Microscopic Modelling of Optoelectronic Quantum Devices: Role of a Predictive Simulation Strategy

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Semiconductor nanostructures have been the subject of impressive research activity owing to their flexibility as model systems for basic research as well as "building blocks" in modern solid-state optoelectronics. Among the most successful applications one must mention a variety of photodetectors as well as unipolar semiconductor lasers.[1] The operation of these intersubband devices involves non-equilibrium carrier dynamics between localised and/or propagating states. In turn, this dynamics is influenced by several factors (intra- and intersubband phonon scattering, carrier concentration and temperature, *etc*.) that depend on the operating frequency and may synergistically couple in a non-intuitive way. For a detailed understanding, a fully three-dimensional description is imperative. Diverse issues that need to be addressed include:

- the physical origin of the hot-carrier relaxation,
- the nature (coherent *vs*. incoherent) of the physical mechanisms governing the injection/extraction processes and therefore the charge transport across the device,
- the validity range and limitations of purely macroscopic models.

I shall review and discuss the first fully three-dimensional quantum-mechanical studies[2,3,4,5] of non-equilibrium carrier dynamics governing unipolar light-emitting devices like quantum-cascade lasers (QCLs). Our non-conventional multisubband quantum Monte-Carlo simulation scheme allows direct access to microscopic details of the electron relaxation without resorting to phenomenological parameters. Moreover, our generalization of the Boltzmann-like treatment into a density-matrix quantum-transport formalism allows us to answer the long-standing question concerning the nature of charge injection/transport processes. Applications are presented concerning both state-of-the-art mid-infrared QCLs as well as novel THz QC emitters. To properly model non-equilibrium carrier dynamics, all the relevant coupling mechanisms are included at a kinetic level. Their relative weights depend on the desired emission wavelength, giving rise to different scenarios. Simulated current-voltage characteristics and gain efficiency well agree with available experimental data for various mid-IR devices. Promising designs for THz QCLs are explored, for which lasing action has recently been demonstrated, therefore validating the predictive character of our approach.

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1. See, e.g., J. Faist *et al.*, *Science* **264**, 553 (1994).
2. R. C. Iotti and F. Rossi, *Appl. Phys. Lett.* **76**, 2265 (2000).
3. R. C. Iotti and F. Rossi, *Phys. Rev. Lett.* **87**, 146603 (2001); *Appl. Phys. Lett*. **78**, 2902 (2001).
4. R. Köhler, R. C. Iotti, A. Tredicucci and F. Rossi, *Appl. Phys. Lett*. **79**, 3920 (2001).
5. R. Köhler *et al.*, *Nature* **417**, 156 (2002).