Device modeling from atomistic first principles

Eric Zhu[1], J. Maassen[2], F. Zahid[3], L. Zhang[4], M. Chan[4] J. Wang[3] and Hong Guo[2,1,3],
[1]Nanoacademic Technologies Inc., Brossard, Quebec, J4Z 1A7, Canada
[2]Department of Physics, McGill University, Montreal, PQ, Canada, H3A 2T8
[3]Department of Physics, The University of Hong Kong, Hong Kong SAR, China
[4]Department of Electronic and Computer Engineering, HKUST, Hong Kong SAR, China
e-mail: guo@physics.mcgill.ca

ABSTRACT

Density functional theory (DFT) carried out within the nonequilibrium Green's function (NEGF) formalism has emerged as the state-of-the-art approach for material specific atomistic first principles modeling of nonlinear and nonequilibrium quantum transport properties of nano-devices[1]. In this work, we report solutions to three most critical problems of NEGF-DFT such that present and emerging solid state semiconductor nanoelectronics can be modeled parameter-free at nonequilibrium.

First, practical devices have large number of atoms –too large for standard DFT codes. Here we report a new NEGF-DFT method and its associated software package NanoDsim[2] (stands for Nano-Device-Simulator) that implements the LMTO representation of DFT[2]. Parameter-free modeling of realistic Si channel structure having ~20,000 Si atomic sites using a very modest computer cluster will be presented.

Second, practical devices have dopant fluctuation that is hard to model atomistically. Here we report the development of a statistical approach within the NEGF-DFT formalism to handle disorder averaging at the Hamiltonian level by coherent potential approximation (CPA), and at the nonequilibrium density matrix level by the nonequilibrium vertex correction (NVC) theory. The combination of CPA-NVC allows one to model effects of atomistic and material specific disorder scattering very efficiently and at any concentration [2].

Third, DFT with the local density approximation (LDA, and other functionals) cannot correctly predict band gaps of semiconductors. This is the most important material parameter for device modeling. Here we report the implementation of the modified Becke-Johnson (MBJ) semi-local exchange [3] that allows one to accurately and efficiently calculate band gaps.

With these important advances, the NanoDsim method can be considered as a new generation of device modeling tool based on atomic first principles. Here we apply it to model quantum transport properties of Si devices with realistic doping at nonequilibrium, and compare results to those obtained from industrial TCAD. We also report disorder scattering in spintronic devices. Our results clearly demonstrate that practical solid state devices can be accurately modelled parameter-free from the NEGF-DFT package NanoDsim.

As an example, in the following we resent first principles calculations of charge transport through a Si nano-channel. Fig.1 plots the atomic structure consisting of the channel region connected to source and drain contacts which are heavily doped Si. The channel region is either uniformly doped by impurity atoms (boron or phosphorus) or delta-doped as shown in the figure. Again, the CPA-NVC method within NEGF-DFT allows configurational average over the randomness of the dopant positions, this is crucial because we dope real atoms. For uniform doping, Fig.2 plots the calculated atomic potential along the channel for two different doping concentrations. Our first principles results are in almost perfect agreement

with those obtained by the Synopsys/Sentaurus which is an industrial standard device simulator based on drift-diffusion coupled with a Poisson solver in real space grids. Clearly, such an agreement is only possible with a correctly calculated band gap of Si (1.11eV, using the MBJ potential of Ref.[3]).

Using the full power of the NEGF-DFT and CPA-NVC as implemented in the NanoDsim package, we investigated how controlled localized doping in nano-scale Si channels can suppress source to drain leakage currents and greatly reduce device-to-device variations[4]. Fig.3 shows the calculated off-state conductance of the channel versus the delta-doping location (the location of the 1.1nm doping region along the channel). If this delta-doped region is located away from the source/drain electrodes at roughly 20% of the channel length L, the tunneling leakage is reduced 2× compared to the case of uniform doping and shows little variation. Oppositely, we find the leakage current increases by orders of magnitude and results in large device-to-device variation. We conclude that doping engineering provides a possible approach to resolve the critical issues of undesirable leakage and device variations in nano-transistors.

ACKNOWLEDGEMENTS

This work is supported by NSERC of Canada, CIFAR (JM, HG) and IRAP (EZ, HG), and the University Grant Council (No. AoE/P-04/08) of the Government of HKSAR (FZ, MC, JW),

REFERENCES

[1] J. Taylor, H. Guo and J. Wang, *Ab initio modeling of quantum transport properties of molecular electronic devices*, Phys. Rev. B **63**, 245407 (2001).

[2] For the NanoDsim software, see www.nanoacademic.ca. See also, Y.Q. Ke, K. Xia, H. Guo, *Disorder Scattering in Magnetic Tunnel Junctions: Theory of Nonequilibrium Vertex Correction*, Phys. Rev. Lett. **100**, 166805 (2008).

[3] F. Tran and P. Blaha, *Accurate Band gaps of Semiconductors and Insulators with a Semi-local Exchange-Correlation Potential,* Phys. Rev. Lett. **102**, 226401 (2009).

[4] Jesse Maassen and Hong Guo, preprint (2012).

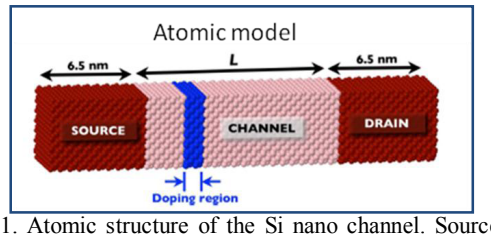

Fig.1. Atomic structure of the Si nano channel. Source and drain are semi-infinite Si leads with periodic cross-section and with doping concentration of $5x10^{19}$ /cm^3. Atomistic doping is handled by CPA-NVC formalism in the channel. The figure shows "delta-doping" where the dopant atoms are randomly reside in a narrow region of D=1.1nm width. When D = L which is the length of channel, we have uniform doping in the entire channel.

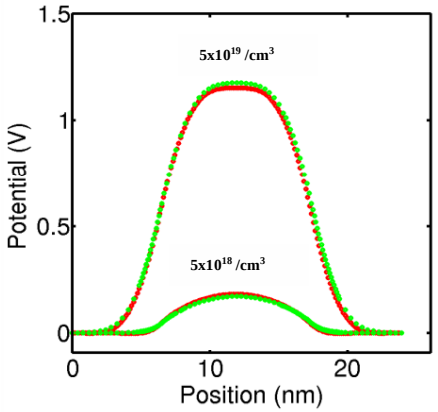

Fig. 2. Potential profiles for the p-n-p structure at different doping concentrations with phosphorus as the dopant in the channel. Solid red: NEGF-DFT by NanoDsim package; dashed green: Synopsys/Sentaurus. Excellent agreements are seen. Note that NanoDsim is completely from atomic first principles and parameter-free.

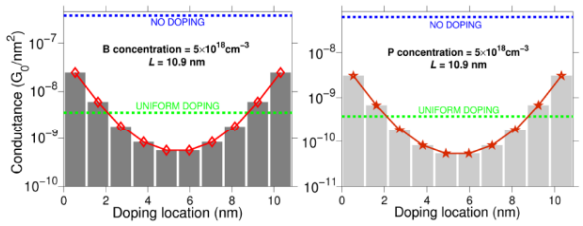

Fig.3. Source to drain conductance (off-state) versus doping location for Boron-doped (n-p-n) and Phosphorus-doped (p-n-p) channel. The doping concentration and channel length *L* are fixed to 5 × 10^{18} cm−3 and 10.9 nm. Each data point corresponds to the doping being localized to a region of 1.1nm in length, as indicated by the width of the bars (see Fig.1). The dashed green line corresponds to uniform doping and the dashed blue line indicates the conductance of channel without doping.