11-8 Nanoscale FET: How To Make Atomistic Simulation Versatile, Predictive, and Fast at 5nm Node and Below

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***Abstract*—Ultra-scaled FET technology requires simulations at the atomic scale. We present the Victory Atomistic tool inherited from Nemo5. Thanks to a combination of non-equilibrium Green's functions and state-of-the-art band structure calculations, versatile, predictive, and fast simulations become accessible within the self-consistent Born approximation, optimized by a generalized low-rank projection.**

Keywords—Atomistic, Simulation, CMOS, FET, NEGF, Scattering, Tight-Binding

I. Introduction

Field Effect Transistor (FET) miniaturization is the workhorse of the microelectronic industry. The FET physical dimensions continue to shrink to five nm node and below, characterized by new types of architectures with nanosheet (NS) and nanowire (NW) shapes [1]. The present choice of material is made of Si, Ge, or SiGe alloy due to their high carrier concentrations. In compliment to III-V technology envisaged for a while, new 2D materials are also investigated, for example the TMDs monolayers. Such nanomaterials and nano-architectures require atomistic simulations for at least two crucial reasons: 1) bulk parameters like the effective masses and forbidden bandgap are no longer pertinent quantities, and 2) the wave nature of charge carriers becomes predominant for predicting I(V) characteristics. Non-equilibrium Green's functions (NEGF) allow us to perform quantum transport simulation of such a device made of two leads and an active region, where carriers move according to a custom band structure [2]. In practice, one needs to build the device's Hamiltonian with a suited set of wave functions, in order to solve the NEGF and Poisson-Schrödinger coupled equations. This comes at the price of a high computational burden, which becomes almost untractable when scattering self-energies of inelastic carrier interactions are included [3]. Thankfully, by generalizing a low-rank approximation (LRA) with a mode space scheme [4], we show how the calculation load can drastically be reduced while preserving accuracy.

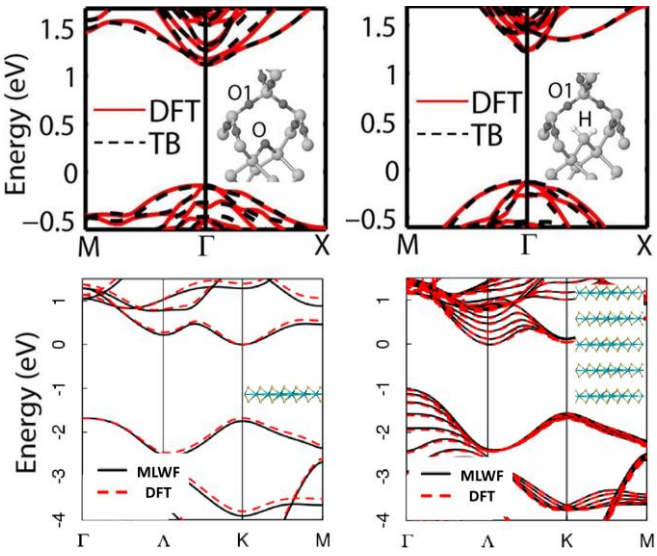

Fig. 1. Top: Tight Binding band structure of Si reproducing the DFT results of the influence of the Si/SiO_2 interface – with a bridging oxygen at the interface (left), with H passivation of Si dangling bonds (right). Bottom: MLWF band structure of MoS_2 TMD reproducing DFT results – for one monolayer, direct gap (left), for five monolayers, indirect band gap (right)

II. Atomistic Simulation Usage

A. Materials and Electronic Bandstructure

One of the most efficient ways to describe the band structure of a material by taking into account its atomic arrangement is the Slater-Koster (SK) tight-binding (TB) model [5]. The set of SK-TB parameters is usually based on accurate experimental measurements and can be extended to state-of-the-art density functional theory (DFT) data, including the most accurate results of hybrid functionals. Passivation chemistry, species alloying, specific mechanical stress can then be included [6]. Eventually, matrix elements of new materials like TMDs 2D layers, topological insulators,

and conductive oxides are derived thanks to maximally localized Wannier functions (MLWF) obtained in hybrid-DFT [7]. As an illustration, band structure results with efficient parametrizations of silicon in contact with SiO_2 and of MoS_2 are shown in Fig. 1.

B. *Quantum Transport*

We simulate a Si NW of different square sections from 2x2 nm^2 to 5x5 nm^2. The contacts are made of highly-doped Si with an intrinsic channel surrounded by SiO_2, see Fig. 2. NEGF calculations are performed using a recursive Green's function [2] and an $sp^3d^5s^*$ Si TB custom basis [6]. I(V) simulations go from ballistic transport up to inelastic scattering by including the self-energies of acoustic and optical phonons, evaluated in the self-consistent sc-Born approximation. This requires computing the G^R (retarded) and $G^<$ (lesser) Green's functions [8]. Note that Victory Atomistic allows treating explicit electrostatic boundary conditions, Ohmic or Schottky contacts, and systematic passivation of the Si dangling bonds.

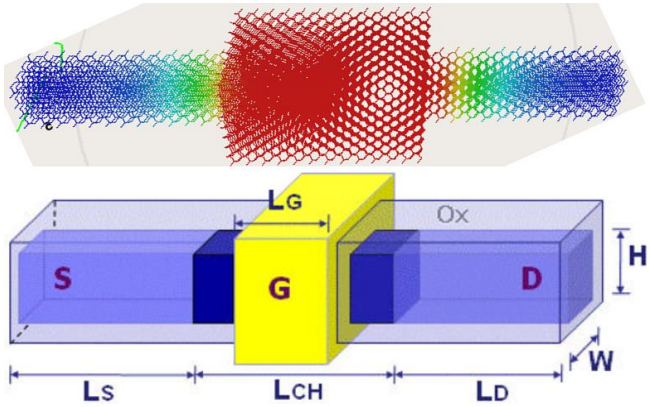

Fig. 2. Si nanowire FET structure of square section. Top: atomistic structure of a 2x2 nm2 nanowire with source and drain of six nm length, and seven nm for the grid. Bottom: drawing of the NW geometry and various characteristic lengths.

C. *Optimization Strategy*

Roughly speaking, the order N of NEGF matrices comes as the product of the number of atoms times the size of the TB basis. In order to reduce the matrix operations of $O(N^3)$ complexity, the scattering mechanisms are often neglected, relegating such simulations to a pure ballistic regime. For keeping the sc-Born approximation, the system's Hamiltonian is reduced by filtering of degrees of freedom that are unlikely to contribute to device operation. This way, our generalized LRA reduces the rank N of the system by a factor of ten or more [9]. We performed a benchmark by qualifying the method against full calculations, see Fig. 3. The obtained speed-up of more than two orders of magnitude is detailed in Table 1.

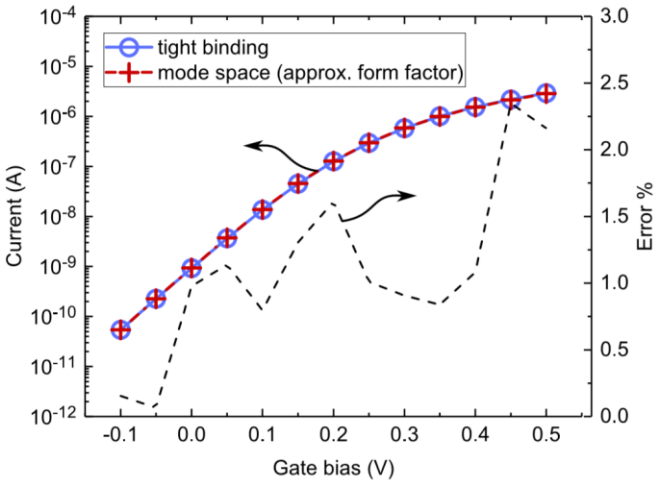

Fig. 3. Benchmark of low rank approximation in mode space including sc-Born inelastic scattering for a nanowire of 3x3 nm^2 and 20 nm length. The LRA (in red) matches the I(V) curve of full band calculation (in blue), with relative error (in black).

TABLE I. SIMULATION TIMES (S) FOR ONE SC-BORN ITERATION FOR VARIOUS SECTIONS, IN FULLBAND AND LRA, WITH SPEEDUP.

Method	**Size nm^2**			
	2x2	***3x3***	***4x4***	***5x5***
Full Band	150	990	4200	17200
LRA	8	9	30	80
Speedup	19	110	140	215

III. SILICON NW FET

Thanks to the LRA approximation, we can study the quantum transport of a silicon nanowire FET transistor, with an affordable computer.

We start with a 2x2 nm^2 structure, see Fig. 2, with a gate-all-around (GAA) structure, for which we draw the I(V) characteristics of the ballistic mode, as shown in Fig. 4.

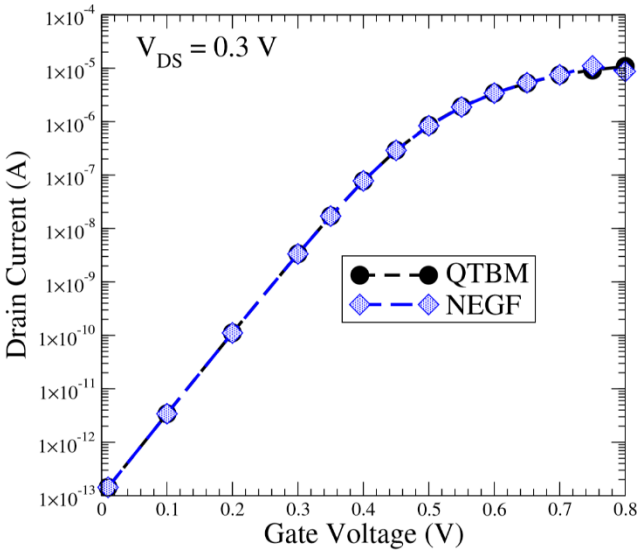

Fig. 4. Id(Vg) characteristics of a GAA Si-nanowire of 2x2 nm^2 and 20 nm long, in balistic mode (QTBM, black circle) and NEGF (blue diamond) at fixed drain voltage Vds.

We use our NEGF with the LRA, and a full quantum transmission boundary method (QTBM) for comparison. Both methods show an excellent agreement for an applied gate voltage Vg of less than 0.7 V. The slight difference observed for larger Vg is mainly due to numerical convergence which is more difficult to achieve with a high ON ballistic current. (Note that our NEGF+LRA is already two times more efficient in terms of simulation time than the QTBM).

Fig. 5 shows the simulation of a 2x2 nm2 Si NW with a double-grid (DG) in ballistic mode with various drain voltages applied, up to saturation. As expected the maximum drain current obtained is lower for a double grid than for a GAA nanowire, due to a less efficient electrostatic control of the gate.

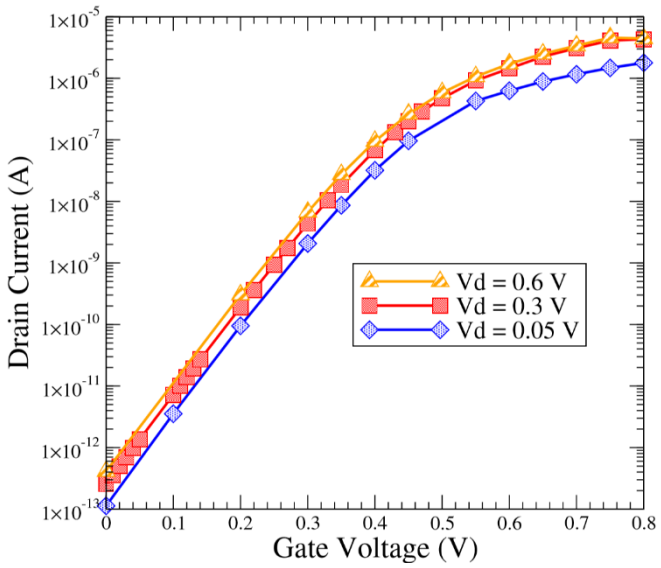

Fig. 5. Id(Vg) characteristics of a DG Si nanowire of 2x2 nm^2 and 20 nm long, in NEGF + LRA for various drain voltages (blue, red, yellow). The simulation is ballistic without including scattering effects.

We performed the simulation of a DG Si NW of 2x2 nm^2 and 20 nm long, by including two scattering effects: the acoustic phonons and optical phonons within the Sc-Born approximation. We limit the Sc-Born number of iterations to ten, which is sufficient to achieve the necessary self-consistency with the outer loop of the Poisson solver. Results are shown Fig. 6 with a net decrease of ON current by 25% approx..

For such a size of a silicon nanowire, the simulation has been performed with a relatively modest number of thirty CPU cores, Intel, (Skylake architecture). One voltage point of the I(V) curve is obtained in 120 minutes, increasing the time of the initial ballistic simulation by a factor no more than 20.

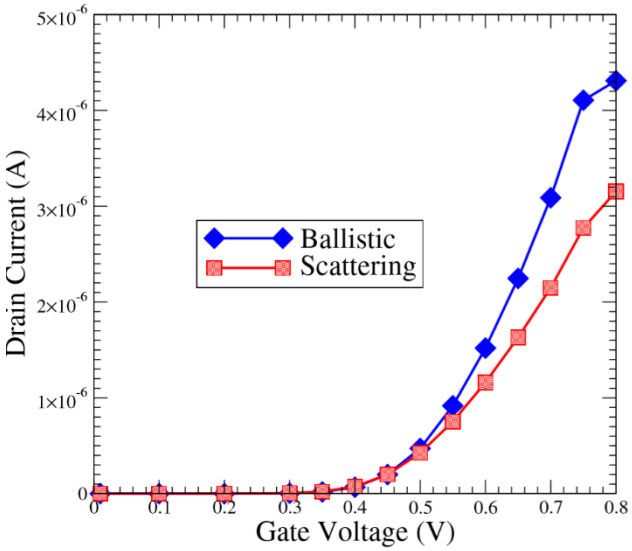

Fig. 6. Id(Vg) characteristics of a DG Si nanowire of 2x2 nm^2 and 20 nm long, in NEGF + LRA a fixed Vds of 0.3 V. With no scattering (blue dimaond), and including acoustic and optical phonons (red square).

We now turn to a larger structure of 5x5 nm^2 and 20 nm long, with DG electrostatic control. As before, we include the acoustic and optical phonons in the Sc-Born approximation, using NEGF+LRA. For performance comparison, one voltage point of the I(V) curve is now obtained in five hours using 240 CPU cores Intel (Skylake), which is consistent with the results of Table I for one Sc-Born iteration.

The energy profile of the conduction and valence bands along the transport direction is visualized Fig. 7.

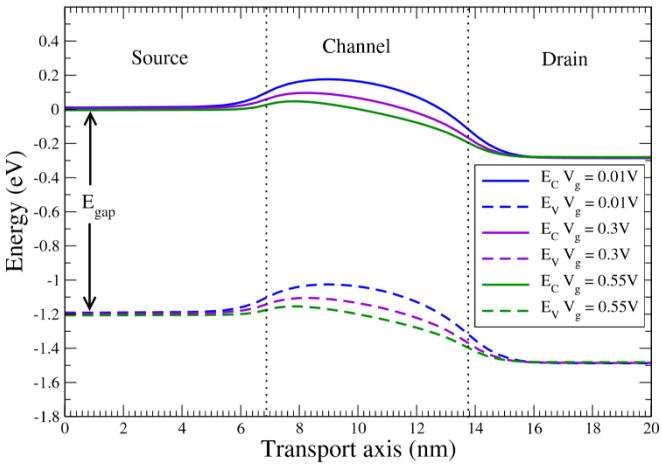

Fig. 7. 5x5 nm^2 Si nanowire, double grid, NEGF+LRA with acoustic and optical phonons. The effective 1-D energy band profiles (conduction Ec and valence Ev) along the transport direction are visualized for different gate voltages and fixed drain voltage of 0.3V. The source is taken as a reference (0 eV).

The band profile of Fig. 7 is directly related to the electrostatic profile of the device. The Poisson potential of the NW-FET is shown in Fig. 8 in three dimensions for illustrative purposes.

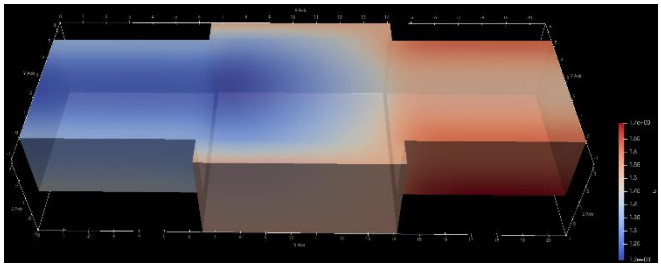

Fig. 8. 5x5 nm^2 Si nanowire, double grid, NEGF+LRA with acoustic and optical phonons. The 3D Poisson potential is visualized with a cut-plane in the middle of the device, where current flows. Voltage in V, dimensions in nm.

Eventually, knowing all our simulations are performed using an atomistic description of the silicon material, this allows us to visualize the electron charge repartition onto each atom. The $sp^3d^5s^*$ Si TB basis components are summed and visualized using VictoryVisual tool, Fig. 9. At Vd = 0.3V, and Vg = 0.55V, this shows a non-intrinsic charge distribution inside the channel, right below the grid (in red) by transparency.

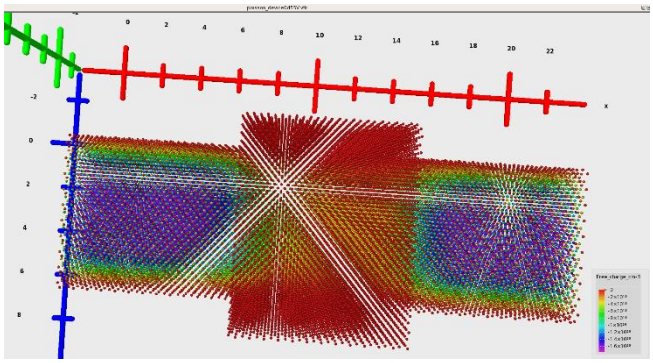

Fig. 9. 5x5 nm^2 Si nanowire, double grid, NEGF+LRA with acoustic and optical phonons. The charge distibution is visualized onto each atomic site, thanks to the VictoryVisual tool. Drain bias is fixed at 0.3 V, and gate voltage at 0.55 V.

IV. Conclusion

Thanks to our new developments, the simulation of a nanoscale FET combining atomic accuracy and inelastic interactions of carriers becomes a daily routine. Moreover, relevant quantities in quantum transport can be safely extracted and visualized. This obviously opens up new perspectives to engineers for simulation of innovative devices in atomistic TCAD. In doing so, the electrostatic of the FET device is revealed at the atomic scale, paving the way to fast and accurate extraction of transistor parameters..

Acknowledgment

Calculations were performed using the Purdue RCAC facilities, Brown's machine.

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