3D Multi-Subband Ensemble Monte Carlo Simulator of FinFETs and Nanowire Transistors

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Abstract—In this paper we present the development of a 3D Multi Subband Ensemble Monte Carlo (3DMSB-EMC) tool targeting the simulation of nanoscaled FinFETs and nanowire transistors. In order to deliver computational efficiency, we have developed a self-consistent framework that couples a MSB-EMC transport engine for a 1D electron gas with a 3DPoisson-2DSchrödinger solver. Here we use a FinFET with a physical channel length of 15nm as an example to demonstrate the applicability and highlight the benefits of the simulation framework. A comparison of the 3DMSB-EMC with Non-Equilibrium Green's Functions (NEGFs) in the ballistic limit is used to verify and validate our approach.

I. INTRODUCTION

In order to fulfill the requirements given by the ITRS for the forthcoming technological nodes [1], the scaling of bulk MOSFETs has ended at the 28/20nm CMOS technology generation with the introduction of a tri-gate transistor by Intel at the 22nm technological node [2]. This difficult decision has been mainly dictated by the high channel doping inherent to bulk transistors that prevents further performance improvement and increases dramatically the statistical variability [3], [4]. FinFETs and nanowire transistors are the preferred present and near-future solution, as they tolerate very low channel doping maintaining good electrostatic integrity allowing the continuation of CMOS scaling and the increase in circuit performance.

On the simulation side, the introduction of these device architectures sets new modeling challenges such as the treatment of carrier transport in highly quantum confined systems, the impact of different crystallographic orientations and fin aspect-ratios and a quasi-ballistic regime of conduction. Therefore, the use of advanced device simulation tools becomes mandatory since several physical effects have to be taken into account keeping an affordable computational effort. In those devices, quantum corrections such Density Gradient (DG) [5] are not enough to accurately represent charge distribution being necessary the use of 2D Schrödinger solvers, Figure 2.

A general simulation approach capable of dealing with all these computational requirements is represented by the 3D Multi Subband Ensemble Monte Carlo (3DMSB-EMC) method targeting the simulation of nanoscaled FinFETs and nanowire transistors. In order to deliver computational efficiency, a self-consistent framework that couples a MSB-



Fig. 1. Electrostatic potential of the FinFET structure used in this work. The oxide is removed for clarity.

EMC transport engine for a 1D electron gas with a 3D Poisson-2D Schrödinger solver has been developed. A FinFET (Figure 1) with a physical channel length of 15nm and a W/H ratio of 5/15 has been used as an example to demonstrate the applicability and highlight the benefits of the simulation framework. A comparison of the 3DMSB-EMC with Non-Equilibrium Green's Functions (NEGFs) in the ballistic limit is used to verify and validate our approach.

II. SIMULATOR METHODOLOGY

The use of MSB is not new in the simulation community as represents one of the best options for the study of ultimate CMOS devices offering a detailed description of carrier transport, catching the main quantum effects and showing balanced computational cost and memory needs. Ultimate-scaled bulk and SOI planar devices [6], [7], [8], have been already studied by means of 2D MSB-EMC codes. However the use of this method for 3D devices is still limited although it is of special interest for the optimization and the prediction in performance of upcoming CMOS technological generations.



domain are coupled by means of the 3D solution of Poisson's equation in order to keep the self-consistency of the simulator. Therefore, MSB-EMC simulators provide one of the most accurate descriptions of carrier transport since detailed scattering models can be included while the main part of quantum effects are taken into account. The flowchart of the 3DEMC-MSB algorithm is shown in Figure 3.



Fig. 2. Drift-Diffusion and CM-NEGF electron density in the center of the device in a cross-section perpendicular to the transport direction at $V_G = 0.0$ V, $V_G = 0.3$ and $V_G = 0.7$ V, showing how the conduction profile changes from bulk-like to surface-like with the applied gate voltage.

The fundamentals of the MSB algorithms are based on the mode-space approach of quantum transport [9], which separates the full 3D problem in a confined and non-confined problems. In this way, the device is divided in several slices containing the confinement plane, where 2D Schrödinger equation is solved and transport properties, considered in the perpendicular direction, are obtained from the Monte Carlo solution of 1D Boltzmann Transport Equation (BTE). The semiclassical and quantum descriptions of the simulation

Fig. 3. Simulation procedure describing the 3DMSB-EMC approach adopted in this work.

After an initial solution that includes a 3DPoisson-2DSchrödinger block and the initialization of the EMC core, the electrostatic potential is used as input for the 2D Schrödinger solver in order to obtain the evolution of eigenenergies, Figure 4, and wave-functions along the transport direction. The transport are computed in a semiclassical way by solving 1D-BTE using the EMC method. As the spacemode approach states, the electric field driving a simulated particle is calculated from the subband's gradient. Therefore, different dynamics are considered to particles belonging to each subbands since drift forces are not the same. After the flight of particles during the time step, the populations of the subbands along the channel, $n_{i,\nu}(x)$, are computed by means of a cloud-in-cell resampling process. The electron concentration, n(x, y, z), is obtained from the subband populations weighted by the distribution functions $|\xi_{i,\nu}(x, y, z)|^2$ for each subband and valley, Eq. 1.

$$n(x, y, z) = \sum_{i,\nu} n_{i,\nu}(x) \left| \xi_{i,\nu}(x, y, z) \right|^2 \tag{1}$$

The way to couple transport direction and confinement plane is by solving 3D Poisson equation in the whole simulation domain whose solver uses as input the previous n(x, y, z). The process is repeated until the convergence is reached.



Fig. 4. The first six subbands profiles along the device length calculated with at $V_G=0.3~V$ and $V_{DS}=50~mV$ CM-NEGF.

III. RESULTS AND DISCUSSION

In order to study the capabilities of the 3DMSB-EMC tool, a set of simulations has been performed on a SOI-FinFET with 15 nm of channel length, and fin height and width of 15 and 5 nm respectively. Its results have been compared with those obtained from well-established tools using different approaches. In particular 3D NEGF and Drift Diffusion (DD) codes [10], [11], [12] have been used to benchmark ballistic and diffusive devices respectively. One of the effects that MSB-EMC codes cannot handle in a direct way is tunneling which may appear through source barrier as channel length is reduced. From density of states calculations (DOS), Figure 5, showing a small DOS inside the barrier, it can be inferred that semi-classical transport neglecting tunnelling terms is still a good approximation for this device.

Concerning electrostatic magnitudes, preliminary 3DMSB-EMC results present a good agreement with those obtained with NEGF regarding charge density along the channel, Figure 6.

Transport properties has been also compared, particularly average velocity profile along the channel which is of special importance in the description of nanodevices where quasiballistic transport regime becomes preeminent, Figure 7. The



Fig. 5. Local density of states (DOS) for simulated device at $V_G = 0.3 V$ and $V_{DS} = 50 \text{ mV}$ with CM-NEGF. The lowest sub-bands (white dashed lines) are also plotted.



Fig. 6. Comparison of 3DMSB-EMC and CM-NEGF electron density along the transport direction at $V_G = 0.3$ V and $V_{DS} = 50$ mV.

simulations shows similar behavior in the ballistic limit for both 3DMSB-EMC and NEGF.

Finally I_D - V_G curves are shown in Figure 8 for the Fin-FET under study considering different approaches including: the present one in the ballistic regime (3DMSB-EMC), 1D ballistic NEGF, 3D-DD with quantum corrections and 2D ballistic electron gas (2DMSB-EMC [13] and NanoMOS [14]) where a fin height correction has been used to establish a fair comparison between 2D and 3D simulators. As expected, all the models behave similarly in subthreshold regime whereas the different transport models play an important role above threshold. As can be observed, the 3DMSB-EMC code developed in this work shows similar behavior in all transport regimes compared to NEGF and 2DMSB-EMC which have already proved their capabilities.



Fig. 7. Velocity profile at $V_G = 0.3$ V and $V_{DS} = 50$ mV along the transport direction derived from 3DMSB-EMC and CM-NEGF approaches.



Fig. 8. I_D -V_G curves calculated with different approaches including Drift-Diffusion, CM-NEGF and MSB-EMC for a fixed $I_{OFF} = 10^{-7}$ A.

These results demonstrate that the semi-classical description of transport provided by the Monte Carlo code remains as an appealing approach for extensive study of ultimate devices. Moreover it can be readily extended to new structures and materials to foresee the performance of future technology nodes.

IV. CONCLUSION

This work presents the development of a 3D Multi Subband Ensemble Monte Carlo (3DMSB-EMC) tool for the simulation of next generations nanodevices with 3D architectures. The self-consistent framework developed for this tool couples a MSB-EMC transport engine for a 1D electron gas with a 3DPoisson-2DSchrödinger solver. The results obtained for a nanoscaled FinFET have been compared to those given by NEGF approach, showing that MSB-EMC codes can be successfully used for the study of future 3D devices with an affordable computational cost.

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