Coupling electrons, phonons, and photons for nonequilibrium transport simulation

Irena Knezevic

University of Wisconsin - Madison, USA

Time-dependent nonequilibrium transport in nanostructures offers a number of exciting basic science challenges, as well as real-world applications. While the low-field and steady-state quantum transport in nanostructures is theoretically well understood, there is incomplete theoretical understanding and a dearth of efficient computational techniques that can address time-dependent quantum transport in nanostructures, where electrons are excited either electrically (by applying a time-varying bias) or optically (by illumination with electromagnetic waves) and transport far from equilibrium that results from large applied biases or electromagnetic waves of high intensity. Simulation of the three-pronged interplay between electrons, lattice, and electromagnetic fields, where simulations proceed in parallel at every time-step and drive each other, is what makes theoretical treatment of realistic transport problems far from equilibrium very different from the linear-regime transport and very challenging.

In this talk, I will present my group's recent work on developing a general and efficient multiphysics simulation framework where electron transport, phonon transport, and electrodynamics will be coupled self-consistently to provide insight into the time-dependent and nonlinear transport in optically or electrically excited low-dimensional electron systems. To achieve this objective, electronic transport [simulated by the ensemble Monte Carlo (EMC) technique] will be self-consistently coupled with the transport of phonons (described by EMC) and electromagnetic field dynamics [described by the finite-difference time-domain (FDTD) technique and molecular dynamics (MD) for subgrid Coulomb interactions]. In particular, I will present our recent work on investigating (1) THz-frequency electronic response of graphene and (2) far-from-equilibrium electron and phonon transport in quantum cascade lasers.

[1] N. Sule, K. J. Willis, S. C. Hagness, and I. Knezevic, "Correlated impurities and carrier transport in supported graphene," submitted (2013).

[2] Y. B. Shi, Z. Aksamija, and I. Knezevic, "Self-Consistent Thermal Simulation of GaAs/Al0.45Ga0.55As Quantum Cascade Lasers," J. Comput. Electron. 11, 144 (2012).

[3] K. J. Willis, S. C. Hagness, and I. Knezevic, "Multiphysics simulation of high-frequency carrier dynamics in conductive materials," J. Appl. Phys. 110, 063714 (2011).