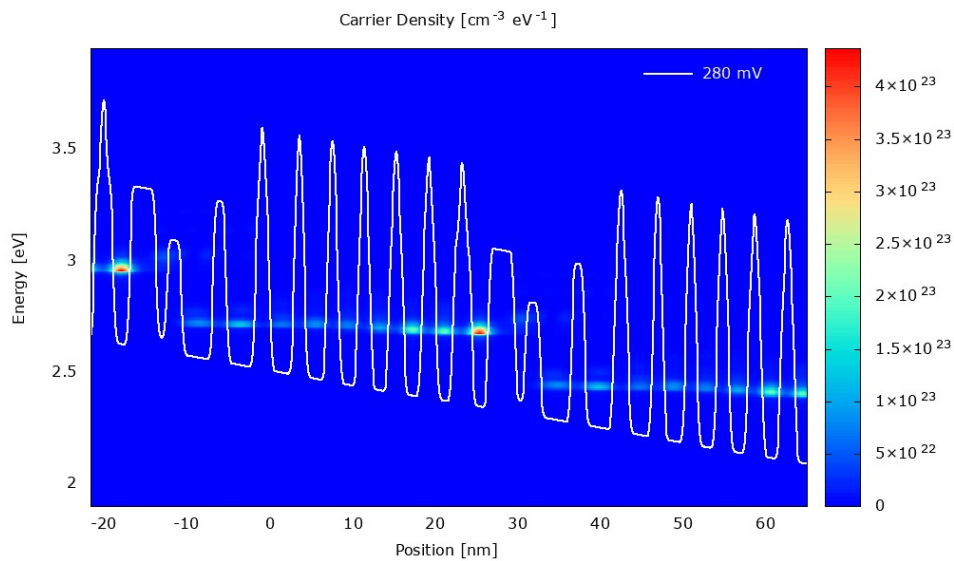


Figure 1: Energy-resolved electron density in a mid-infrared QCL [4] simulated using the nextnano.NEGF software considering grading of the interfaces.

[1] T. Grange, *Phys. Rev. B* **92**, 241306 (2015).

[2] Online documentation at [www.nextnano.com/nextnano.NEGF](http://www.nextnano.com/nextnano.NEGF)

[3] T. Grange et al, *Phys. Rev. Appl.* **13**, 044062 (2020)

[4] Y. Bai, et al, *Appl. Phys. Lett.* **98**, 181102 (2011).