Hybrid models for electron transport in Carbon Nanotube Field-Effect Transistors

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The peculiar electronic properties of Carbon Nanotubes (CNT) make them promising components in future nanoelectronics, e.g. for their potentiality in high speed and low voltage switching in Field-Effect Transistors (FET). Their electronic behavior strongly depends on the geometry of the tube. In particular, the strong quantum confinement affects the energy bands, so that bulk material quantities cannot be used in simulations. Atomistic ab-initio computations give accurate description of electron transport but they are computationally too demanding and are not feasible in a device design framework. The goal is to develop computationally efficient models which still accurately describe the most relevant features of the devices.

In [1] an envelope function decomposition has been used to derive from a three dimensional (3D) Schrödinger equation a one dimensional (1D) longitudinal effective mass model, where effective quantities take into account the periodic longitudinal lattice potential and the lateral confinement. In the non degenerate case, adiabatic decoupling occurs and the model consists of a sequence of 1D effective Schrödinger equations, one for each conduction band.

Here we present a macroscopic collisional transport model, which includes the quantum effects through an effective Bohm potential. The novel Quantum-Drift-Diffusion (QDD) model is derived extending the approach of [2] to strongly confined structures and incorporating the atomistic quantities derived in [1]. Also, in order to improve the accuracy in the active region, a spatial hybrid approach is proposed: the macroscopic collisional QDD model is used in the Source/Drain regions, and the transport Schrödinger equations of [1] are used in the active region. As it is done in [3], we impose interface conditions that preserve the continuity of the total current and of the electron density.

In order to model a gate-all-around FET, self-consistent computations include the resolution of the 3D electrostatic problem. A comparison of the different models is presented for the simulation of a zig-zag single-walled CNTFET.

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References

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