Improving subthreshold MSB-EMC simulations by dynamic particle weighting

Carlos Sampedro*, Francisco Gámiz*, Andrés Godoy*, Raul Valín‡, and Antonio Garcia-Loureiro§
*Dep. de Electrónica y Tecnología de Computadores, Universidad de Granada, 18071 Granada (SPAIN). Email: csampe@ugr.es
‡College of Engineering, University of Swansea, Swansea (UK)
§Departamento de Electrónica y Computación, Universidade de Santiago de Compostela, Santiago de Compostela 15782 (SPAIN)

***Abstract*— The study of current and futures nanodevices demands a special focus on the subthreshold regime for switching and power consumption considerations. MSB-EMC simulators represent one of the best options for the study of ultimate CMOS devices offering the most detailed description of carrier transport. However, several issues derived from the charge discretization process and the statistical nature of the technique limit the application to subthreshold regime. This paper presents a method for statistical enhancement including dynamical calculation of electron-particle equivalent (EPE) values with position and bias dependence in order to extend the application of MSB-EMC simulators to subthreshold regime in a feasible way from a CPU and memory requirements point of view.**

I. Introduction

As semiconductor devices are aggressively scaled down in the search for improved performance and lower power consumption, the semiconductor industry must face important challenges arising from the use of new geometries and materials at the nanoscale in order to fulfill the requirements given by the ITRS for the forthcoming 14/11 nm nodes [1]. To accomplish such extreme scaling, it is necessary to control Short Channel Effects (SCEs) and to enhance transport properties including arbitrary channel orientations or strain materials to increase the device performance. At this point, standard bulk-MOSFET technology cannot provide good enough solutions for sub-22 nm nodes due to the limited control of SCEs and variability problems coming from a highly doped channel [2]. Two are the mainstream Silicon based options to reduce SCEs based on novel device structures: the use of multiple gate devices (MuGFETs) and the extension of planar technology by means of SOI. The first option, thanks to an outstanding SCEs control [3], [4], is able to extend the end of the roadmap by means of different candidates (FinFETs, Trigate and Gate-All-Around). The second option tries to take advantage of the benefits provided by SOI devices. More precisely, Extremely Thin Fully Depleted SOI devices (ET-FDSOI or simply ETSOI) are chosen thanks to the extra control over SCEs provided by the thin silicon channel, the buried oxide (BOX) and their simpler fabrication process compared to planar bulk architectures and, of course, 3D devices. This fact allows a reduction in the overall cost and an almost straightforward layout transfer from bulk to SOI [5] in opposition to the implementation of MuGFET technology, where a complete redefinition of the fabrication flow and the introduction of new processing steps are mandatory.

Within this framework, the use of advanced device simulation tools offers several advantages for the development of upcoming technological nodes. On the one hand, it is possible to predict the performance of different architectures and technological choices. On the other hand, the development stage can be reduced in terms of cost and time. Another important advantage is the possibility of studying the impact of each technological booster separately to explain experimental results and to determine which one is the most effective in improving the device performance.

Depending on the required accuracy, the computational resources and time available to perform the simulations, different approaches from classical to full quantum could be considered. However simple tools based on drift diffusion models should not been employed since confinements effects are of special importance. At the opposite end of the spectrum, full quantum simulators based on numerical solutions of the Schrödinger equation or the Non-Equilibrium Green's Functions theory (NEGF) have also been developed [6]. The introduction of scattering in the simulations involves a very high computational cost and for this reason, only simplified models can be used in practical quantum simulations [7].

In this scenario, Multi-Subband Ensemble Monte Carlo simulators (MSB-EMC) [8] represent one of the best options for the study of ultimate CMOS devices offering the most detailed description of carrier transport, catching the main quantum effects and showing balanced computational cost and memory needs. However, at subthreshold regime the main limitation of this method becomes of special relevance. The study of device characteristics below threshold voltage has became of special interest in the last years due to the exponential grown of mobile application where stand-by power consumption is of paramount importance. The stochastic nature of MC techniques limits the maximum accuracy in current calculations due to the inherent statistical noise. This fact, that can be reduced increasing the number of flights in one-particle approaches, is difficult to be dealt with when the self-consistency between the electrostatics and the particle ensemble must be kept. The quantization introduced in the charge density in the conversion process from a continuum to a particle-based description adds rounding errors which are non-negligible

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in the study of current and future nanodevices where off-current and subthreshold slope reduction drive scaling in low power applications. This work deals with the use of statistical enhancement techniques based on particle dynamic weighting and their application on MSB-EMC codes to minimize CPU costs in the study of subthreshold regime of nanodevices.

II. Simulator Description

Our Multi-Subband Ensemble Monte Carlo code (MSB-EMC) has been successfully applied for the study of different nanodevices including bulk [9], DGSOI [8] and FDSOI [10]. Based on the mode-space approach of quantum transport [11], MSB-EMC simulators provide one of the most detailed descriptions of carrier transport that includes in a natural way the particularities of carrier transport in ultra-short devices as those considered in this work.

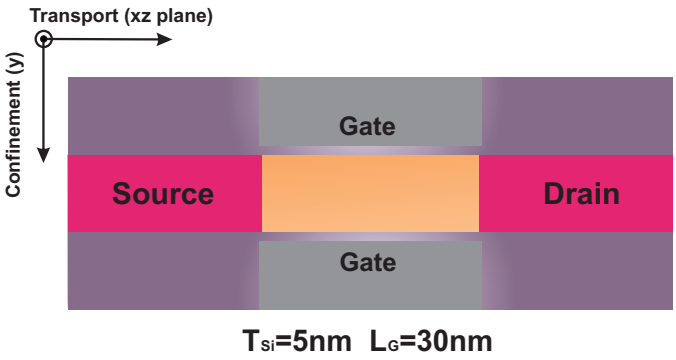

Fig. 1. Benchmark DGSOI device used in this study with $L_G = 30$ nm, $T_{Si} = 5$ nm, EOT= 1 nm and $N_D = 10^{20}$ cm^{-3}.

This approach decouples the problem for the transport plane and the confinement direction. In this way the transport is treated as semiclassical whereas 1D Schrödinger equation is solved for different slabs in the confinement direction (*XZ* plane and *Y* direction in Figure 1 respectively).

The electrostatics of the system is obtained from the coupled solution of 2D Poisson and 1D Schrödinger system. Therefore the evolution of the eigen-energies and wavefunctions for the *i-th* valley and the ν-*th* subband is obtained along the transport direction. To evaluate the transport properties, the Boltzmann Transport equation (BTE) is solved by the Ensemble Monte Carlo method (EMC) considering a non-parabolic conduction band approximation in both confinement [12] and transport directions. According to the space-mode approach, the driving field undergone by a simulated particle is calculated from subband's gradient corresponding to a different driving force for each the subbands. The subband population needed to calculate the electron density is then obtained from a re-sampling of the particles weighted by the corresponding distribution function $|\xi_{i,\nu}(x,y)|^2$ using the cloud-in-cell method. Finally, the electrostatic potential is updated by solving the 2D Poisson equation using the previous $n(x,y)$ as input. This approach is especially appropriate for the study of 1D confinement in nanoscale devices since the computational impact of the inclusion of quantum effects is partially overcome thanks to the efficient parallel implementation of the code [13]. Concerning scattering models, the simulator includes acoustic and intervalley phonons [12], surface roughness scattering [14] and Coulomb interaction.

III. Simulation Set-up and Results

The combination of highly doped source and drain regions to reduce parasitic resistance and the low populated channel under subthreshold conditions represents the biggest challenge for standard EMC codes for the study of nanodevices, like the DGSOI shown in Figure 1, where each particle inside the simulation domain represents the same amount of charge.

In this way, a correct representation of the charge inside the channel demands small electron-particle equivalent (EPE) values and, therefore, a huge amount of particles in source and drain regions resulting in a non feasible simulation run from both memory and CPU time requirements. Bigger EPE values reduce simulation time and memory requirements as less particles are simulated. However, it could cause quasi-empty regions in the discrete to continuous charge representation process.

The use of bigger values of EPE does not impact in an important manner in the subband distribution under subthreshold regime as observed in Figure 2. The reason arises from the small carrier density found at such bias conditions. It is true that the carrier concentration is better represented in the channel for small EPE values, however the change of this value is not big enough to affect in an important way the shape of the quantum well which determines the position of the subbands.

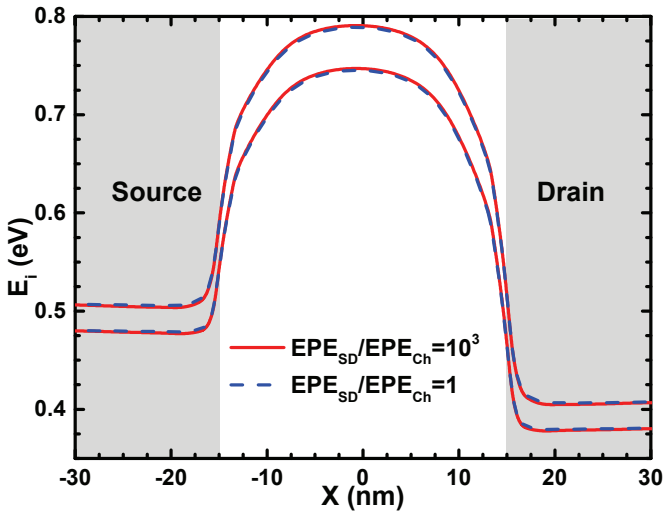

Fig. 2. Fundamental and first excited subband profile along transport direction under V_{GS}=0.4 V and V_{DS}=0.1 V for $EPE_{SD}/EPE_{Ch}=10^3$ (red) and 1 (blue).

On the contrary, there is a non-negligible impact on the accuracy in the determination of drain current characteristics and transport properties when big EPE values are used. These issues are carrier concentration-related and come from two main sources: the first one is the miss-population of the excited subbands as a consequence of discretization errors leading to

differences on carrier concentration as shown in Figure 3. The second one arises from the poor statistics that superparticles show in the source region where only a very small fraction of them have enough energy to overcome the barrier since the tail of energy distribution is poorly represented.

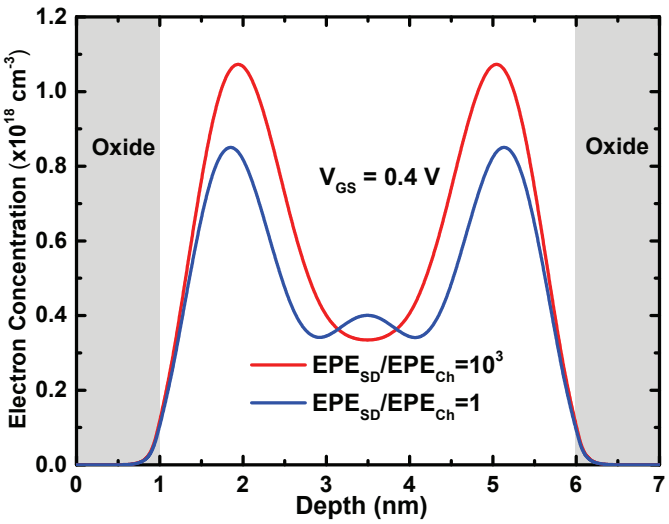

Fig. 3. Carrier concentration at midpoint of the channel under V_{GS}=0.4 V for $EPE_{SD}/EPE_{Ch}=10^3$ (red) and 1 (blue).

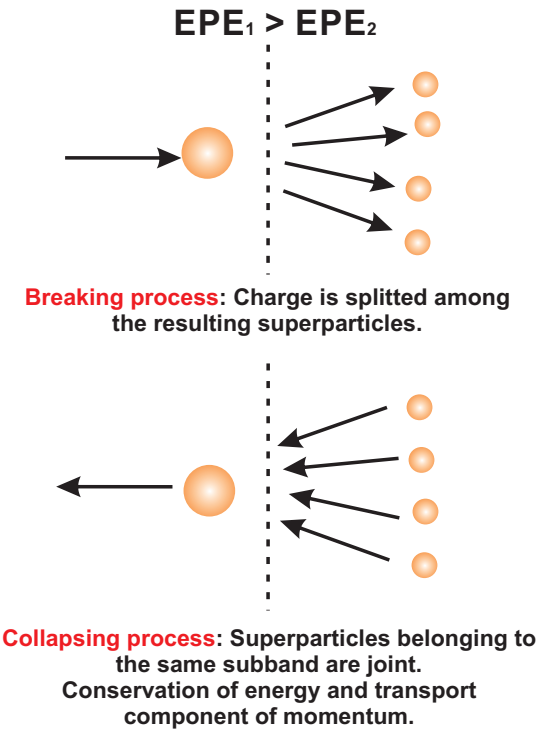

Fig. 4. Representation of the breaking (top) and collapsing (bottom) processes when particles cross a boundary between two regions with different EPE.

This work proposes the use of different EPE values in S/D and channel regions as it was already employed in bipolar semiclassical EMC codes [15]. In the case of MSB-EMC, spatial charge distribution, momentum and energy are conserved as in the semiclassical case, however it is also necessary to keep the population of each subband constant, specially in the collapsing processes occurring when several particles with small EPE reach a region with a bigger EPE assigned, Figure 4. The proposed algorithm has been implemented in the OpenMP parallelised version of MSB-EMC simulator [13]. This code optimizes the free flight of carriers distributing the total number of simulated particles among threads and evaluating the charge neutrality condition at the Ohmic contacts with an unique and efficient algorithm. The breaking and collapsing processes are independently evaluated for each particle allowing a fair parallel scaling. These processes are controlled by a threshold value which guarantees a defined amount of particles into the channel region. To enhance the statistics on the injection of particles into the channel, the breaking boundary has been set some grid points before the virtual source increasing the number of flights near the barrier.

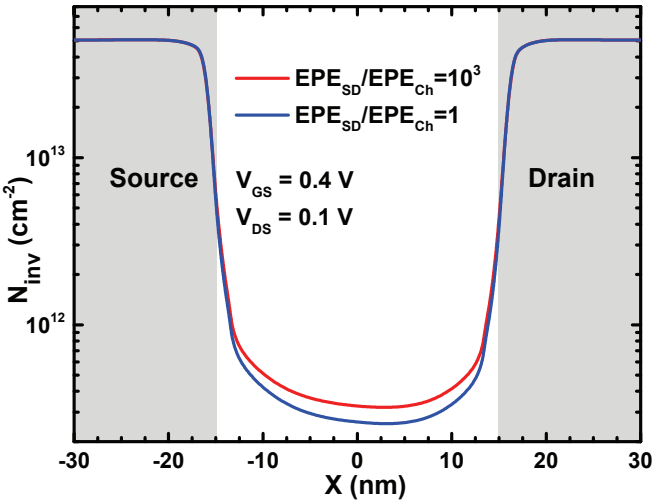

Fig. 5. Inversion charge for $EPE_{SD}/EPE_{Ch}=10^3$ (red) and 1 (blue) when $V_{GS} = 0.4$ V and $V_{DS} = 0.1$ V. The charge enhancement can be only notice in the small concentration region (channel)

As Figure 5 shows, the only difference on charge density appears in the channel region whereas in S/D there is no difference between both cases. The main drawback of this method is an important increase in the CPU time as the EPE_{Ch} is reduced as shown in table I. This penalty on the execution time is mainly caused by the increase on the total number of simulated particles which jeopardizes the performance of the simulator increasing the computational time of the key subroutines.

To reduce this overhead, an adaptive algorithm that dynamically calculates the EPE_{Ch} focusing on keeping the total amount of particles around a target value has been used. In order to assure a correct representation of carrier concentration in the channel for low bias conditions, an initial EPE_{Ch} value is obtained from the self consistent solution of the Poisson-Schrödinger problem at $V_{DS} = 0$ V. From this point on, the MSB-EMC run starts increasing or decreasing

Device	EPE_{SD}/EPE_{Ch}	CPU time (s)
a	1	20040
b	10	25440
c	100	92100
d	1-2000	42900

TABLE I

CPU TIME FOR DIFFERENT EPE CONFIGURATIONS (A-C) AND A DYNAMICAL WEIGHT ADJUSTMENT (D) FOR THE CALCULATION OF THE I-V CURVE IN FIGURE 6 WHERE 88 PS WERE CONSIDERED. ALL THE SIMULATIONS WERE PERFORMED USING 8 PARALLEL THREADS.

EPE_{Ch} in a dynamic way as bias conditions or the number of superparticles is changing. As a result, the EPE in the channel tends to the value considered in source and drain regions as the gate voltage increases decreasing the needed CPU time for the calculation of states above the threshold voltage (Table I). In this way, there is an important optimization of the use of High Performance Computing resources (HPC) keeping the accuracy of the simulations performed considering small and constant EPEs as shown in the case of drain current characteristics in Figure 6.

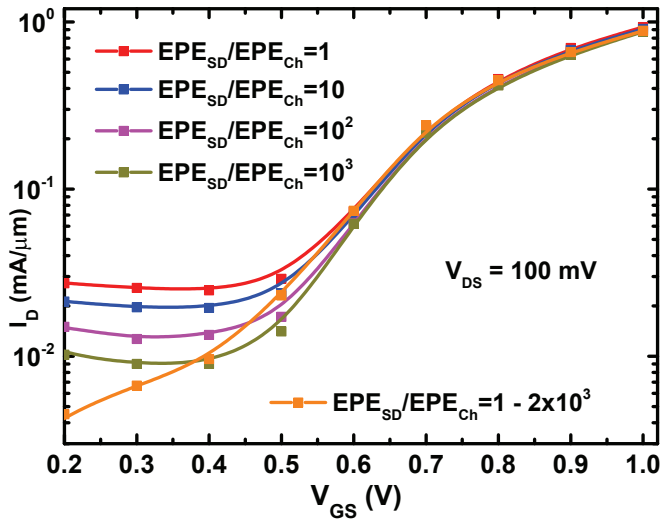

Fig. 6. I_D vs. V_{GS} for different EPE ratios and the dynamic particle weighting.

IV. CONCLUSION

This work presents a method for statistical enhancement of MSB-EMC simulators to increase the accuracy of their results in the subthreshold regime which has become of paramount importance specially in the field of low power applications. The proposed technique includes dynamical calculation of EPE values with position and bias dependence. The implementation of breaking and collapsing processes keeps the advantages of the parallel characteristics of the simulator enabling feasible CPU and memory requirements for such kind of simulations.

V. ACKNOWLEDGMENT

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