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A semiempirical surface scattering model for quantum corrected Monte-Carlo simulation of unstrained Si and strained Si/SiGe PMOSFETs

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Abstract

A new hole surface scattering model for FBMC simulations is presented for unstrained Si and biaxially strained Si/SiGe PMOSFETs. The new scattering model was developed for quantum corrected spatial hole charge distributions at the Si/SiO_2 interface, where the quantum correction is based on the improved modified local density approximation (IMLDA). To extract channel mobility efficiently, a new linear response (LR) MC method has been developed. The new LRMC method, which is faster than standard MC by about three orders of magnitude, allows to extract the parameters of the surface scattering model for holes from the available measurements in an efficient manner. The model has been calibrated and verified for a wide range of doping levels (7.8×10^{15} to 6.6×10^{17} cm^{-3}), temperatures (223–443 K) and Ge-content up to 30% by comparison to experimental data. A 23 nm PMOSFET with and without a strained Si layer on top of the substrate has been simulated with our new FBMC model. Drain current enhancement due to biaxial strain is found to be reduced in comparison to the NMOSFET case.

Keywords: Surface scattering; Linear response Monte-Carlo method; Warped structure of valence bands; Biaxially strained Si; PMOSFETs

1. Introduction

Since the macroscopic drift diffusion (DD) and hydro dynamic (HD) models fail for nanoscale MOSFETs (Fig. 1), an accurate and efficient FBMC model including a consistent treatment of surface scattering and quantum correction is required. In this paper, a new hole surface scattering model for FBMC simulations is presented for unstrained Si and biaxially strained Si/SiGe PMOSFETs. For holes, due to the warped band structure, reflection of holes at the boundaries of the potential well is not necessarily specular [1], and the low-field mobility tensor is therfore no longer diagonal. Thus, the numerical integration method [2] is not valid for FB holes. To extract low-field inversion layer mobility efficiently, a completely new LRMC method has been developed. The form of the new scattering model and the implementation of the new scattering model into our FBMC simulator are similar to the electron case [3]. The improved modified local density approximation (IMLDA) [4] is used in all simulations to correct the charge densities near the Si/SiO_2 interface according to the size quantization effect.

2. Surface scattering rates

In [3], a surface scattering model which reproduces excellently low-field mobility measurements has been developed for electrons. The form of the this scattering model can also be applied to holes. However, the new surface scattering model for holes contains only surface roughness scattering and surface phonon scattering mechanisms.

As in the electron case, the formula in [5] is used to calculate the surface roughness scattering rate:

$$S_{\mathrm{sr}} = 2\pi \frac{m^* q^2}{\hbar^3} \left(\frac{\varepsilon_{\mathrm{si}}}{\varepsilon_{\mathrm{ox}} + \varepsilon_{\mathrm{si}}} \right)^2 \Delta^2 L^2 E_{\perp}^2, \tag{1}$$

where $\hbar$ is the Plank constant, $\varepsilon_{\mathrm{si}}$ and $\varepsilon_{\mathrm{ox}}$ the dielectric constants of the Si layer and SiO_2. The effective hole mass and positive electron charge are denoted with m^* and q. L and Δ are the correlation length and r.m.s height of the Si/SiO_2 interface roughness. $E_{\perp}$ is the local confining field which is perpendicular to the Si/SiO_2 interface.

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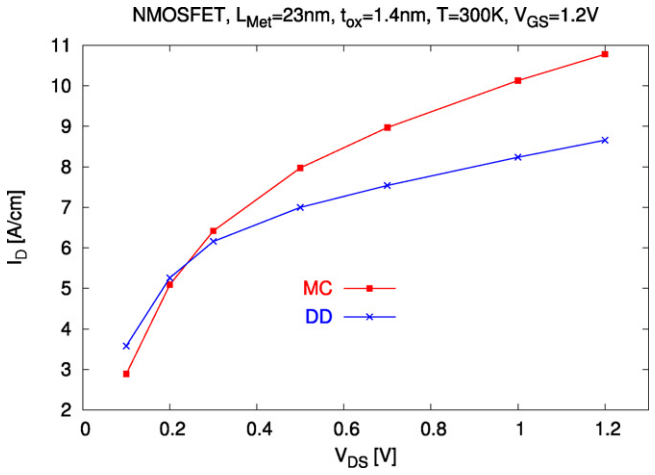

Fig. 1. I_D–V_{DS} characteristic of unstrained Si 23 nm NMOSFETs simulated by MC and DD models which are consistent for homogenous channel conditions.

In order to reproduce low-field mobility measurements, an additional term is introduced into the conventional formula for surface phonon scattering rate [6]:

$$S_{sac} = \frac{m^* k_B T}{\rho c_s^2 \hbar^3} \frac{\Xi_{ph}^2}{W} + \frac{q}{m^*} \frac{1}{K_{pha}}. \quad (2)$$

The additional term related to K_{pha} creates a new degree of freedom for shifting the effective mobility curve up or down. In (2) ρ is the Si mass density, c_s the speed of sound in Si, k_B the Boltzmann constant, T the lattice temperature, Ξ_{ph} the deformation potential of surface phonons and K_{pha} is the surface acoustic phonon limited mobility of strained Si. Similarly to the electron case, the thickness of the surface inversion layer W is modeled as the weighted sum of the classical and quantum layer widths divided by the Fuchs scattering factor p_f [7,8]:

$$W = \frac{\gamma W_{cl} + \delta W_{qt}}{p_f}, \quad (3)$$

where the parameters γ and δ are the classical and quantum weight factors. The normalized classical and quantum inversion layer widths are modeled similar to [6,8]:

$$W_{cl}(E_\perp, T) = T_n \frac{k_B T}{q} E_\perp^{-1}, \quad (4)$$

$$W_{qt}(E_\perp) = \left(\frac{12 m^* q}{\hbar} E_\perp \right)^{-1/3}, \quad (5)$$

respectively. T_n is the normalized temperature $T_n = T/300\,\mathrm{K}$. The Fuchs factor is modeled similar to [7]:

$$p_f(p_s, T) = p_{fT} T_n + p_{fN} \left(\frac{p_s}{p_0} \right)^{p_{pf}} \frac{1}{T_n}, \quad (6)$$

where p_s is the hole screening density, p_{fT}, p_{fN}, p_{pf} the adjustable parameters and p_0 is the normalizing hole screening density with a fixed value of $10^{16}\,\mathrm{cm}^{-3}$.

In contrast to the electron case, there is no need to modify the hole impurity scattering due to surface effects. Moreover, it turns out that there is no need to generalize the parameters of the hole surface scattering model for unstrained Si when switching to a strained Si/SiGe structure. Therefore the parameter set of the new hole surface scattering model ($L = 2.0\,\mathrm{nm}$, $\Delta = 0.133\,\mathrm{nm}$, $\Xi_{ph} = 11\,\mathrm{eV}$, $K_{pha} = 2000\,\mathrm{cm}^2/\mathrm{V\,s}$, $\delta = 0.08$, $\gamma = 1.6$, $p_{pf} = -1.0$, $p_{fT} = 0.5$, $p_{fN} = 0.5$) has a smaller number of elements than for the electron case.

The new surface scattering model for holes is implemented into our FBMC simulator [2] in the same manner as in the electron case [3]. The quantum correction potential calculated by the IMLDA model [4] is also implemented into our FBMC simulator through an additional force [9] as in the case of electron. This force drives the particles away from the Si/SiO_2 interface, therefore sets the inversion hole density to zero at the interface.

3. Low-field mobility extraction

Due to the warped structure of the valence bands, the reflection of a hole at the potential well is not necessarily specular [1]. This leads to off-diagonal elements in the mobility tensor, and the numerical integration method for the channel mobility, that works for electrons [2], fails for holes. We have developed a new LRMC method for holes. The Boltzmann equation is linearized with the first order perturbation δf as the unknown in response to a small driving field δE_y applied along a 1D homogenous channel in y-direction. Neglecting second and higher order terms, the linearized BTE has the form:

$$\underbrace{\left(\frac{\partial}{\partial t} + \frac{qE_x}{\hbar} \frac{\partial}{\partial k_x} + v_x \frac{\partial}{\partial x} \right) \delta f = -\frac{\delta f}{\tau}}_{\text{BTE with unknown } \delta f} + \underbrace{\frac{q \delta E_y v_y}{k_B T} f_0}_{\text{source term}}, \quad (7)$$

where t denotes the time, E_x the confining field, k_x the momentum in x-direction, and v_x, v_y the group velocity in x-,

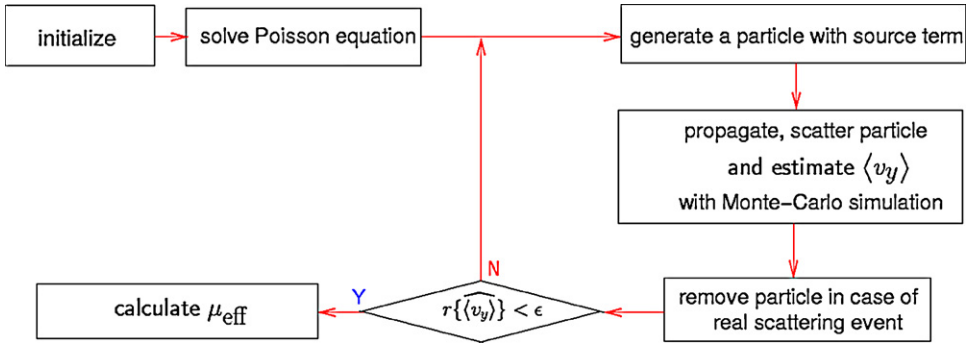

Fig. 2. Flow chart of LRMC method.