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Coupled Mode Space versus Real Space Approach for the Simulation of CNT-FETs

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Carbon Nanotube Field Effect Transistors (CNT-FETs) are considered a promising alternative to CMOS technology at end of the ITRS Roadmap [1]. Fabrication technology still poses serious challenges, such as the selection of semiconducting CNTs, the poor control of the contacts and the large CNT diameter dispersion. As with silicon technology, device simulation tools capable to address very general structures with limited computational resources, can represent a precious tool to explore device architectures, and provide fabrication guidelines. In this work, we present a three-dimensional code that can deal with general architectures, based on the self-consistent solution of the Poisson and Schrödinger equations, within the NEGF formalism, using a tight-binding Hamiltonian with an atomistic (p_z-orbitals) basis set both in the real [2] and in the mode space, by means of the Recursive Green's Functions method. In particular, the mode space approach is based on the reduction of the order of the real space Hamiltonian matrix, by means of a simple basis transformation. Compared to other mode space approaches, the one we propose intrinsically includes intersubband scattering, which is present when the coaxial symmetry of the potential is broken.

The simulated device has the structure depicted in Fig. 1 : the CNT is embedded in SiO_2, and n-doped CNT extensions at the source and drain ends are considered. In Fig. 2 we show the transfer characteristics of a (10,0) CNT with oxide thickness t_{ox} =1 nm and channel length $L = 10$ nm, computed with the real (solid line) and the mode space approach considering only 2 modes (circles). As can be noticed, for this kind of structure, the results obtained with the two different approaches give the same results, since only the first two subbands contribute to electron transport. In Fig. 3 the time required to solve the Schrödinger equation with NEGF for 1684 values of energy on a 1.8 GHz AMD Athlon 64 bit processor is shown. The mode space approach with an analytical expression for the self-energy [3] is 5 times faster than the real space approach (analytical self-energy) when 2 modes are considered, whereas it is slower when 10 modes are considered, due to the additional operation required by the basis transformation. As can be seen, when iterative methods [4] are used for the calculation of the self-energy, the computing time is much larger. For the real space we have for example encountered a speed enhancement of almost a factor of 4. In Fig 4, the transfer characteristics of a (25,0) $L =$ 7 nm CNT computed with the real space and mode space (4 modes) approach are compared. Here, the advance in terms of computing time is more significant, as shown in Fig. 5 since the number of atoms in the carbon ring (which determines the complexity of the problem) is much larger than the number of modes.

In conclusion, the coupled mode space approach results to be an efficient and accurate approach for the investigation of CNT device architectures with reduced computational cost. The authors gratefully acknowledge Prof. Mark Lundstrom for his support during this work. We also gratefully acknowledge support from the EU through the Network of Excellence SINANO (EC Contract n. 506844), and NSF grant # EEC-0228390.

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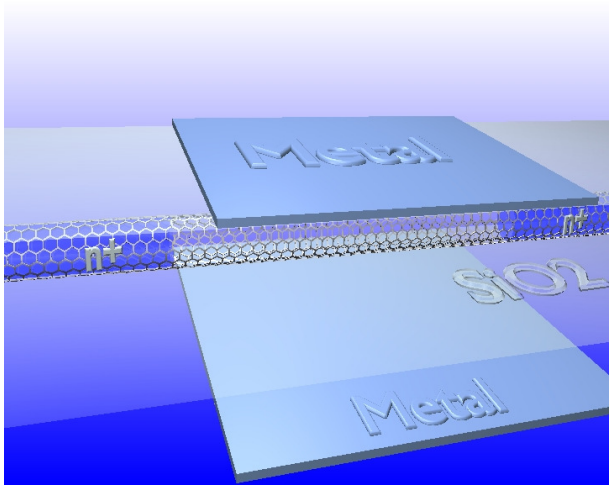

Fig. 1. Simulated device architecture: double gate CNT FET with SiO_2 dielectric and metal gates, n-doped source and drain extensions.

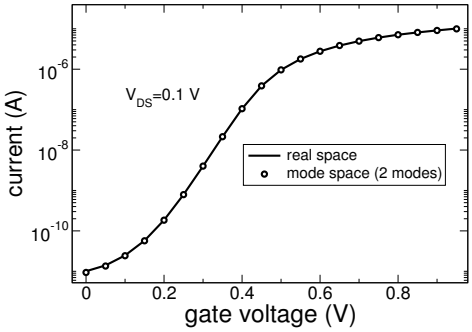

Fig. 2. Transfer characteristics for a (10,0) CNT with t_{ox} =1 nm and L = 10 nm computed with the real space and mode space approach (two modes).

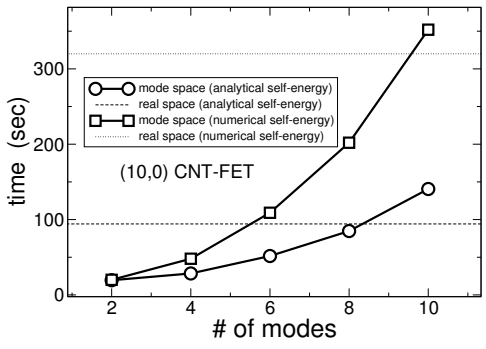

Fig. 3. Time required to solve the Schrödinger equation with NEGF in a CNT with 10 atoms per ring, 280 rings, on a 1.8 GHz AMD Athlon 64 bit processor, as a function of the number of modes with analytical self-energy (circles) and numerical self-energy (squares). The dashed line represents the time required with the real space approach.

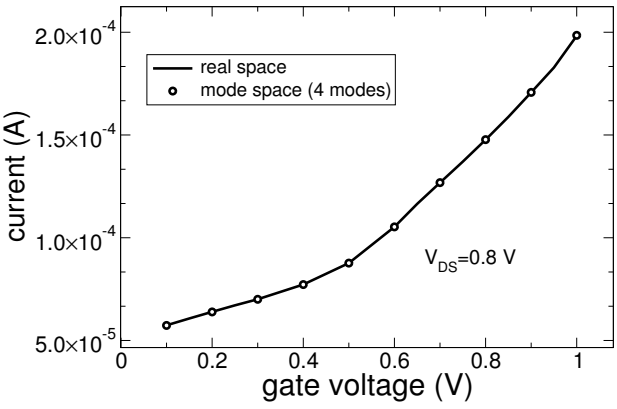

Fig. 4. Transfer characteristics of a $L = 7$ nm (25,0) CNT-FET computed with the real space and the mode space approaches (four modes). V_{DS}=0.8 V.

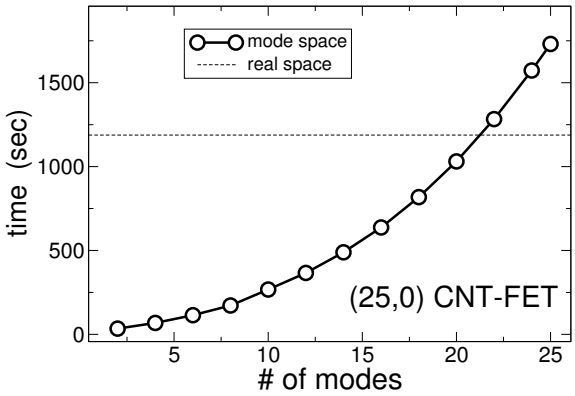

Fig. 5. Time required to solve the Schrödinger equation in a CNT with 25 atoms per ring, and 358 rings, on a 1.8 GHz AMD Athlon 64 bit processor, as a function of number of modes. The dashed line represents the computing time required by the real space approach.