Monte Carlo simulation of ultimate DGMOS based on a Pearson Effective Potential formalism

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***Abstract*— These last years, the effective potential approach has become very attractive for assessing the impact of first order quantum effects on electron transport in nanoscale MOSFETs. In this paper the Gaussian function is replaced by a Pearson IV function for improving the description of the electron wave-packet. The new effective potential implemented into a semi-classical Monte-Carlo particle simulator gives an excellent representation of the electron density profile. A 2D extension of the model in the transport direction allows us to qualitatively evaluate the impact of quantum confinement effects on I-V electrical characteristics of double-gate nMOSFET with a channel length L_c= 10 nm.**

Keywords: Effective Potential; Quantum effects; Monte-Carlo method; double-gate MOSFET

I. INTRODUCTION

To investigate electron transport in ultimate MOSFET architectures, the traditional semi-classical transport theory can no longer be applied. Transport approaches including quantization effects are now required. In the last few years, some works investigated the possibility to develop quantum models based on a particle description [1-7]. Within full quantum transport theory, one method consists in including the Wigner function into an ensemble Monte Carlo simulation [1,2]. This approach describes well the wave-like nature of particles but it is so far limited to the 1D simulation of resonant tunneling diode [1] or to the non self-consistent study of MOSFET [2]. Within classical transport, one may couple the 1D Schrödinger equation with standard particle-based simulators for a multi-sub-band description of the 2D gas including appropriate scattering rates [3]. This approach properly accounts for quantization effects but is very time consuming and may be difficult to extend to all device architectures. An alternative to this approach is the Effective Potential method [4-7]. This formalism has been demonstrated as a possible correction method for describing quantization effects in Monte Carlo device simulation. By the effective potential, electron 'classical' trajectory is modified during the free flight, and the scattering rates are assumed to be the same as in the semi-classical Monte-Carlo simulation. Electrons are thus submitted to a *quantum* trajectory. The usual Gaussian Effective Potential (GEP) is defined in the confinement direction x by the convolution of the Poisson potential by a Gaussian function describing the electron wave-packet [4]

$$GEP(x)=\frac{1}{\sqrt{2\pi}\,\sigma_x}\int_0^{T_{Si}} V_p(x')\times\exp\left(-\frac{|x-x'|^2}{2\sigma_x^2}\right)dx' \qquad (1)$$

with σ_x the standard deviation of the Gaussian function and $V_p(x')$ the Poisson potential. If the GEP formalism is proved to be useful for the estimation of quantum influence on overall electrostatics, some discussions on the validity limits of this method have been recently reported [6-7]. In a previous paper [7], we have demonstrated using a methodology based on a design of experiment that the usual formalism of the effective potential is not able to accurately reproduce the Schrödinger-Poisson carrier density profile. The Gaussian function used in (1) to derive the effective potential is not the most appropriate function to describe the wave-packet. It induces an overestimation of repulsive electric field at SiO_2/Si interfaces. In section II we propose an alternative formalism based on a Pearson distribution. The results of electron density profile calculated with the usual and our new formalism are compared with the Schrödinger–Poisson results (SP) in section III. Then, quantum confinement effects on electrical characteristics I-V of nanoscale DGMOS are evaluated in Section IV, while in Section V the conclusions are drawn.

II. THE PEARSON EFFECTIVE POTENTIAL APPROACH

The Pearson Effective Potential (PEP) is calculated as the convolution of the potential obtained from the solution of 2D Poisson's equation with a Pearson distribution in the confinement direction. As previously described [7], '*padding regions*' are used on the edge of the device to fix appropriate boundary conditions on the Poisson potential for the calculation of convolution. An energy barrier E_B = 3.1 eV is used for electrons at Si/SiO_2 interfaces and satisfies $V_{ox}=V_p-E_B$. In analogy with the GEP (Eq. 1), our Pearson effective potential is then defined as:

$$PEP(x)=\int_0^{T_{Si}}\left[V_p(x')\times P_{IV}\left(R_p(E_x,T_{Si})-x'\right)\right]dx' \qquad (2)$$

where $V_P(x')$ is the Poisson potential along the confinement direction x, T_{Si} is the silicon film thickness, E_x is the local

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electric field and P_{IV} is a Pearson IV distribution. In order to improve the description of the wave-packet of a particle close to the oxide barrier we use an optimized Pearson IV distribution which matches the squared modulus of the first level Schrödinger's wave function $|\psi_0|^2$. The Pearson IV distribution is characterized by its first four moments related to the average position (R_p), the standard deviation (σ_p), the skewness (γ) and the kurtosis (β) of the distribution, respectively [9]. Considering that $|\psi_0|^2$ looks like a Pearson IV law, its first four theoretical moments have been extracted as a function of the interfacial electric field in MOS capacitors. The values of parameters R_p and γ have been chosen by fitting the squared modulus of the first level wave function. The standard deviation σ_p has been considered as the unique adjustable parameter. It is chosen in order that the Pearson penetration into the oxide barrier induces a repulsive electric field reproducing correctly the electron density profile. The kurtosis β of the distribution is arbitrarily calculated as a function of the skewness γ [9] so as to be minimal and close to the Gaussian value.

III. Validation of the Approach

To validate the Pearson effective potential formalism we have simulated a long-double gate nMOSFET with a channel doping $N_A = 10^{15}$ cm^{-3}, an oxide thickness $T_{ox} = 1.1$ nm and a silicon thickness $T_{Si} = 5$ nm. Self-consistent simulations have been performed for a large range of perpendicular effective field (10^5 V×cm^{-1} ≤ E_{eff} ≤ 10^6 V×cm^{-1}). Figure 1 compares the Poisson potential resulting from the PEP correction (the PEP is represented in full lines with open circles and the GEP is represented in dotted line with crosses) with the Poisson potential resulting from SP simulation. An excellent agreement is obtained between both approaches.

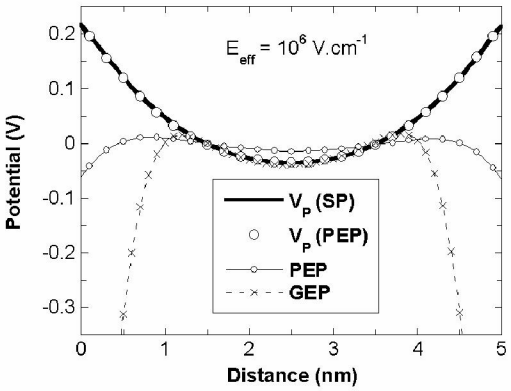

Fig. 1. Self consistent Poisson Potential resulting from SP simulation (V_P (SP)) and from PEP correction (V_P (PEP)) and effective potentials from PEP and GEP corrections extracted from a DGMOS ($T_{ox} = 1.1$ nm et $T_{Si} = 5$ nm).

Figure 2 compares the results of the SP approach with that obtained from the GEP model (the value $\sigma_x = 0.5$ nm has been chosen, as in ref. [4][6]) and from the PEP model. We can notice an excellent agreement between the SP data and the PEP results for an effective field varying from 10^5 V×cm^{-1} to 10^6 V×cm^{-1}. As expected, the electron density profile calculated with the GEP model is unrealistic close to the Si/SiO_2 interfaces due to an unsuitable description of the particle wave-packet.

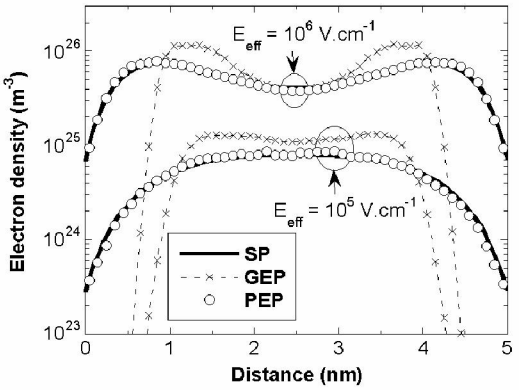

Fig. 2. Electron density in a double-gate nMOSFET with $T_{Si} = 5$ nm and $T_{ox} = 1.1$ nm using SP, GEP and PEP models.

A more detailed validation of this model has been recently presented in [10] for the same range of effective field. An excellent agreement on electron density profile has been shown between PEP and SP data for another channel doping (10^{16}cm^{-3}), a large range of oxide thickness 0.5 nm ≤ T_{OX} ≤ 2 nm and a large range of silicon thickness 5 nm ≤ T_{Si} ≤ 20 nm.

For simulating ultra-short double-gate MOSFETs, the PEP and GEP quantum corrections have been extended in 2D. In the transport direction a Gaussian function (defined by σ_y=1nm [4]) has been used.

IV. Device Simulation

At first the influence of quantum confinement effects induced by the PEP model are discussed at low drain voltage (V_{DS}=0.05V) and compared with those resulting from the GEP model. Then we will analyze the evolution of the carrier confinement all along the channel when the drain voltage is increased. The simulated device is a double-gate nMOSFET with a channel length equal to 10nm, an oxide thickness $T_{ox} = 1.1$ nm and a silicon thickness $T_{Si} = 5$ nm. The source/drain regions are uniformly doped to 1×10^{20}cm^{-3} and the P-type residual doping level in the channel is 1×10^{15} cm^{-3}. The scattering mechanisms included in the model are acoustic intravalley phonon scattering, three *f* and *g* intervalley phonon scattering, and electron-impurity scattering. To make easier the comparison between standard and quantum corrected simulations, surface roughness scattering is not included here.

A. Low drain voltage

The device output characteristic I_{DS}-V_{GS} calculated at V_{DS}=0.05V without quantum correction and using the GEP and PEP corrections is shown in figure 3. We can note a reduction of the drive current when quantum corrections are included. It is essentially explained by the repulsion of

electrons at SiO_2/Si interfaces which reduces the inversion charge.

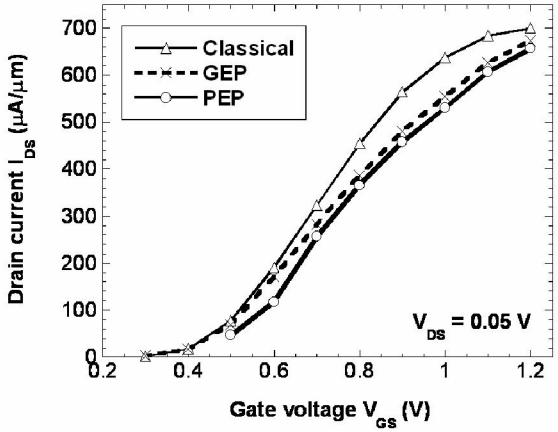

Fig. 3. Output I_D-V_{GS} characteristics using classical, GEP and PEP models.

A cartography of electron density inside the channel is shown in figure 4. We clearly see the two conduction channels located at about 1nm from both interfaces. We plot the electron density profile resulting from PEP and GEP corrected Monte-Carlo simulations extracted in the middle of the channel along the confinement direction. In comparison to the GEP model, the carrier repulsion is now clearly reduced at SiO_2/Si interfaces (in good agreement with figure 2)

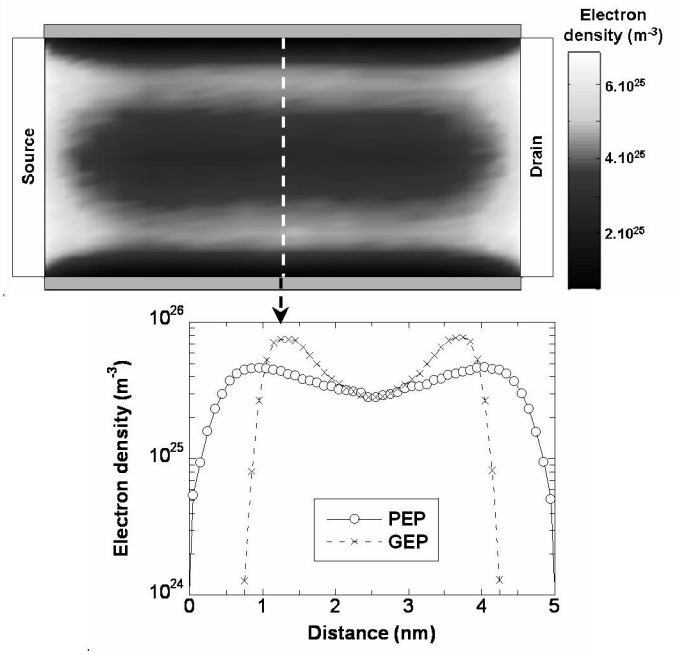

Fig. 4. Cartography of the electron density induced by our PEP model for V_{GS} = 1.2 V and V_{DS} = 0.05 V. The electron density profiles are extracted at the middle of the channel for PEP and GEP models.

B. High drain voltage

The device output characteristic I_{DS}-V_{DS} calculated for a gate voltage V_{GS}=1.2V is shown in figure 5. As observed at low drain voltage the drain current calculated with PEP and GEP are reduced in comparison to the classical one. Figure 6 shows a cartography of electron density inside the channel for a gate voltage V_{GS}=1.2V and a drain voltage V_{DS}=0.7V. The two conduction channels do not appear as clearly as at V_{DS}=0.05V. To focus on the electron density values, two cuts have been performed at different positions along the channel. The curvature of the conduction band in the x direction is less sensitive to the drain voltage at the source-end of the channel than at the drain-end. Consequently, the repulsion progressively decreases all along the channel.

Here we would like recall that surface roughness is not taken into account. Moreover, even if carrier density profiles are different, the SP inversion charge is accurately reproduced with both GEP and PEP corrections. That is why no difference is observed on the drain current. By using the same surface roughness model, significant differences on the drain current may appear due to the respective electron density profile.

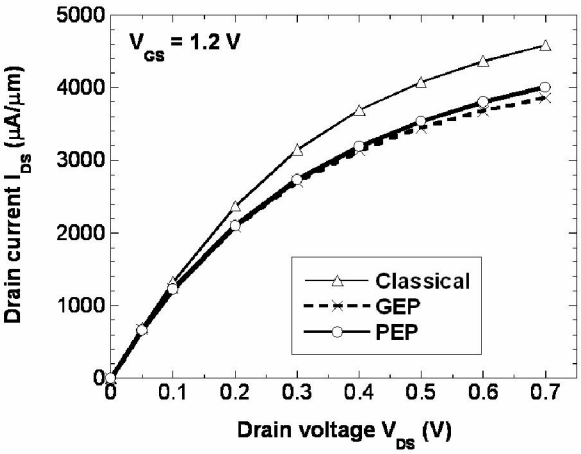

Fig. 5. Output I_D-V_{DS} characteristics using classical, GEP and PEP models.

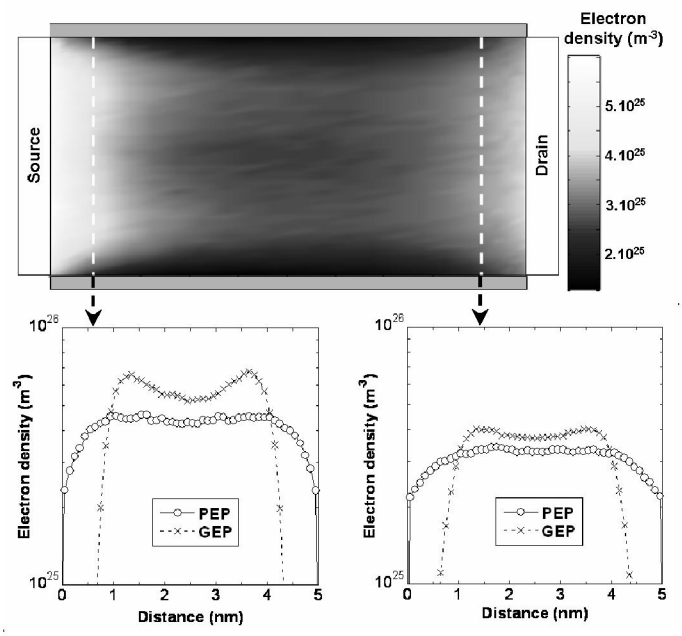

Fig. 6. Cartography of the electron density induced by our PEP model for V_{GS} = 1.2 V and V_{DS} = 0.7 V. The electron density profiles are extracted at the source-end and at the drain-end of the channel for PEP and GEP models.

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V. CONCLUSION

A new effective potential based on a Pearson IV distribution has been developed to accurately reproduce quantum confinement effects in ultimate double-gate MOSFETs. In comparison to the usual Gaussian distribution, this new formalism give an excellent representation of the electron density profile inside silicon film. The model including 2D quantum confinement effects (in the vertical direction and along the transport direction) has been used for simulation of electron transport in a 10nm long DGMOS with a silicon thickness T_{Si}=5nm. The impact of quantization effects are evaluated at low and high drain voltage. In comparison with non-corrected simulation, a slight degradation of drain current of about 16% and 13% are observed using the PEP correction at V_{DS}=0.05V and V_{DS}=0.7V, respectively.

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