Fast Convergent Schrödinger-Poisson Solver for the Static and Dynamic Analysis of Carbon Nanotube Field Effect Transistors

M. Pourfath, W.J. Park, H. Kosina, and S. Selberherr

Carbon nanotube field-effect transistors (CNTFETs) have been studied in recent years as a potential alternative to CMOS devices, because of the capability of ballistic transport. In order to account for the ballistic transport we solved the coupled Poisson and Schrödinger equations for the analysis these devices. Conventionally the coupled Schrödinger-Poisson equation is solved iteratively, by using a damping parameter. If a high damping factor is selected the simulations may oscillate and will not converge and if a low damping factor is selected then a long time for simulations is required. In this work a nonlinear Poisson equation is solved. In each iteration after solving the Schrödinger equation and calculating the carrier concentration an exponential relationship between the carrier concentration and the potential is assumed. By using this method most of the simulations converge in a few iterations.

First we studied the static behavior of CNTFETs. Depending on the difference between the work function of the contact metal and the electron affinity of the CNT, Schottky barriers at the metal-CNT interface are formed. We performed simulations for devices with different Schottky barrier heights. In agreement with experimental results simulations indicate that because of narrow band gaps in CNTs the ambipolar behavior limits the performance of these devices. To suppress this ambipolar behavior, we proposed a double gate structure in which the first gate controls carrier injection at the source contact and the second one controls carrier injection at the drain contact. Simulations show that in a double gate structure the ambipolar behavior is suppressed and improved device characteristics is achieved.

To perform small signal analysis for the CNTFETs, a Quasi Static Approximation was used. In this approximation, by sweeping the contact potential, ie. the gate voltage, over a voltage range with small steps the total charges injected from different contacts are calculated. By numerically differentiating over the data, the capacitance between different contacts can be also obtained. By calculating the small signal model the frequency response of the device can be achieved. Simulation results indicate that the quantum capacitances have less effect on the dynamic response of the device and to improve the dynamic response of the device the parasitic capacitances between the gate, source and drain contacts should be reduced.