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The variability of the surface scattering coulombian mobility in dielectric interface of Si-Nanowire GAA-MOSFET at 20 nm Length channel

Abderrezak Bekaddour and Gérard Ghibaudo

***Abstract*—We present a strong methods of two studies that were reviewed, which demonstrated a well bounded case of the trap-charge-induced variability of surface scattering coulombian mobility in silicon-nanowire FETs. By using full-quantum 3-D NEGF simulations, we proof and analyse the effective mobilities $\mu_{eff} - V_G$ and $\mu_{eff} - N_{inv}$ in the attendance of discrete trap charges at different positions in the gate-stack surface, and we calculate the probability density function of these 2D randomly distributed impurities. Entertaining a Poisson distribution for the trap charge numbers, we compute approximation of the statistics of the surface scattering coulombian mobility shift induced by such charged defects and evaluate the mean value and the standard deviation, of the coulombian mobility for typical trap density values and also its errors.**

***Index Terms*—Nonequilibrium Green's functions (NEGF) method, remote Coulomb scattering (RCS), Negative Bias Temperature Instability (NBTI), Hot Carrier Injection (HCI), GAA silicon-nanowire (Si NW) transitors (GAA-SNWTs), variability.**

I. Introduction

THE scattering coulombian mobility in the inversion charge layer of nanowire MOSFET's has been a subject of extensive studies [4], [11], for the reason that its importance has an influence on the drain current. The theoretical work in [6] supplies a foundation for understanding the various physical phenomenon of charge transport in the surface inversion layer. Dopant densities and trap charges in the channel are corresponding increase of the electric fields in the direction normal to the Si-SiO_2-High-κ interface makes quantization of the channel electron gas significant even above room temperature [3], [6]. In addition, mobility degradation due to scattering with ionized dopants and traping charges becomes important and cannot be neglected.
To study of the nanowire MOSFET performance requires predictive physical models for the carrier transport. However quantum studies sugested in a nanoscale metal-oxyde-semiconductor (MOS) devices [2],[8],[9]. This is why, our main goal is the physics of the electronic transport is inspected very closely visualizing the most important internal properties with the assistance of a self-consistent three-dimensional (3D) nonequilibrium Green's functions (NEGF) quantum mechanical code has investigated [1], [7].
The aim of this work is to model the exact of scattering at different spacial locations along the channel and extension regions of silicon n-MOSFETs [3], [5]. We consider only surface trap charges interface layer, which is in significant scattering mechanism in nanowire with undoped channels[11].

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In this work, the paper is organized as follows. We are propose the problem of scattering coulombian mobility and their implications on NW device reliability as intrduction. First, part 2 presents the discrete trap charges disctrubuted, background and the theory for noise degradation from the perspective of Reaction-Diffusion phenomenon . Physical models are presented in section III . The impact of noise, degradation on GAA NW MOSFET characteristics is investigated in section IV. Future directions are provided and conclusions in section V.

II. Physical models

As the transport below a gate dimension of 10 nm cannot be treated anymore with classical physics [5], [6]. However, in the nanometer regime, particles must be described by their wave functions $\psi(\mathbf{r}, \mathbf{t})$, which can be derived from the time-dependent single particle Schrdinger equation

$$H_b\psi(\mathbf{r}, t) = i.\hbar\partial_t\psi(\mathbf{r}, t) \quad (1)$$

Implicitly, to taking in consideration effect of times evolution in the wive function, we moast apply Fourier transform of the equation (1); then the equation becam spectral probelem:

$$H_b\Psi(\mathbf{r}) = E.\hbar\Psi(\mathbf{r}) \quad (2)$$

Numerical simulations are performed by self-consistently solving the 3-D Schrodinger and Poisson equations in the coherent transport regime in the presence of fixed charge centers trapped at the Si-SiO_2-high-κ dielectric interface.
As we consider Nb independent valleys for the electrons within the effective mass approximation [22], [23]. The Hamiltonian of valley b is

$$H_b(\mathbf{r}) = \frac{-\hbar^2}{2}\left[\nabla\cdot\left(\frac{1}{m^b}(\mathbf{r})\nabla\right)\right] + V(\mathbf{r}) \quad (3)$$

where $\frac{1}{m^b}(\mathbf{r}) = \left(\frac{1}{m_x^b}, \frac{1}{m_y^b}, \frac{1}{m_z^b}\right)$ are the components of the effective mass in valley b [10], [11], [12].
The purpose of this paper is to describe development of a particular approach, namely the NEGF approach, comparison of various methods is not the purpose of this paper. Numerical simulations are performed by self-consistently solving the 3-D

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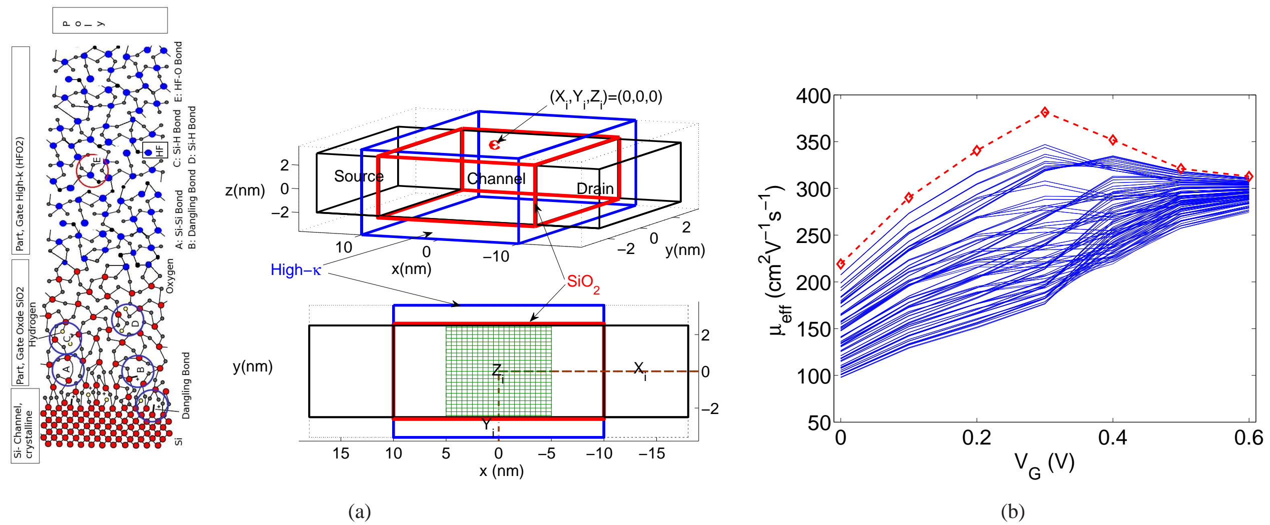


(a) (b)

Fig. 1. (left (a)) Si, Si/SiO$_2$ interface, SiO$_2$/high-κ interface, high-κ, and oxide/high-κ defect structure and dangling Si bonds are shown. (right (a)) Schematic view of the GAA Si-NW FET consisting of a 20-nm undoped channel and 10-nm S/D regions nominally doped at 10^{20}cm^{-3}. The cross section of the devices is 5×5nm^2, and the SiO$_2$ oxide and High-κ thickness are 0.2-nm, 0.8-nm respectively. (b) (Solid blue lines) $\mu_{eff} - V_G$ characteristics of the GAA nanowire Si-MOSFET with the single charge trapping $M_i = (x_i, y_i, z_i)$ inside of channel. (Dashed red line) The smooth device is also shown for comparison.

Schrödinger and Poisson equations in the coherent transport regime in the presence of fixed charge centers trapped at the SiO$_2$/high-κ dielectric interface.

In order to reduce the numerical burden the coupled mode space (CMS) approach is used within the NEGF formalism [2], [20], [21]. According to the CMS approach the discrete electron correlation function reads:

$$G^{<}(i_1,i_2,j_1,j_2,k_1,k_2;E) = \sum_{n,m} G^{<}_{\mathrm{ms}}(i_1,i_2,n,m;E)\phi^{n}_{i_1}(j_1,k_1)\phi^{m*}_{i_2}(j_2,k_2) \ , \quad (4)$$

where $\{\phi^n_i\}_{n=1,2,\ldots,N_yN_z}$ is the orthonormal set of eigenfunctions solution of the 2-D Schrödinger problem for the ith slice of the device, $G^{<}_{\mathrm{ms}}$ is the mode-space counter part of the real-space Green's function and $N_y(N_z)$ indicates the number of discretization nodes along the $y(z)$ confinement direction. The solution in the transverse plane is obtained assuming close boundary conditions with vanishing wave functions at the gate-oxide interface. The Green's functions in the mode space are obtained as solution of the two of kinetic equations

$$[E - H_{\mathrm{ms}} - \Sigma_{\mathrm{ms}}]\, G_{\mathrm{ms}} = I \quad (5)$$
$$G^{<}_{\mathrm{ms}} = G_{\mathrm{ms}}\Sigma^{<}_{\mathrm{ms}}G^{\dagger}_{\mathrm{ms}},$$

where $\Sigma^{<}_{\mathrm{ms}}$ and Σ_{ms} are the lesser-than and retarded self-energies describing the ideal infinite equipotential contacts, H_{ms} is the mode-space Hamiltonian and I is the identity matrix, for every energy E, and then evaluating the real space electron density through the integral:

$$n_{i_1,i_2,i_3} = -\frac{ig_vg_s}{\Delta x}\int \frac{\mathrm{d}E}{2\pi} G^{<}(i_1,i_1,i_2,i_2,i_3,i_3;E) \ , \quad (6)$$

where $g_{v,s}$ are the valley and spin degeneration coefficients, respectively.

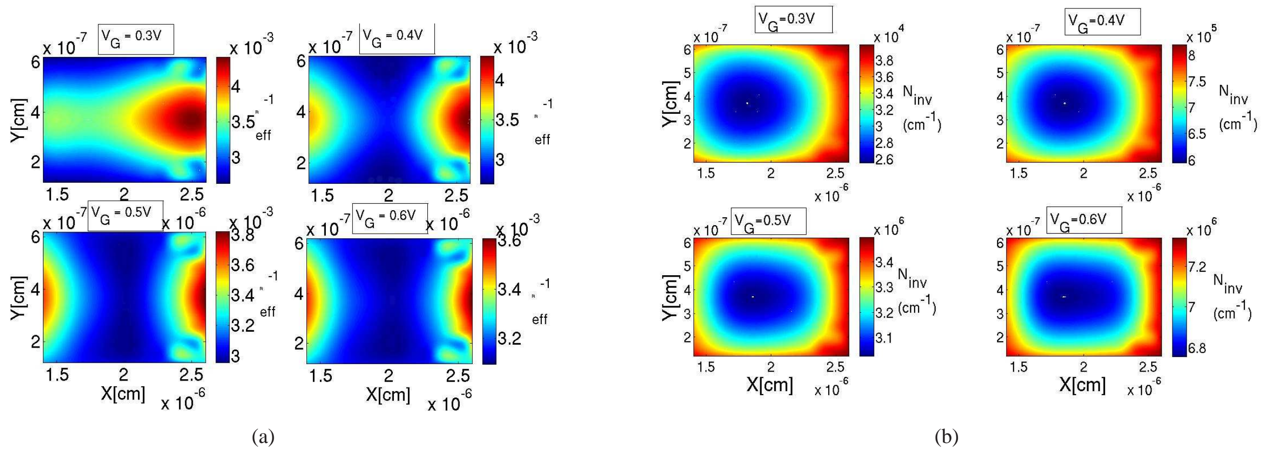
The Poisson equation

$$-\nabla\cdot(\epsilon(\mathbf{r})\nabla\phi(\mathbf{r})) = \rho(\mathbf{r}) \quad (7)$$

is solved in the 3-D domain using the box-integration method, where $\epsilon(\mathbf{r})$ is the position dependent dielectric constant, $\rho(\mathbf{r})$ is total charge density accounting for both electrons and fixed charges, and $\phi(\mathbf{r})$ is the self-consistent electrostatic potential [13], [3], [15].

III. Results and Discussion

For the evaluation of the quantum study models a state-of-the-art three-dimensional N- channel GAA nanowire structure was chosen. The nanowire geometry can be seen in Fig. 1 (left (a)). We consider, the silicon [100] fin has a cross section area of 5×5 nm^2 and gate length of 20 nm. The source and drain regions are heavily n-type doped whereas the channel itself remains undoped. The S/D regions are 10 nm long with a donor-doping concentration of $N_D = 10^{20}$ cm^{-3}. An interfacial layer of silicon oxide with thikness $t_{\mathrm{IL}} = 0.2$ nm is placed between the silicon channel and the high-k gate dielectric (HfO_2). The dielectric propreties of the high-k and of SiO$_2$ interfacial layer are assumed thikness independant. Discrete charged defects can be located inside the gate-stack volume at position (x_i, y_i, z_i) and the Si/SiO$_2$ interfaces. Applied source-drain voltage is V_{DS} =10mV, and the temperature is $T = 300$ K. The tansfer characteristics of such devices in the presence of a single trap carge located at the Si/SiO$_2$/ high-κ interfaces and at different positions along the $x - y$ surface are shown in Fig. 1(right (a)), where the on- turn curve of a clean device is plotted as the reference. We notice a systematic positive effective mobility shift due to the additional barrier on the device subbands induced by the negatively charged defect.
The low-field effective mobility in SNFETs is calculated for traping charge NWs and for a perfect NW from the electron



(a) (b)

Fig. 2. (a) The effective mobility shift as a function of the position of single trap charge at the interface and along the $x-y$ plane for different value of V_G. (b) The corresponding of inversion charge layer shift as a function of the position of single trap charge at the interface and along the $x-y$ plane for different value of V_G respectively

density and the conductance using the expression [16], [17], [18], [19]

$$\mu_{eff} = \frac{G.L_{ch}}{q.N_{inv}} \ , \tag{8}$$

where G is the conductance at low drain bias and N_{inv}, the inversion density is calculated by intergrating the electron density in the domain of the channel under the gate where the electron density is nearly flattening [22], [23], [24]. Assuming that the ballistic mobility is the effective mobility for perfect nanowire.

The dependence of the effective mobility shift on the position along the two spacial directions of the single charged impurity is studied, such that; we calculated effective mobility μ_{eff}, expressed in formulation (8) and corresponding the different values of V_G: $0.3, 0.4, 0.5, 0.6$ as represented in Fig. 1 (b) .

By fastening the trap-charge defect at the interface, it was possible to systematically study the influence of the position on the surface interface layer (x,y) of the trap on the effective mobility variability and to generate by 2-D extrapolation the effective mobility variation map shown in left of Fig. 2. However, at low V_G and inferior of device threshold voltage V_{th}, we found a stronger decrease of assymmetric parabolic forms effective mobilities as far as the impurity is moved away from the interface along the vertical direction shown in top of Fig. 2 (a) . This behavior is primarily due to the usual remote coulomb scattering effect depicted in (8) and additionally due to the different permittivities present in the SiO_2 layer dielectric in the gat stack as well as for the wive-function penetration inside the dielectric. On the other hand, at strong V_G and superior of device threshold voltage V_{th}, we shown in the bottom of Fig. 2(a), that the parabolic forms divided in two half no symmetrically parabolic forms converging to Drain and Source, when V_G increasing. Note that, as drain voltage is nicely have an influence, so the corner effect is shown clearly (as rotation phenomenon) near of borders. In parallel we remark that the inversion densities assymmetric parabolics for different V_G are deviate a center in a right of Fig. 2, because the strong electrostatic effects of drain and its corner especially .
As clearly the assymmetric of effective mobilities in the linear region i.e at low drain bias is create theoritical peoblem, the correction of effective mobilities is necessary and that expressed by:

$$\mu_{eff,coul} = \frac{\mu_{eff}.N_{inv}}{N_{inv,ball}} \ , \tag{9}$$

To investigate single-charge generation in this configuration, from the Matthiessen rule, namely,

$$\frac{1}{\mu_{coul}} = \frac{1}{\mu_{eff,coul}} - \frac{1}{\mu_{ball}} \ , \tag{10}$$

where $\mu_{eff,coul}$ is the effective mobility for the scattering coulombian in NWs. The scattering coulombian limited mobility μ_{coul} plotted by maps in left of Fig. 3, corresponding the different values of V_G: $0.3, 0.4, 0.5$ and $0.6\ V$

IV. Variability and statistical study of the scattering coulombian mobility in NWs

From 2D-maps shown in left of Fig. 3 and by exploiting these data, we estimated the statistical properties of a single charge trap randomly distributed in the surface. Here, this is achieved by generating 40401 (201 x 201) random positions uniformly distributed on the surface for each V_G value and hence by calculating the corresponding PDF shown in middle of Fig. 3 for strong V_G and in right of Fig. 3 for low V_G.
In order to obtain an almost continuous curve, a discretization step $\delta\mu_{coul} = 0.4\ cm^{-2}.mv.s$ has been considered. Such a deterministic approach has the advantage to be expensive than a statistical treatment consisting in computing a complete set of simulation for a given set of random positions.

Moreover, we notice that such an approach can be easily extend to charged traps localized on specific spacial regions as grain-boundary lines of Si/SiO_2 interface materials. This is particularly beneficial for $3-D$ NEGF quantum simulations

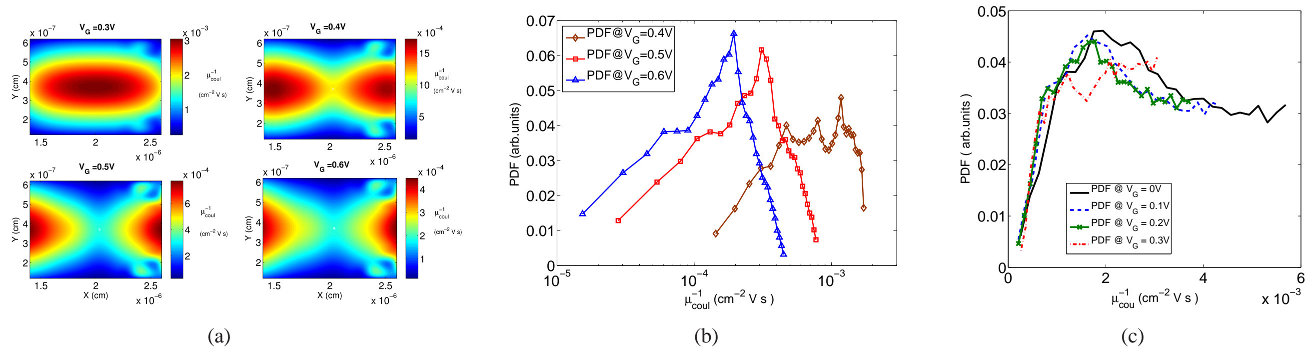


Fig. 3. (a) The inverse scattering coulombian mobility shift as a function of the position of single trap charge at the interface and along the $x-y$ plane for different value of V_G. (b) Effect of strong value V_G on the PDF of having a determined value of inverse scattering coulombian mobility shift due to a single discrete trap charge at the Si/SiO_2 interfaces. (d) At low V_G, Keeping of PDF form of the inverse scattering coulombian mobility shift due to a single discrete trap charge at the Si/SiO_2 interfaces

which are very much time consuming. In order to evaluate the variability induced by discrete trap charges in the Si/SiO$_2$ of small devices, we have to consider that the number of these impurities is statistically distributed according to a Poisson law with the mean value determined by the nominal surface trap density N_{st}.

We verified that the addition of two or more trap charges in the Si/SiO$_2$ is almost independent of each other and that it gives rise to an overall μ_{coul} cumulating the single-charge contributions.

Therefore, we assume that, for each device, the global μ_{coul} shift, $\mu_{coul,\text{tot}}$, is given by

$$\mu^j_{coul,\text{tot}} = \sum_{j=1}^{N^j_{st,\text{tot}}} \mu_{coul,i} \tag{11}$$

where $\mu_{coul,i}$ is the contribution of the ith trap and $N^j_{st,\text{tot}}$ is the number of trap charges in the jth simulated device. The number of traps $N^j_{st,\text{tot}}$ is randomly generated from a Poisson law having a mean value $N_{st}S$, S being the area of the device active surface (here $S = 400$ nm^2). The $\mu_{coul,i}$ are randomly generated using the PDF of the elementary charge μ_{coul} distribution. and for different V_G value. By this methode, we could obtain, as shown in Fig. 4(a), (b), the evolution with the average trap surface charge density N_{st} of the first two statistical moments of the μ_{coul} probability distribution. The behavior of the mean value as shown in Fig. 4(c) for different V_G, and of the standard deviation shown in Fig. 4(d) also for different V_G, at the large value of N_{st} is determined by the Poissonian distribution of the number of surface interface trap charges. In particular, we observe an almost linear increase of the mean threshold voltage shift, a power-law increase of the standard deviation with N_{st}. Finally, of course, the simulation of the present paper to have an influence on the future researchs of experimentally or simulation and the characterization (same nanoscale) of NW-MOSFET; this is why the important part of this work that, no only explain the mechanism physic but the statistical characteristic quantities can either be calculated or measured in order to fit an assumed frequency function to experimentally determined versus V_G for different trapping charges surface

TABLE I
COEFFICIENTS FOR $Mean\ \mu^{-1}_{coul}\ (cm^{-2}.mv.s)$ VERSUS V_G ON DIFFERENT SURFACE TRAP CHARGES DENSITIES N_{st}.

$N_{st}\ (cm^{-2})$	5.10^{11}	10^{12}	$2\cdot10^{12}$	$3\cdot10^{12}$	$4\cdot10^{12}$	$5\cdot10^{12}$
a_0	0.00181	0.00312	0.00541	0.00765	0.00994	0.01234
a_1	-0.0011	-0.0014	-0.0058	-0.008	-0.0125	-0.0119
a_2	-0.0762	-0.140	-0.184	-0.265	-0.303	-0.427
a_3	0.6138	0.1106	0.1574	0.2245	0.2690	0.3574
a_4	-1.522	-2.718	-3.979	-5.669	-6.920	-8.988
a_5	0.000	0.000	0.000	0.000	0.000	0.000
a_6	4.230	7.500	11.182	15.943	19.743	25.162
a_7	-3.794	-6.720	-10.038	-14.324	-17.794	-22.570

N_{st}.
Fig. 4(c) and Fig. 4(d) describe the importance of the quantities of the surface traps on the mean scattering coulombian mobility and its standard deviation respectively in NWFETs for different value of V_G.
On the Fig. 4(e) and Fig. 4(f) shown the importance of the quantities effect of the mean of inversion charge layer of nanowire MOSFET's on the mean of inverse scattering coulombian mobility and its standard deviation respectively for different surface trap charges density N_{st}.
However, we propose the easiest approach for that task is a simple polynomial fit:

$$Mean(\mu^{-1}_{coul}) = \sum_{i=0}^{n} a_i.V^i_G \tag{12}$$

$$\sigma_{\mu^{-1}_{coul}} = \sum_{i=0}^{n} b_i.V^i_G \tag{13}$$

just find the inverse problem; the coefficients for such polynomials are given in Table I and Table II for different surface trap charges densities N_{st}. The dimension of the coefficients a_i, b_i are $cm^{-2}.V.s\ per\ i-th$ power of the units used for gate voltage, usually V in the range $[0.0, 0.6]$ in GAA NWFETs . The maximum errors of $\sigma_{\mu^{-1}_{coul}}$ by Mean μ^{-1}_{coul} shown in Fig. 5(b) as describe the importance of the quantities of the surface traps in NWFETs for different value of V_G. In parallel, no impact of V_G on the errors of $\sigma_{\mu_{coul}}$ by Mean μ_{coul} , for different surface trap charges density N_{st}, that shown in Fig. 5(c).

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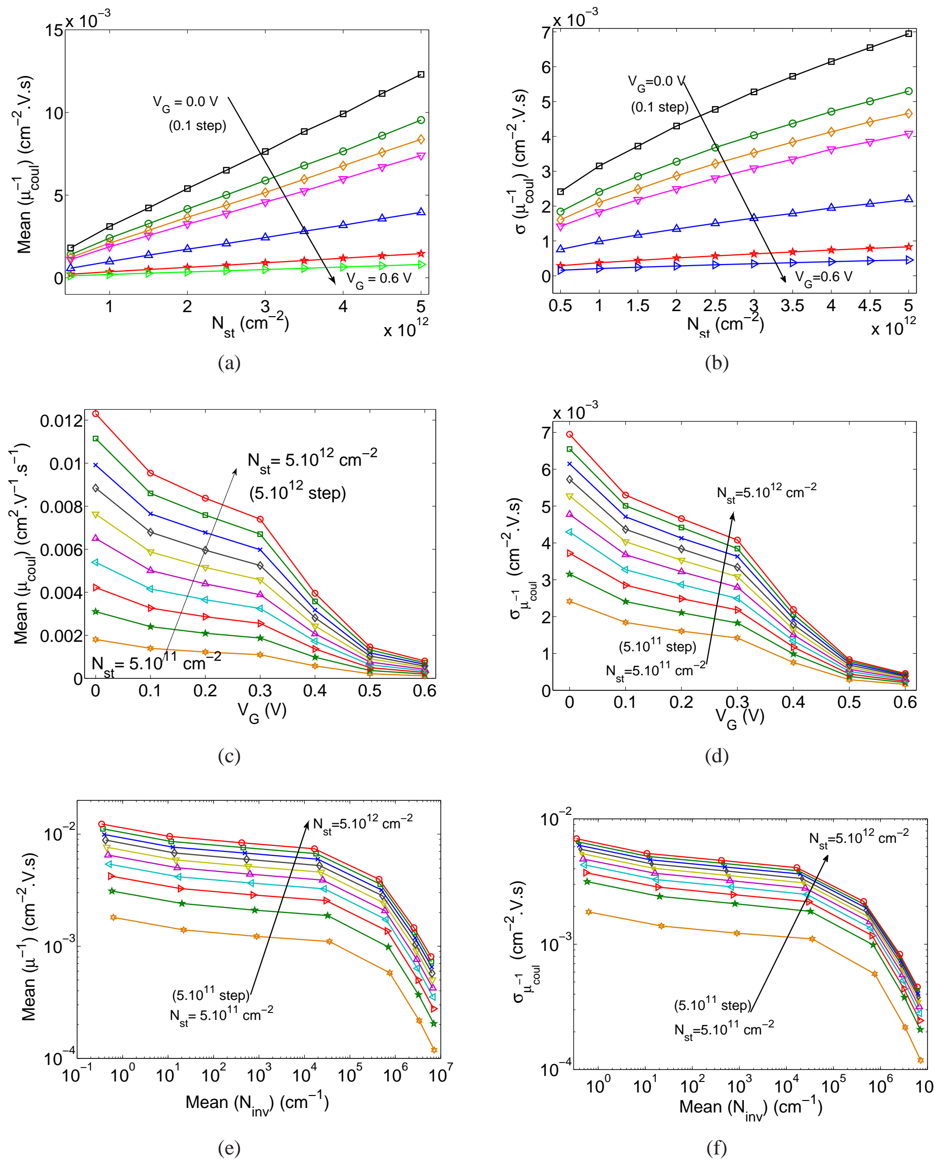

Fig. 4. (a), (b) the mean of inverse scattering coulombian mobility and its standard deviation respectively versus gate voltage V_G of having a determined value of due to a given surface trap charges density N_{st}. (c), (d) the mean of inverse scattering coulombian mobility and its standard deviation respectively versus gate voltage V_G for different surface trap charges density N_{st}. (e), (f) effect of the mean of inversion charge layer of nanowire MOSFET's on the mean of inverse scattering coulombian mobility and its standard deviation respectively for different surface trap charges density N_{st}.

The skewness and the kurtosis has not been approximated in this way, although there in principal no problem, but for construction of distributions for which an accurate value of the skewness and the kurtosis are required.
Certainly quite a few other frequency functions have also been sugested to describe the scattering coulombian mobility, for exmple; the Gram-Charlier series wich is based on an expression of the Gaussian frequency function into Hermite Polynomials. However, the drawback of most of the more sophisticated frequency functions as the tendency to oscillate, or very complicated calculus for the coefficient evaluation are usually too seevere for practical application

TABLE II
COEFFICIENTS FOR $\sigma_{\mu_{coul}}^{-1}$ $(cm^{-2}.mv.s)$ VERSUS V_G ON DIFFERENT SURFACE TRAP CHARGES DENSITIES N_{st}.

N_{st} (cm^{-2})	5.10^{11}	10^{12}	$2 \cdot 10^{12}$	$3 \cdot 10^{12}$	$4 \cdot 10^{12}$	$5 \cdot 10^{12}$
b_0	0.00242	0.00315	0.00430	0.00529	0.00616	0.00697
b_1	-0.0026	-0.0051	-0.0072	-0.0073	-0.0081	-0.0110
b_2	-0.0845	-0.0765	-0.1026	-0.1550	-0.1860	-0.1828
b_3	0.7138	0.7231	0.9853	0.1378	0.1644	0.1707
b_4	-1.795	-1.889	-2.587	-3.531	-4.209	-4.445
b_5	0.000	0.000	0.000	0.000	0.000	0.000
b_6	5.0333	5.4357	7.4746	10.027	11.942	12.765
b_7	-4.520	-4.902	-6.749	-9.025	-10.747	-11.513

V. CONCLUSION

We have studied the importance of the quantities of the surface traps present in the gate stack on the scattering coulombian mobility in GAA NWFETs for different value of V_G. By performing 3D self consistent simulations with in the NEGF formalism, we have first evaluated the effect on the effective mobility of the single trap charge located inside the

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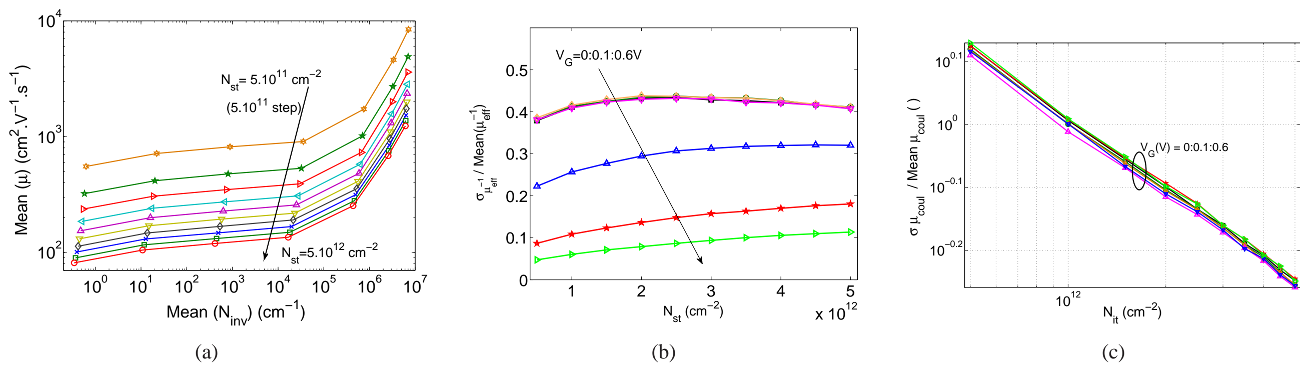

Fig. 5. (a) Effect of the mean of inversion charge layer of nanowire MOSFET's on the mean of scattering coulombian mobility for different surface trap charges density N_{st}. (b) The errors of $\sigma_{\mu_{coul}^{-1}}$ by Mean μ_{coul}^{-1} and the importance of the quantities of the surface traps in NWFETs for different value of V_G. (c) No impect effect of gate voltage on the errors of $\sigma_{\mu_{coul}}$ by Mean μ_{coul} , versus different surface trap charges density N_{st}

insulator.
Hence, we have presented statistical methods after huge simulation of NEGF exploiting the PDF due to Poissonian number of discrete single traps.
The electron mobilityis serously degraded by Coulomb scattering from charged interface traps; this so-called roll-off region. As the effective field increase (especially at stong V_G), the mobility becomes independent of the channel charged interface traps and all the samples approach the so-called universal curve.

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