11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

Non-Equilibrium Green's Function (NEGF) Simulation of Metallic Carbon Nanotube Transistors: Impact of Vacancy Defect

Neophytos Neophytou, Shaikh Ahmed and Gerhard Klimeck
School of Electrical and Computer Engineering, Purdue University, 465 Northwestern Ave.
Network for Computational Nanotechnology
West Lafayette, Indiana 47907-2035, USA.
E-mail: ssahmed@purdue.edu, Phone: (765) 494 9034, Fax: (765) 494 6441

Carbon nanotube (CNT) based devices are promising structures for future electronic applications. An accurate treatment of quantum effects is necessary for short channel CNT devices. In this work, we describe a method to simulate realistic 3D CNT field effect transistors (CNTFETs) based on Finite Element Method (FEM) for the electrostatic treatment and nearest neighbour Tight-Binding (TB) method for electron transport, employing Non-Equilibrium Green's Function (NEGF) techniques.

The device geometry treated is shown in Fig. 1. The continuous grid includes the positions of the carbon atoms of the CNT and the charge distribution is treated as delta functions (point charges). The mesh created is fine enough to capture atomistic resolution for the potential on the shell of the CNT. The solution of the Poisson equation is self-consistently coupled to the transport part of the simulator where we employ three different techniques: (1) a semiclassical ballistic transport model, (2) an uncoupled mode space, and (3) a real space Nearest Neighbor Tight Binding (NNTB) p_z orbital model using the NEGF technique [1]. The simulator can treat both MOSFET-like devices using open boundary conditions, and Schottky-Barrier devices using a phenomenological model of metallic contacts. We have used two different algorithms in the computation of the Green's functions in the transport kernel of the simulator: (1) the LAPACK routines for solving a complex system of linear equations utilizing the LU decomposition with partial pivoting and row interchanges, and (2) the recursive Green's function (RGF) approach. Fig. 2 shows a comparison of the two approaches as a function of the Hamiltonian size (corresponding to the total number of atoms in the nanotube as the length of the nanotube is changed) through non-self-consistent simulation experiments. Noticeable is the superior performance with the RGF algorithm as the system size increases.

The simulator has been used to study the effects of vacancies on the performance of metallic CNTFETs. The model device used is a (12,0) metallic CNT within a 3D geometry (Fig. 1). We introduce a single vacancy in the mid-region of the channel by raising the on-site energy of the vacancy and thus preventing any hopping of electrons to that particular site. Fig. 3 shows the local density of states (LDOS) in the vicinity of the vacancy and transmission (Tr) calculated from non-self consistent simulations. For comparison, we also show the results for a device without a vacancy. We find that the presence of a single vacancy locally modulates the LDOS significantly. More importantly, regardless of the chirality of the nanotube, the transmission is reduced throughout the entire energy spectrum (note the reduction by one quantum unit in some regions) in agreement with [2, 3].

We also address the efforts and on-going activities on building and deploying community nanotechnology software tools on nanoHUB.org which currently provides the nanoscience research community with interactive on-line simulation and educational resources such as tutorials, seminars, and on-line courses. One such community tool is the CNTFET which is going to be publicly released and has recently been expanded in its capabilities through detailed numerical performance analysis. Fig. 4 shows the graphical user interfaces for this simulator used in an interactive session.

ISBN 3-901578-16-1

REFERENCES

[1] J. Guo, S. Datta, M. Lundstrom, and M. P. Anantram, *Multi-Scale Modeling of Carbon Nanotube Transistors,* The International Journal on Multiscale Computational Engineering, **2**, 257 (2004).

[2] N. Neophytou, D. Kienle, E. Polizzi, M.P. Anantram, *Influence of Defects on nanotube transistor performance,* Appl. Phys. Lett. , 2005 (submitted).

[3] L. Chico, L. Benedict, S. Louie and M. Cohen, *Quantum conductance of carbon nanotubes with defects,* Phys. Rev. B **54**, 4 (1996).

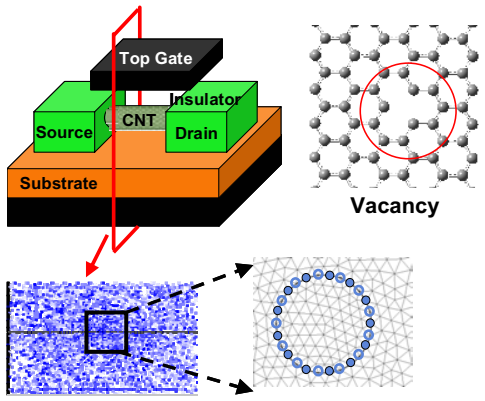


Fig. 1. The device structure and the creation of finite element mesh.

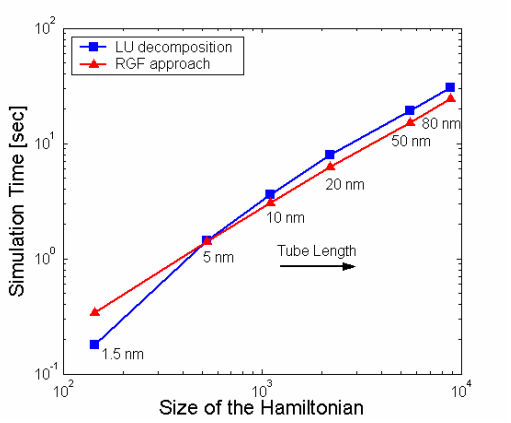
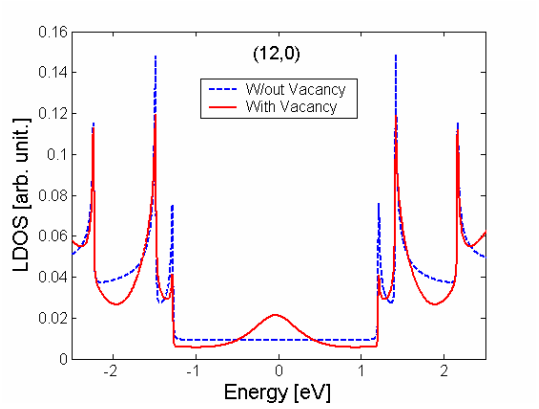
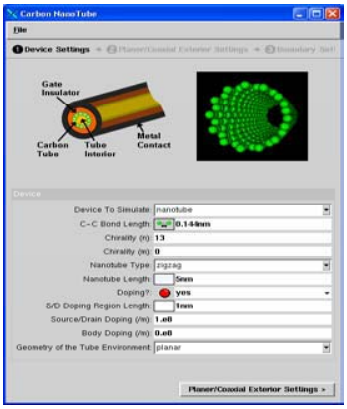
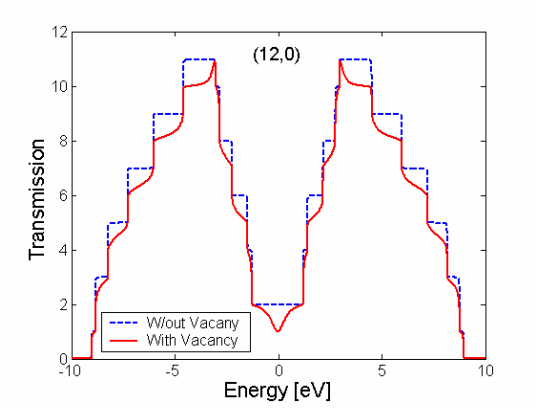


Fig. 2. Comparison between RGF and LU approaches.







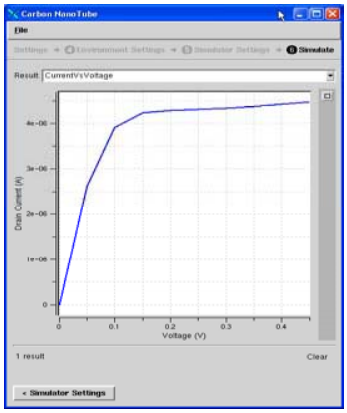


Fig. 3. (Left panels) Simulated local density of states (LDOS) in the vicinity of a vacancy and transmission for (12,0) metallic CNT.

Fig. 4. (Right panels) The rappturized graphical user interfaces for the CNTFET simulator.