Pearson versus Gaussian Effective Potentials for Quantum Corrected Monte-Carlo Simulation

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These last years, the Gaussian Effective Potential (GEP) has become a very attractive approach for assessing the impact of quantum effects on the classical potential. This formalism was already used for including quantum effects into the simulation of ultra-short channel MOSFETs [1-4]. However, discussions on the validity limit of this method have been recently reported [3-4]. They highlight that, even if the GEP model is able to conserve the Schrödinger-Poisson (SP) inversion charge, the Gaussian function is unsuitable for reproducing the carrier density profile. Our motivation is here to demonstrate the ability of a more general concept based on the Pearson Effective Potential (PEP) to accurately reproduce both the SP electron density profile and the inversion charge.

The GEP induces an overestimation of the carrier repulsion at SiO_2/Si interfaces [1-4], which is due to the fact that the electron presence probability is represented by a Gaussian function all along the silicon film thickness [4]. At SiO_2/Si interfaces, this description is not realistic with regard to SP. This preliminary study leads us to propose a new Effective Potential formulation using a function inspired by the shape of the SP wave functions. As the GEP formalism, our PEP formalism is based on the convolution of the Poisson potential by a function representing the non zero-size of the electron wave-packet [1]. Our 1D PEP is defined as:

$$PEP(x,y) = \int_{-T_{ox}}^{T_{Si}+T_{ox}} \left[V_P(x',y) * \text{Pearson IV}\left(E_{x,y}, T_{Si}, x'\right) \right] dx'$$

where $V_P(x',y)$ is the potential energy, T_{Si} and T_{ox} are the silicon film and oxide thicknesses, $E_{x,y}$ is the local electrical field in the confinement direction. The first four moments of the Pearson IV distribution are then calculated as a function of T_{Si} and $E_{x,y}$ so as to qualitatively follow the evolution of squared modulus of the first level Schrödinger's wave function. Figure 1 compares the Gaussian and Pearson IV distributions for different carrier positions in the confinement direction of a double-gate device. The shape of the Pearson IV distribution close to the SiO_2/Si interfaces is more realistic than that observed with the Gaussian one.

To validate our PEP formalism, a long double-gate nMOSFET has been simulated with $N_A = 10^{16}$ cm^{-3}, $0.5\ nm \le T_{OX} \le 2\ nm$ and $5\ nm \le T_{Si} \le 10\ nm$. Simulations have been performed for a large range of effective field ($10^5\ V.cm^{-1} \le E_{eff} \le 10^6\ V.cm^{-1}$). Figures 2 to 5 show the electron density profiles calculated for two different effective fields in various double-gate devices. In all the cases, an excellent agreement is obtained between SP and PEP results with an average error on the inversion charge of about 3.2%. As the SP electron density profile is accurately reproduced, the Poisson potential is now correct. Figure 6 shows the Poisson potential resulting from semi-classical Monte-Carlo, SP, PEP simulations and the Effective Potential for $T_{Si} = 10$ nm and $E_{eff} = 10^6\ V.cm^{-1}$.

To conclude, we demonstrate that our PEP approach is able to accurately reproduce the SP electrostatic confinement effects in various double-gate MOSFETs. The calculated potential inside the silicon film is correct and can be used for improved quantum corrected Monte-Carlo simulation. The extension of the PEP model for T_{Si} = 20 nm is currently underway.

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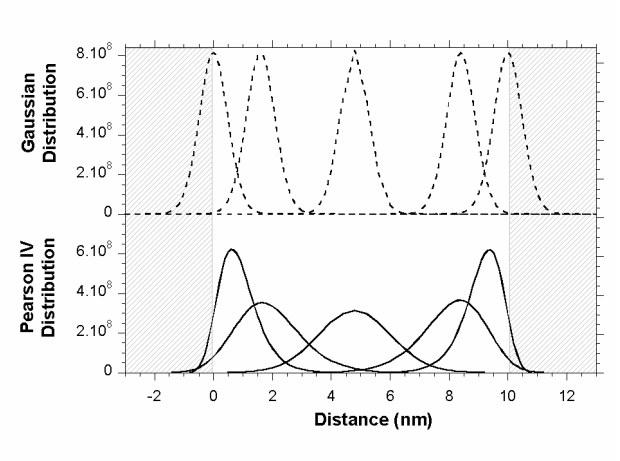

Fig. 1. Gaussian and Pearson IV distributions for different carrier positions in a double-gate device with T_{Si} = 10nm.

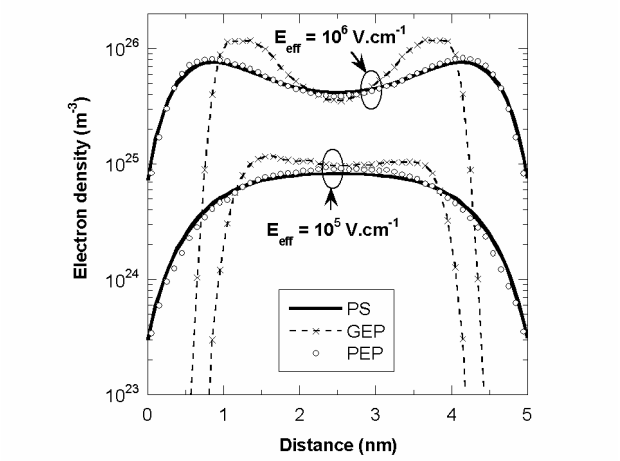

Fig. 2. Electron density in a double-gate nMOSFET with T_{Si} = 5 nm and T_{ox} = 1nm using SP, GEP and our PEP.

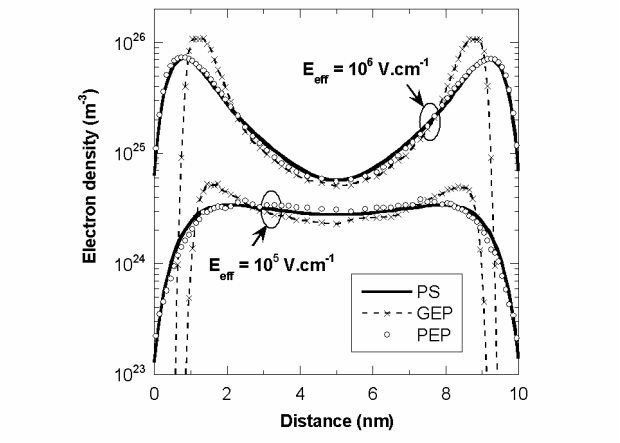

Fig. 3. Electron density in a double-gate nMOSFET with T_{Si} = 10 nm and T_{ox} = 1 nm using SP, GEP and our PEP.

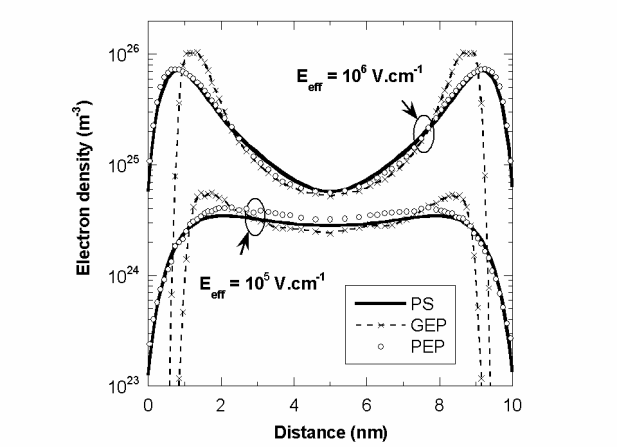

Fig. 4. Electron density in a double-gate nMOSFET with T_{Si} = 10 nm and T_{ox} = 0.5 nm using SP, GEP and our PEP.

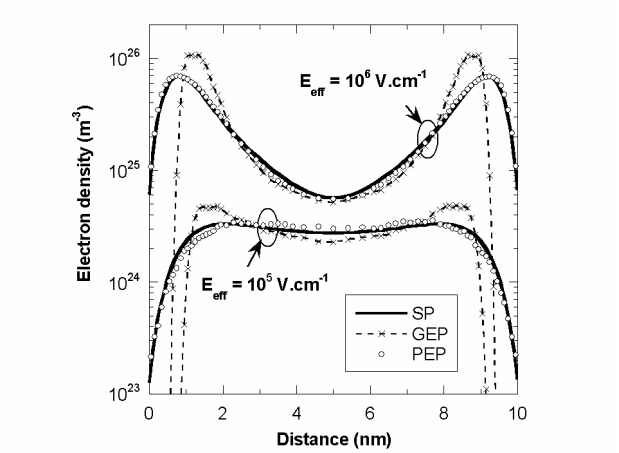

Fig. 5. Electron density in a double-gate nMOSFET with T_{Si} = 10 nm and T_{ox} = 2 nm using SP, GEP and our PEP.

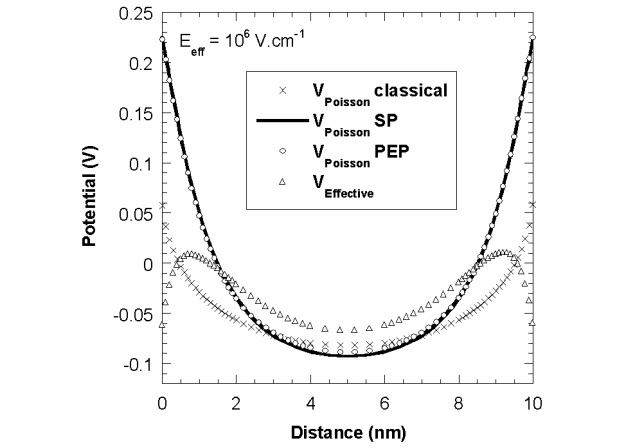

Fig. 6. Poisson Potential resulting from semi-classical Monte-Carlo, SP, PEP simulations and Effective Potential in a double-gate device with T_{Si} = 10 nm, T_{ox} = 1 nm.