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Non-equilibrium Green's function (NEGF) simulation of metallic carbon nanotubes including vacancy defects

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Abstract The electronic behavior of metallic carbon nanotubes under the influence of externally applied electric fields is investigated using the Non-Equilibrium Green's function method self consistently coupled with three-dimensional (3D) electrostatics. A nearest neighbor tight binding model based on a single *pz* orbital for constructing the device Hamiltonian is used. The 3D Poisson equation is solved using the Finite Element Method. Carbon nanotubes exhibit a very weak metallic behavior, and external electric fields can alter the electrostatic potential of the tubes significantly. A single vacancy defect in the channel of a metallic carbon nanotube can decrease its conductance by a factor of two. More than one vacancy can further decrease the conductance.

Keywords Carbon Nanotubes · Defects · Vacancies · Non-Equilibrium Green's Function · Finite Element Method

1 Introduction

Single wall carbon nanotubes (CNTs) are of great interest for future electronics because of their excellent electronic and optical properties. Near-ballistic transport with exceptionally high mobilities, is one of their characteristics which make them attractive for circuit implementations. Transistor structures that demonstrate high-performance operation have been reported [1, 2]. On the other hand, metallic nanotubes have also been given large attention for the possibility of their use as interconnects in VLSI circuits [3], and field emission devices as electron sources [4].

A lot of theoretical work has been done in investigating the performance of perfect CNT devices. The understanding of the performance of defected structures is however also important, especially when CNTs are used in a high radiation environment, such as space applications. In a previous work, we investigated the performance of vacancy defected semiconducting carbon nanotube field effect transistors (CNTFETs) [5]. In this work, the behavior of metallic carbon nanotubes under the influence of external electric fields or vacancy defects is examined.

2 Approach

The metallic CNTFETs simulated are shown in Fig. 1. The Poisson equation in 3D cylindrical and rectangular coordinates using the Finite Element Method [6] is solved self consistently with the non-equilibrium Green's function (NEGF) method. The Hamiltonian of the device is constructed by using a nearest neighbor tight binding model based on a single *pz* orbital. Standard NEGF equations are been solved [7, 8]. The atom-to-atom tight binding matrix element is chosen to be 3 eV to provide the correct bandstructure.

In the case of the vacancy, the on-site energy of the vacancy element is raised to a significantly high value, essentially repelling the carriers from that particular site [9]. To connect the discrete atomistic tight binding resolved charge to the continuum finite element mesh, the mesh is built using nodes on the position of the carbon atoms of the CNT and point charges are assumed on those nodes as shown in Fig. 1.

The model device is a 20 nm long CNT with a high *k*-dielectric 4 nm thick gate oxide (HfO_2, with $k = 16$), with metallic source/drain contacts. A midgap Schottky barrier

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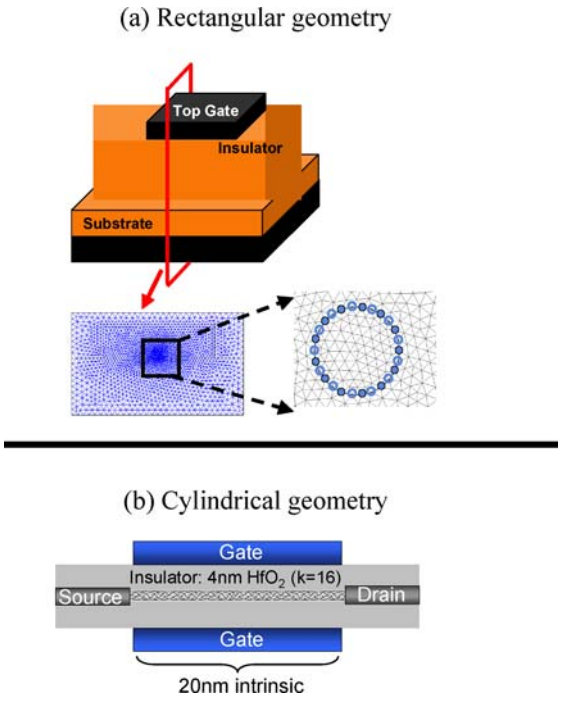

Fig. 1 The devices simulated. (a) The 3D planar device. A 2D finite element mesh is built on the atoms of the CNT and repeated along the length of the device to form the 3D device. (b) The cylindrical CNT device geometry. The gate oxide is assumed to be HfO_2 ($k = 16$). The CNT is a (12,0) metallic nanotube with 1 nm diameter and 20 nm length. The source/drain is assumed to be metallic contacts

for electrons between the metal contacts and the nanotube is assumed. Flat band conditions for the gate, are also assumed so the gate tends to keep the CNT intrinsic.

In the self consistent simulations, the most computationally expensive part is the Green's function calculation at every energy point. The size of the Hamiltonian can be up to 7000 $\times$ 7000, block-tri-diagonal. Depending on the required energy resolution, the equations need to be solved 1000 times for every Poisson iteration. Two different solution methods for the Green's function elements are utilized, the Recursive Green's Function (RGF) technique [10], and the LAPACK based LU decomposition sparse matrix solver. In both cases the only elements that need to be calculated are the first and last n columns of the Green's function (where n is the block size which is equal to the number of atoms in a CNT ring) that will be used for the density of states and transmission calculation (valid in the ballistic case). Using RGF we also obtain the diagonal elements that can be useful in the case where scattering is included in the simulator in the future. In order to reduce the computational burden, the MPI (message passing interface) parallelization scheme has been implemented in the solver in the independent computation of Green's function at each point along the energy spectrum. Figures 2 (a) and (b) show the performance characteristics of the MPI. A satisfactory speed-up and scaling for up to 20 processors

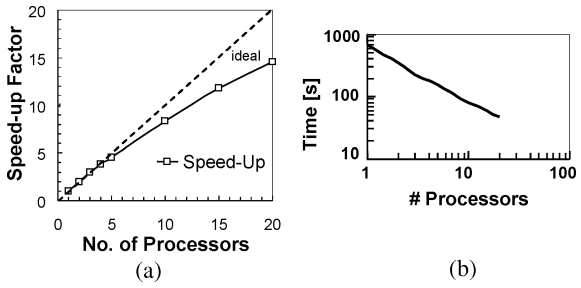

Fig. 2 The performance characteristics of the MPI. (a) The speed up factor vs. number of processors. (b) The simulation time vs. number of processors

has been realized. The reason of a declining speed-up behavior beyond 15 processors is attributed to the increasing amount of time used in various MPI communication calls that are implemented immediately after the parallel computation in order to exchange and gather large amount and size of data among the processors.

3 Results

Although metallic conductors are expected to have a large density of states around their Fermi level so that they are able to accumulate large quantities of charge on their surfaces and screen any external electric fields, this is not the case for metallic CNTs. The low density of states of the metallic CNTs around the Fermi level, as indicated in Fig. 3(a), does not allow them to screen external electric fields. Figure 3(b) shows the potential energy along a channel of a metallic (12,0) CNT in the cylindrical geometry of Fig. 1(b). The potential is strongly gate dependent, indicating weak screening by the metallic tube. Therefore, for the relevant operating bias regions, the CNT behaves as a very weak metal or even as a simple resistor.

Introduction of a vacancy defect in the channel of the CNT, however, alters both the density of states and the transmission of the CNT as shown in Fig. 4(a) and (b). Here, the non-self consistent simulated $DOS(E)$ and $T(E)$ for a (12, 0) CNT is shown, with and without vacancy in the channel, using open boundary conditions for the contacts. The density of states around the Fermi level rises due to the broken pi

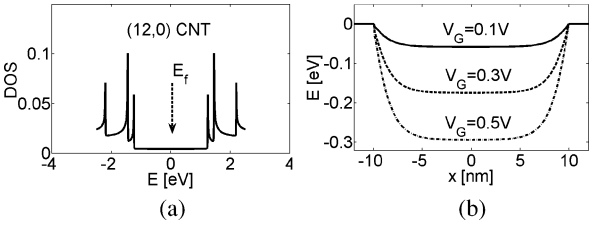

Fig. 3 (a) The density of states of a (12,0) zig-zag metallic CNT. (b) The electrostatic potential energy in along the channel of the metallic (12,0) CNT for different gate biases ($V_G = 0.1, 0.3, 0.5$ V)

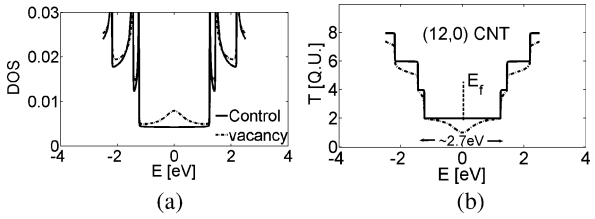

Fig. 4 (a) The total density of states of two unit cells of a (12,0) nanotube with and without a vacancy on the shell of the CNT. (b) The transmission of the (12,0) CNT with and without a vacancy on the shell of the CNT

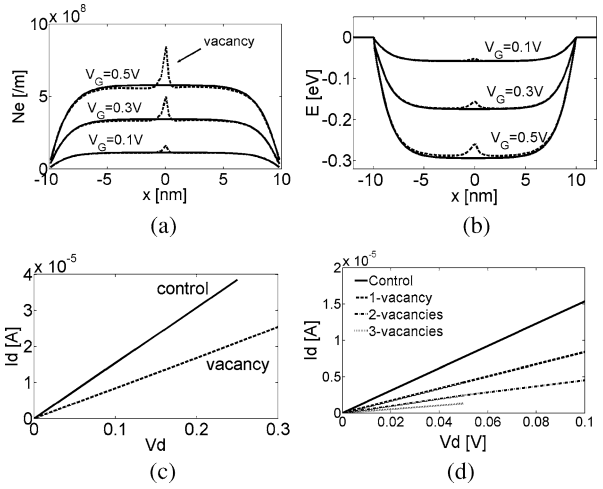

Fig. 5 (a) The charge profile along the channel of a (12,0) CNT for various gate biases for cases with and without a single vacancy in the middle of the channel. (b) The electrostatic potential energy. (c) The current of the device with and without the vacancy defect. (d) The current in the device with none, one, two and three vacancies on the shell of the CNT for small drain biases

network at the vacancy site. The transmission on the other hand decreases close to one quantum unit (q^2/h per spin) in the vicinity of the Fermi level in agreement with [11]. The self consistent simulated charge and potential energy distribution along the channel of the coaxial CNTFET is shown in Fig. 5(a) and (b). They indicate an accumulation of charge in the middle of the channel where the vacancy was placed, which is associated with an increased DOS. The amount of charge increases as the bias on the gate electrode increases, because more of the vacancy induced states are now filled with electrons. This charge accumulation raises the electrostatic energy of the channel locally (Fig. 5(b)).

The reduction in the transmission probability of the device results in 50% reduction in the current of the metallic CNT device, as indicated in Fig. 5(c). The (12,0) CNT that is used as the model device has a diameter of 1nm. Larger diameter nanotubes (>4 nm), however, do not suffer as much by the presence of a single vacancy in their channel because of the fact that the carriers have now a larger area and more pathways to move on the surface of the CNT.

The effect of multiple vacancies in the channel of the device is also investigated. Specifically, two and three vacancies are considered. The two vacancies are placed at $L/3$ and $2L/3$ in the channel, where L is the channel length, and the three vacancies at $L/4$, $L/2$ and $3L/4$. Figure 5(d) shows the I_{ds} vs. V_{ds} for these devices. The more defects we have in the channel of the device, the larger the current degradation in the device.

Finally, we would like to address the efforts of the Network for Computational Nanotechnology (NCN) in deploying nanotechnology simulation tools for the scientific community. NCN is a multi-university, NSF-funded initiative, with a mission to connect theory, experiment, and computation in a way that makes a difference to the future of nanotechnology. It provides new models, algorithms, approaches, and

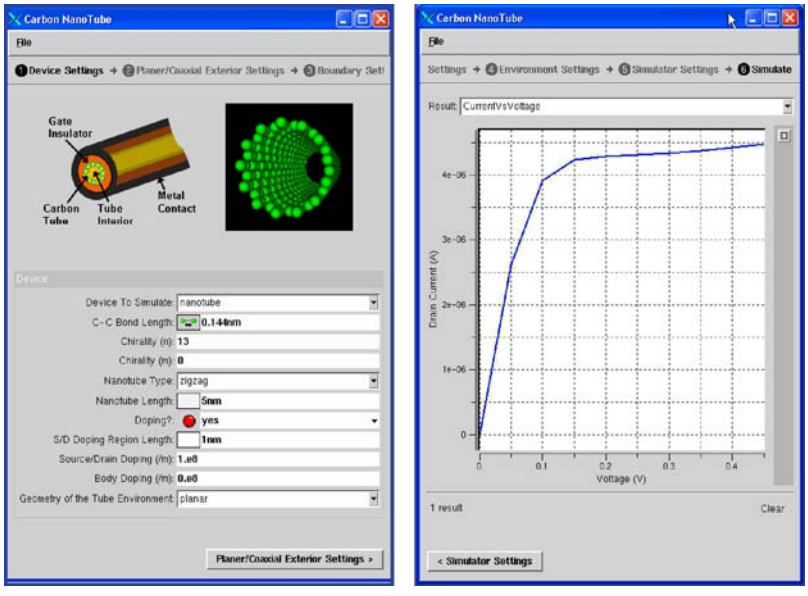

Fig. 6 The graphical user interface (GUI) for the CNTFET simulator used in an interactive session

a comprehensive suite of simulation tools for both conventional and novel nanoscale devices with capabilities not yet available commercially. As an example, the above-described carbon nanotube simulator (named as CNTFET) has been deployed and on the process of being publicly released on nanoHUB.org which currently provides the nanoscience research community with interactive on-line simulation. The necessary computational resources are further assigned to the simulation dynamically by the web-enabled middleware, which automatically allocates the necessary amount of CPU time and memory on the NCSA TeraGrid cluster. The end user, therefore, has access not only to the code, but also to the scientific and engineering community responsible for its maintenance, as well as computational resources necessary to run it. Figure 6 shows the snapshots of the graphical user interface (GUI) for this simulator used in an interactive session.

4 Conclusions

The effect of vacancy defects in the performance of metallic transport devices is examined. The device is described by a nearest neighbor *pz* orbital tight binding Hamiltonian and the NEGF technique coupled to a 3D Finite Element Poisson solver is used to calculate electron transport through the CNT. Recursive Green's Function technique and LU decomposition within MPI implementation are implemented. Our results show that metallic CNTs are greatly influenced by external electric fields due to their very low density of states near their Fermi level. A single vacancy defect can however decrease the metallic nanotube conductance by a factor of two, whereas multiple defects can cause even further conductance degradation.

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References[a]

1. Javey, A., Guo, J., Wang, Q., Lundstrom, M., Dai, H.: Ballistic carbon nanotube field-effect transistors. Nature **424**, 654–657 (2003)
2. Javey, A., et al.: High dielectrics for advanced carbon nanotube transistors and logic. Nature Mater. **1**, 241–246 (2002)
3. Kreup, F., Graham, A.P., Liebau, M., Duesberg, G.S., Seidel, R., Unger, E.: Carbon nanotubes for interconnect applications. Electron Dev. Meeting, IEDM Techn. Digest 683–686 (2004)
4. Saito, Y., Uemure, S., Hamaguchi, K.: Cathode ray tube lighting elements with carbon nanotube field emitters. Jpn. J. Appl. Phys. **37**, L346–L348 (1998)
5. Neophytou, N., Kienle, D., Polizzi, E., Anantram, M.P.: Influence of defects in nanotube transistor performance. J. Appl. Phys. accepted (2006)
6. Polizzi, E., Abdallah, B.N.: Self-consistent three-dimensional models for quantum ballistic transport in open systems. Phys. Rev. B. **66**, 245301 (2002)
7. Datta, S.: Electronic Transport in Mesoscopic Systems. Cambridge University Press, Cambridge, UK (1995)
8. Guo, J., Datta, S., Lundstrom, M., Anantram, M.P.: Multi-scale modeling of carbon nanotube transistors. Intl. J. Multiscale Comput. Eng. **2**, 257 (2004)
9. Anantram, M.P.: Conductance of carbon nanotubes with disorder: A numerical study. Phys. Rev. B. **58**, 4882–4887 (1998)
10. Svizhenko, A., Anantram, M.P., Govindan, T.R., Biegel, B.: Two-dimensional quantum mechanical modeling of nanotransistors. J. Appl. Phys. **91**(4), 2343–2354 (2002)
11. Chico, L., Benedict, L., Louie, S., Cohen, M.: Quantum conductance of carbon nanotubes with defects. Phys. Rev. B. **54**, 4 (1996)

[a]Elements of this work have been summarized in an extended abstract published by IEEE.