Benchmarking of Atomistic *Ab initio* Model for nanoFET Device Simulations

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ABSTRACT

Quantum transport modeling based on density functional theory (DFT) and the nonequilibrium Green's function (NEGF) formalism have been very successful for studying molecular conductors in recent years. However, for modeling practical solid state devices, NEGF-DFT methods have not been quite useful due to three major issues: (i) practical systems have large number of atoms - too large for DFT; (ii) doping and random disorder averaging are very difficult to handle; (iii) band gaps of semiconductors/oxides are typically under-estimated by conventional DFT. Recently, we have developed an NEGF-DFT method which resolved all the above issues: a TB-LMTO representation of DFT [1] is adopted which can handle more than 10,000 atoms; random disorders are treated by coherent potential approximation (CPA) at the Hamiltonian and single particle Green's function level, and by the nonequilibrium vertex correction (NVC) at the nonequilibrium density matrix level [2,3]; the modified Becke-Johnson (MBJ) semi-local exchange functional [4] is implemented which provides accurate band gaps for semiconductors and oxides (see Table 1). Our code has been successfully employed to model MRAM devices [5] and Cu interconnects [6].

Here, we present a detailed benchmarking study of our atomistic *ab initio* model (NanoDsim software package) with Synopsys/Sentaurus, an industrial standard device simulator which is based on drift-diffusion coupled with a Poisson solver in real space grids. We choose a Si nanoFET device with periodic cross-section as the test system (see Fig. 1). Our *ab initio* modelling shows excellent agreement with the Sentaurus results for many different situations: device structures (p-i-n, p-n-p and n-p-n), dopants (Phosphorus and Boron), doping concentrations, and doping profiles (uniform and delta doping). A few representative benchmarking results have been presented in Figs. 2, 3 and 4. Our results clearly indicate that practical solid state devices can be accurately modelled parameter-free with the NEGF-DFT package, NanoDsim.

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	Expt.	VASP (PBE)	NanoDsim (MBJ)
Si	1.12	0.59	1.11
Ge	0.66	0.00	0.68
HfO_2	5.63	3.77	5.50

Table. 1. Theoretical and experimental band gaps in eV. MBJ functional, as implemented in NanoDsim software, provides very reasonable band gaps for semiconductors and oxides.

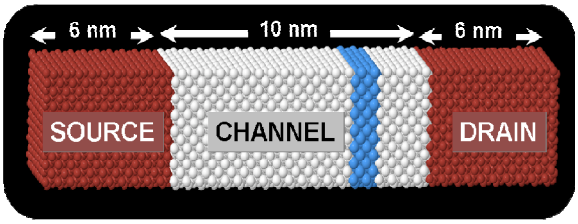

Fig. 1. Atomic structure of the Si nanoFET device with around 800 atoms in the center region. Source and drain are semi-infinite Si leads with periodic cross-section and with doping concentration of $5x10^{19}$ /cm^3 within the Virtual Crystal Approximation (VCA). The doping in the channel region is treated atomistically within the CPA-NVC formalism with dopants, doping concentrations and doping profiles as variables.

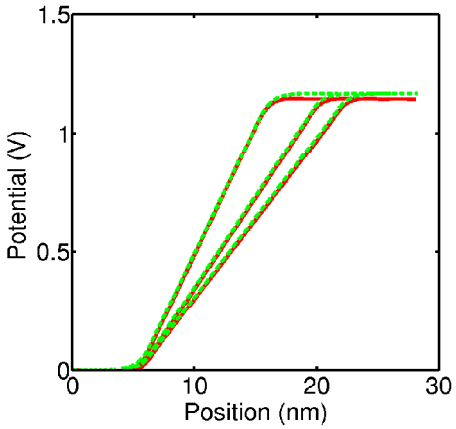

Fig. 2. Potential profiles for the p-i-n structure at equilibrium with channel lengths of 8, 12 and 14 nm. Solid red lines represent the NanoDsim results while the dashed green lines are for the Sentaurus simulations.

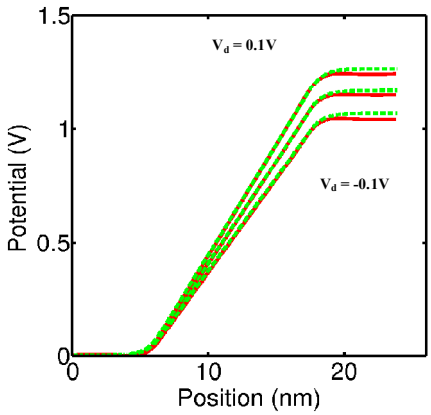

Fig. 3. Potential profiles for the p-i-n structure at reverse bias (V_d = 0.1V) and forward bias (V_d = -0.1V) for 10 nm channel length. Lines on the middle are for the equilibrium case. Solid red: NanoDsim; dashed green: Sentaurus.

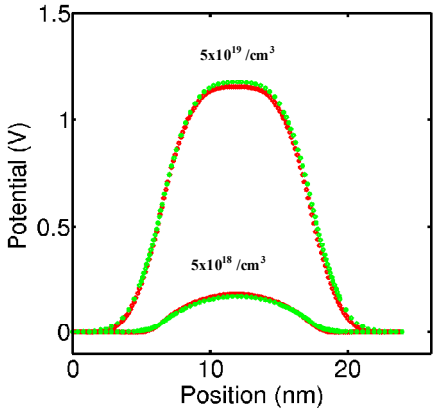

Fig. 4. Potential profiles for the p-n-p structure for different doping concentrations with phosphorus as the dopant in the channel region. Solid red: NanoDsim; dashed green: Sentaurus. Excellent agreement with the Sentaurus simulation results for different doping concentrations validates the CPA-NVC formalism as implemented in the NanoDsim software.