Self-Forces in 3D Finite Element Monte Carlo Simulations of a 10.7 nm Gate Length SOI FinFET

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***Abstract*—Particle-mesh coupling in ensemble Monte Carlo simulations of semiconductor devices results in unphysical self-forces when using unstructured meshes to describe the device geometry. We develop a correction to the driving electric field and show that self-forces can be virtually eliminated on a finite element mesh at a small additional computational cost. The developed methodology is included into a self-consistent 3D finite element Monte Carlo device simulator. We simulate an isolated particle and show the kinetic energy conservation down to a magnitude of 10^{-10} meV. The methodology is applied to a 10.7 nm gate length FinFET simulation and we find that for a large enough ensemble of particles, the impact of self-forces on the final I_D-V_G is almost negligible.**

I. Introduction

Monte Carlo (MC) methods have been widely used to simulate carrier transport in semiconductor devices [1], [2], [3]. As semiconductor devices are shrunk into deep nanoscale dimensions in order to boost their performance, the carrier transport becomes highly non-equilibrium requiring advanced physically based simulation models. The self-consistent ensemble MC is one of such methods, providing a detailed insight into transport and an accurate prediction of current characteristics of nanoscale transistors [4], [5].

Nanoscale non-planar multi-gate transistor architectures [6] such as FinFETs are replacing conventional bulk transistors during the scaling into nanometre dimensions [7], [8]. Their 3D device geometry at nanoscale has unique shapes created by the fabrication process [4] which leads to new serious challenges for physically based device modelling. In order to precisely describe such fluctuating device geometry, the finite element method (FEM) provides unparalleled advantages. However, the use of unstructured meshes in a self-consistent ensemble Monte Carlo (MC) [2] simulation requires careful evaluation of the particle-mesh coupling to avoid unphysical self-forces on the particles [9], [1], [10].

The impact of self-forces in semiconductor device particle simulations has been extensively studied in the past [1], [10], [3] and various methods have been proposed to minimise them. However, most of these works have achieved a satisfactory result only for orthogonal meshes [10]. In this work, we present a methodology to evaluate and suppress the self-forces in a finite element (FE) MC device simulator based on tetrahedral elements [5]. The structure of the paper is as follows. Section II describes the main features of the EMC simulator used in the study and the methodology we have developed for the determination of the self-force. Section III presents and analyses two simulation studies. The first one focuses on the impact of the self-force on a single particle, and in the second one we show the impact of the self-forces on the drain current of a 10.7 nm gate length SOI FinFET. Finally, Section IV summarises the main conclusions of this work.

II. Methodology

A. Monte Carlo simulations

The 3D FE ensemble MC simulation method that we employ [5] uses an analytic non-parabolic anisotropic model for the dispersion relation in the valleys of the conduction band of silicon [2], [11]. The scattering mechanisms included in the simulations are acoustic phonon scattering, non-polar optical phonon scattering (g, f-processes) [2], [12], [13], ionized impurity scattering using the third body exclusion model by Ridley [14], [15] and interface roughness (IR) scattering using Ando's model as described in [16]. For an exponential autocorrelation function, the IR scattering rate is given by

$$\Gamma(\mathbf{k}) = \frac{m^* e^4}{\hbar^3 \varepsilon_S^2} \frac{\Delta_{RMS}^2 \Lambda^2 E_\perp^2}{\sqrt{1+k^2\Lambda^2}} \times \mathcal{E}\left(\frac{k\Lambda}{\sqrt{1+k^2\Lambda^2}}\right), \quad (1)$$

where Δ_{RMS} is the RMS height of the fluctuation at the interface, Λ is the correlation length for the fluctuations, $E_\perp$ is the local transverse field (i.e. the one normal to the interface), $\mathcal{E}$ is the complete elliptic integral of the first kind and all other symbols have their usual meaning. The values used for Δ_{RMS} and Λ are 0.57 nm and 1.7 nm, respectively. The value for Δ_{RMS} was taken from experimental data in Si FinFETs [17] and verified in the simulation of a 25 nm gate length FinFET [5], whereas the correlation length Λ is assumed to be as in planar MOSFETs [18], [19]. Quantum corrections are included through the density gradient approach [20] and they are assumed to be fixed during the MC simulation [21].

B. Self-force correction

For the calculation of the self-force on the unstructured mesh, we need the potential created by a point charge in every node of the mesh. Therefore, for a given mesh and for every node, we calculate the *reference electrostatic potential* for a unit charge assigned to the node p, $\psi^{p,R}$:

$$\nabla^2 \psi^{p,R} = \delta(\vec{r} - \vec{r}_p), \quad (2)$$

$$\psi^{p,R}|_{\partial\Omega_D} = \frac{k_C}{|\vec{r} - \vec{r}_p|}, \quad (3)$$

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where $\partial\Omega_D$ is the external boundary of the domain, with Dirichlet boundary conditions applied. This reference potential mimics the potential that the particle would create in an infinite domain without any other charge and with the boundary condition $\lim_{|\vec{r}-\vec{r}_p|\to\infty} \psi^{p,R} = 0$.

To calculate the reference potential, we use the Ritz–Galerkin approximation and apply the FEM based on tetrahedral elements with piecewise linear base functions θ_i [22]. We then obtain the following weak formulation of the equation (2) [23]:

$$\sum_{j=1}^{K} \psi_j^{p,R} \int_\Omega \nabla\theta_j \cdot \nabla\theta_i d\Omega = -\delta_{ip},\ \forall i = 1,\dots,K, \quad (4)$$

where K is the number of nodes in the mesh and we have used the fact that p is in the position of a node.

On the other hand, during the simulation, we solve the Poisson equation to obtain the electrostatic potential at every time step:

$$\nabla(\varepsilon(\vec{r})\nabla\psi(\vec{r})) = \sum_p q_p \delta(\vec{r}-\vec{r}_p) + \rho(\vec{r}), \quad (5)$$

where $\varepsilon(\vec{r})$ is the permittivity of the medium and $\rho(\vec{r})$ is a continuous charge distribution. Using the same discretisation method, we obtain the following weak formulation of the equation:

$$\varepsilon \sum_{j=1}^{K} \psi_j \int_\Omega \nabla\theta_j \cdot \nabla\theta_i d\Omega = - \sum_p q_p \theta_i(\vec{r}_p) - \sum_{j=1}^{K} \int_\Omega \rho_j \theta_j \theta_i d\Omega,\ \forall i = 1,\dots,K. \quad (6)$$

For every particle, we correct this electrostatic potential using the reference electrostatic potential (4) since it corresponds to the self-interaction term. For a particle p in element e with nodes i, we calculate the force as:

$$\vec{F}(\vec{r}_p) = -q_p \sum_{i\in e} \left(\psi_i - \varepsilon(\vec{r}_p)\psi_i^{i,R}\right) \nabla\theta_i(\vec{r}_p). \quad (7)$$

III. Numerical results

To test the proposed method, we carry out two types of simulations. First, we simulate a domain with a single charged particle with Dirichlet boundary conditions representing the Coulomb potential of the particle. Any force that the particle feels in these conditions is artificial and corresponds with the self-force. In this way, we can quantify the self-force in a given mesh and also evaluate its impact in terms of conservation of the energy. Later, we evaluate the impact of the self-force on the current-voltage characteristics of a semiconductor device, since this is the final quantity of interest and, therefore, the key indicator about the quality of the method in terms of reliability of the results.

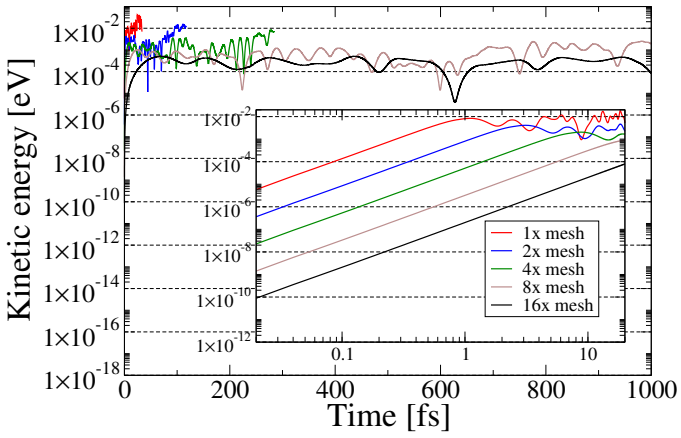

Fig. 1. Dependence of the kinetic energy with the simulation time for different mesh scalings. A detailed view for small simulation times is shown in the inset in a log-log scale.

A. Single particle simulations

To measure the self-force, we set up a simulation reproducing as closely as possible a single charged particle in an infinite homogeneous domain. To approximate this ideal system, we simulate self-consistently a single particle in an element e far enough from the boundaries of the simulation domain. As a first experiment, we simulate the evolution of a single particle with zero initial kinetic energy. The movement of the particle is carried out using the semiclassical equations of motion without any scattering mechanism. Any force that the particle feels in these conditions is artificial and corresponds to the self-force. We evaluate its impact in terms of conservation of the energy. We also study the impact of the mesh size using the same mesh scaled by a factor up to 16 times larger than the original one. Fig. 1 shows the time evolution of the kinetic energy during 1 ps for the differently scaled meshes. There is a clear artificial increase of the kinetic energy caused only by particle-mesh coupling. The increase in the energy of the particle decreases with increasing size of the mesh. The inset shows the evolution of the kinetic energy during the first 20 fs. For a free flight time of 0.5 fs, the artificial kinetic energy increase can be as large as 3 meV for the smallest element size, which is unacceptable during a simulation.

Applying the correction for the self-force described in (7) for every time step, we can suppress the self-force during the simulation. Fig. 2 shows that the artificial kinetic energy has been greatly reduced after applying the correction and it remains below 2×10^{-13} eV after a simulation of 1 ps for the worst case. For all the cases, the error in kinetic energy remains zero for free flights of at least 30 fs in the worst case and, for a scaling of the original mesh by a factor 4 or 8, it remains zero for the whole simulation time.

B. Device simulations

We apply the self-force correction within our 3D FE MC simulation toolbox including density gradient based quantum corrections [5] to study the impact of self-forces in a 10.7 nm gate length SOI FinFET designed following the ITRS 2012 description [24]. The device has a silicon body with a height of 15 nm, a width of 5.8 nm, and an equivalent oxide

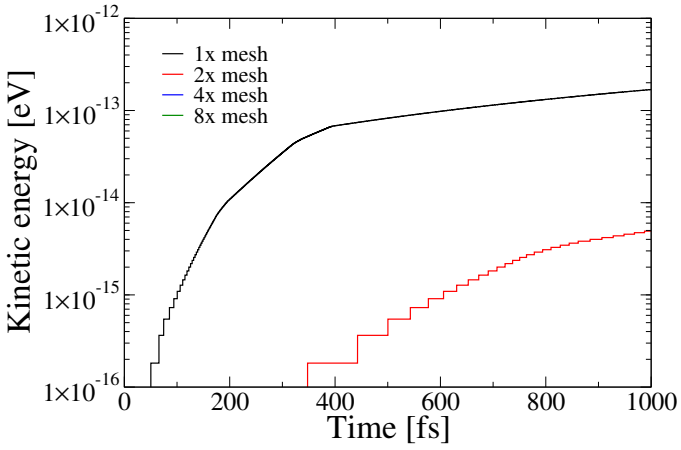

Fig. 2. Dependence of the kinetic energy with the simulation time for different mesh scalings using the corrected force calculation.

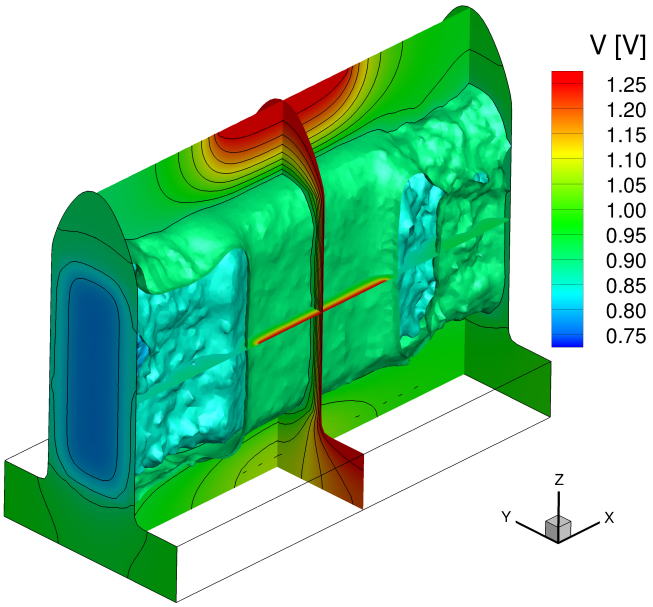

Fig. 3. Electrostatic potential inside the studied 10.7 nm gate length, n-channel SOI FinFET at $V_D = 50$ mV and $V_G = 0.9$ V.

thickness (EOT) of the dielectric layer of 0.62 nm. The n-type doping in the source and drain (S/D) regions has a maximum concentration of 10^{20} cm^{-3} with a Gaussian decay of $\delta = 3.45$ nm, while the p-type channel is nominally undoped to 10^{15} cm^{-3}. All simulations are done at a low drain bias of $V_D = 50$ mV since self-forces will be more important at low external fields. The electrostatic potential inside the device at $V_D = 50$ mV and $V_G = 0.9$ V is shown in Fig. 3.

Fig. 4 shows the dependence of the drain current at $V_D = 50$ mV and $V_G = 0.9$ V with the number of superparticles with and without self-force correction. For a large number of superparticles, the self-force is smaller and negligible compared to other fields (external and of other particles). However, as the number of superparticles in the simulation domain increases, the self-force starts being more important and the error in the current increases to $\sim 10\%$. We can also see a decrease in the current as we decrease the number of superparticles, as also shown in Fig. 5 for the $I_D - V_G$ characteristics at a low

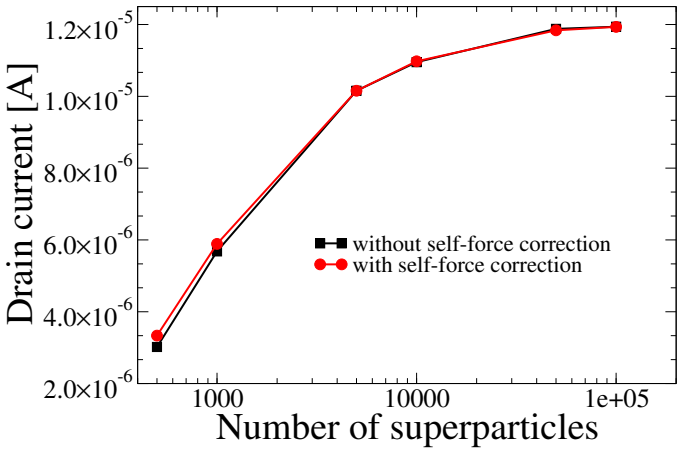

Fig. 4. Dependence of the drain current at $V_D = 50$ mV and $V_G = 0.9$ V with the number of superparticles with and without self-force correction for the studied 10.7 nm gate length SOI FinFET.

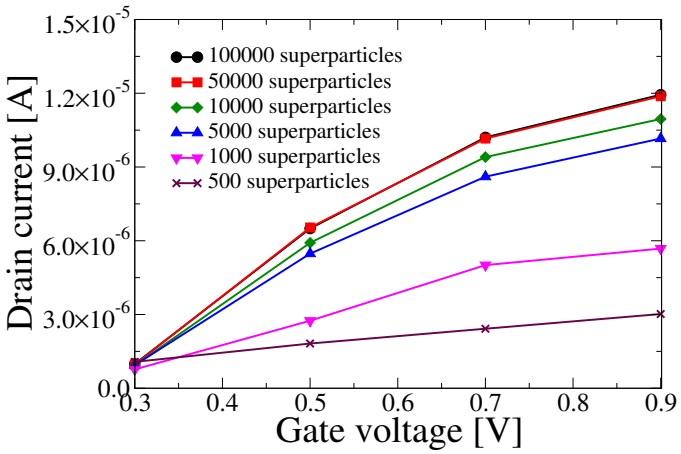

Fig. 5. $I_D - V_G$ characteristics of the 10.7 nm gate length SOI FinFET at a low drain bias $V_D = 50$ mV for different number of superparticles.

drain bias $V_D = 50$ mV for different number of superparticles. As the number of superparticles decreases, the nature of the long range electron-electron interaction changes from quasi-continuum (many superparticles with a small charge) to particle-like (few superparticles with an electron charge), introducing an extra scattering.

IV. Conclusion

In this work, we have present a methodology which allows the suppression of the self-forces in a FE MC device simulator based on tetrahedral elements [5]. We found that self-forces could have a very important impact on the kinetic energy of an isolated particle without collisions. However, simulations of a 10.7 nm gate length SOI FinFET demonstrated that when we take into account external forces (from other charges and external potentials) and scattering processes, the net impact of the self-forces on the current of the device is quite limited unless a small number of superparticles is used.

We have also studied the impact of the change in the number of superparticles on the current. Due to the change in the electron-electron interactions, if a small number of

superparticles is used, the drive current can be significantly underestimated. For example, the current drops by 50% when reducing the number of superparticles from 100000 to 1000.

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