Multiscale Transport Simulation of Nanoelectronic Devices with NEMO5

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Abstract— The downscaling of electronic devices has reached a regime where quantum and atomistic effects govern the active part of the device while semi-classical physics still plays a very important role for the remaining parts. A multiscale transport simulation approach is therefore developed in NEMO5 tool to address this issue. In this approach, nonequilibrium Green's function (NEGF) equations with atomistic tight-binding Hamiltonian are employed to calculate the ballistic current through the tiny central device, while drift-diffusion (DD) equations (with quantum charge density) are used to model the surroundings where scattering and relaxation dominate. These two sets of equations are coupled through quasi-Fermi levels, which are determined by continuity equation. With Poisson equation solved self-consistently, device characteristics such as the I-V curves are obtained. Using this approach we demonstrate two examples. For the first example, we consider a recently fabricated nitride tunneling diode that consists of a GaN-InNGaN heterojunction. The band-to-band tunneling through the strained heterojunction is accurately modeled by the NEGF method while the serial resistance of the leads is accounted for by potential drop from the contacts obtained by solving the DD equation. Further, the contact resistance is taken into account by computing the tunneling through the Schottky barrier (also via NEGF method). For the second example, we simulate a two-dimensional III-V MOSFET, featuring wrapped-around leads. The channel part of the transistor is modeled by the NEGF method to capture source-to-drain tunneling leakage, which is critical for short-channel devices scaled to sub-10 nm. The (relatively) long leads, are again assigned to the DD solver to calculate the non-trivial potential drop from the external contacts. We benchmark the simulation results with the experimental measurements and then optimize the device design parameters.