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Microscopic modeling of contact resistance in carbon nanotubes

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Electrical properties of low-dimensional devices are dominated by the contact resistance. Contact resistance has always been a key problem for carbon nanotubes field effect transistors (CNT-FETs) which reflects a complex interplay of many factors. With advances in scaling, the contact resistance and transfer length are becoming even more critical. We have developed a general purpose CNT device simulator which is unique in including quantum-mechanical tunneling, both acoustic and optical-phonon scattering, as well as the crucial transfer of carriers between the CNT and metal contact. Self-consistent electrostatics is implemented for a wrap-gate geometry. Quantum mechanical tunneling is matched by the appropriate boundary conditions to a semi-classical transport model.

To illustrate the unique capabilities relative to existing approaches such as non-equilibrium Green's function (NEGF) formalism, we predict the scaling of on-state current with contact length. The behavior is surprising. The transfer length is roughly a factor of two shorter at a typical drain voltage than at low bias. This reflects the onset of optical-phonon scattering underneath the metal contact for a ballistic channel. We find systematic differences in transfer length between good contacts and poor contacts. Even the best contacts give transfer lengths a factor of two shorter than in metallic CNTs. The contact resistance at high bias is about twice as large as compared to the simulation results in the absence of optical phonon scattering. The model can also address the crossover from diffusive to ballistic transport, short channel effects, self-heating effects, and ambipolar devices characteristics.