Simulation Standard

Connecting TCAD To Tapeout

A Journal for Process and Device Engineers

Schrödinger Approach and Density Gradient Model for Quantum Effects Modeling

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Abstract

We describe here two approaches to model the quantum effects that can no more be neglected in actual and future devices. These models are the Schrödinger-Poisson and Density-Gradient methods fully integrated in the device simulator ***ATLAS***. Simulations based on such methods are compared to each other on electron concentration and C-V curves in a MOS-capacitor.

1. Introduction

Advanced silicon technology tends towards ever thinner and shorter gate oxide resulting in significant quantum effects. The most relevant effect is the confinement of the carriers. For instance, in a Metal-Oxide-Semiconductor capacitor C-V characteristic, the threshold voltage is shifted and the apparent oxide thickness is increased compared to the C-V characteristic expected with a semi-classical approach. To model this confinement accurately in a device simulator based on a drift-diffusion approach, two methods are treated in this paper. The first one, and the most accurate, is to include the Schrödinger equation into a self-consistent computation with the Poisson equation. Unfortunately this solution, due to its non-locality, has a significant numerical cost and cannot be efficiently coupled with the continuity equations giving the current flow in practical applications. All the same this method is used in 1D as a reference: the C-V characteristic and the carrier density profiles are useful to validate simpler methods. Different simpler methods compatible with the drift-diffusion approach have been developed [1, 2]. In this paper we describe a density gradient model which introduces a quantum potential correction in the continuity equations. In the following, we present first the Schrödinger-Poisson model, then the density gradient model and the comparison to each other.

2. Schrödinger-Poisson Model (S-P)

The confinement effect appears in very thin oxide devices where the barrier of potential at the interface SiO_2/Si is larger and deeper than a thick oxide device. This quantum confinement is well described by solving the single particle Schrödinger equation. Solved self-consistently with the Poisson equation, it provides the eigenvalues and eigenvectors along the three directions of the k-space. Considering ml, mt1 and mt2 the electron longitudinal effective mass and the electron transverse effective masses respectively, the electron density is written as:

$$n(x) = \frac{2k_B T}{\pi\hbar^2} \left\{ \sqrt{m_l m_{t1}} \sum_i |\Psi_{li}(x)|^2 \ln\left[1 + \exp\frac{E_F - E_{li}}{k_B T}\right] + \sqrt{m_l m_{t2}} \sum_i |\Psi_{t1i}(x)|^2 \ln\left[1 + \exp\frac{E_F - E_{t1i}}{k_B T}\right] + \sqrt{m_{t1} m_{t2}} \sum_i |\Psi_{t2i}(x)|^2 \ln\left[1 + \exp\frac{E_F - E_{t2i}}{k_B T}\right] \right\}$$

where x is the position along a vertical slice (normal to the gate oxide), Ψ_{li}, E_{li} (resp. Ψ_{ti}, E_{ti}) are the i-th longitudinal (resp. transverse) eigenvector and eigenvalue, k_B is the Boltzmann

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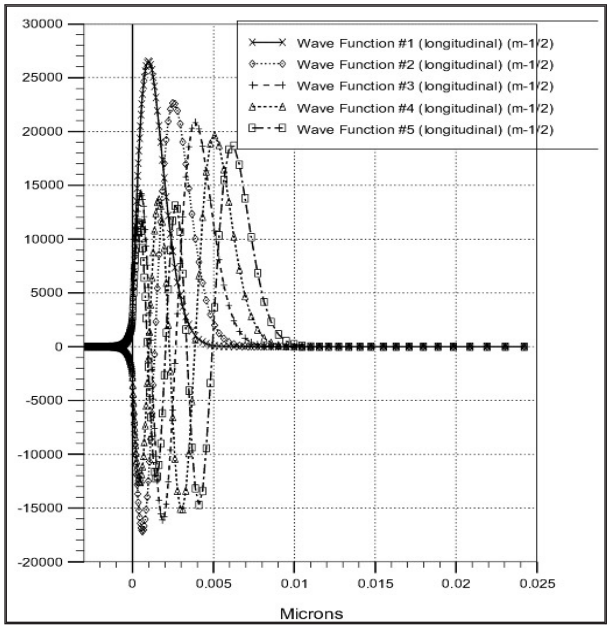

Figure 1a. 5 first longitudinal wave functions.

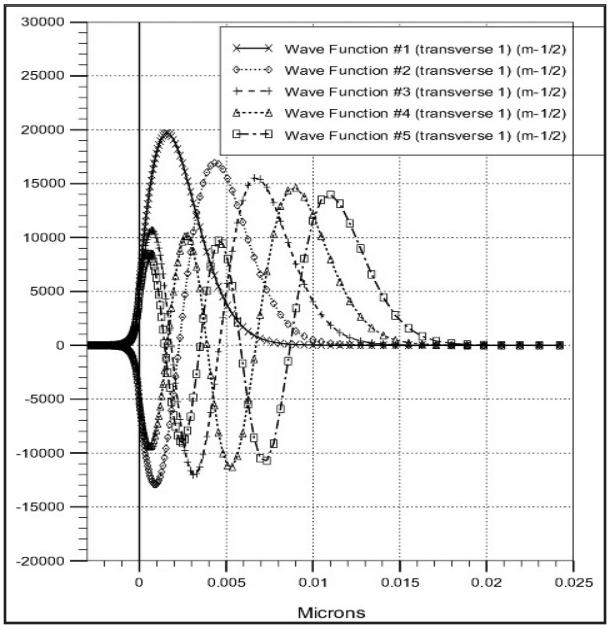

Figure 1b. 5 first transverse wave functions.

constant, T is the temperature, ħ is the Planck constant and E_F is the Fermi level. For the holes, a similar expression is obtained with the light and heavy holes effective masses. For a 2D device, the S-P equation is solved along a set of 1D parallel slices under the gate. At the ends of each slice an infinite potential is set as a boundary condition. As this assumption is unphysical at the SiO_2/Si interface, the S-P model has been designed to include the gate oxide in the solver so that the eigenvectors and thus the carriers could penetrate in the oxide. In the silicon oxide effective masses for electrons and holes have been defined, with value 0.3 and 1.0, respectively. A full description of this S-P model is presented in [3] with the works presented in [4, 5].

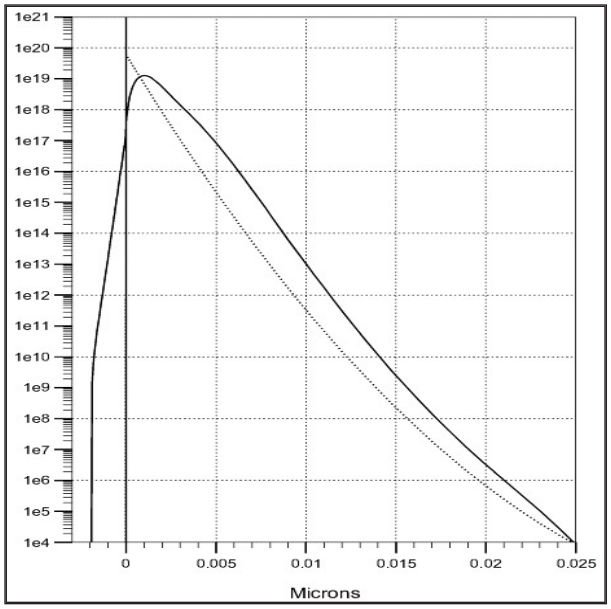

Figure 2. Semi-classical (dotted line) and quantum (solid line) electron concentration in log scale.

To illustrate this model, one defines a MOS-capacitor with 1e18 cm^{-3} p-type doped substrate and a 3 nm gate oxide thickness. In inversion mode (Vgate=1.0 V), Figure 1 shows the 5 first longitudinal and transverse eigenvectors (ml=0.98, mt1=mt2=0.19 have been set). The corresponding electron concentration is depicted in Figure 2 and compared with a semi-classical profile. It shows the peak in the quantum simulation is no more at the interface (x=0 coordinate) as in the semi-classical simulation. The quantum confinement is correctly modeled.

3. Density Gradient Model (DG)

The density gradient method is an approach compatible with the drift-diffusion treatment used in device simulator. Different methods have been proposed [6-8], one presents here one of these models. It applies a quantum potential correction _ in the density current expression:

$$\vec{J}_n = qD_n\vec{\nabla}n - qn\mu_n\vec{\nabla}(\Psi - \Lambda) - \mu_n n k_B T\vec{\nabla}\ln n_{ie}$$

with:

$$\Lambda = -\frac{\gamma\hbar^2}{6m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}}$$

where:

$$D_n = \frac{k_B T}{q}\mu_n$$ (if Boltzmann statistics is assumed),

μ_n is the electron mobility,
Ψ is the electrostatic potential,
n_{ie} is the intrinsic carrier concentration,
m is the electron effective mass,
γ is a fit factor.

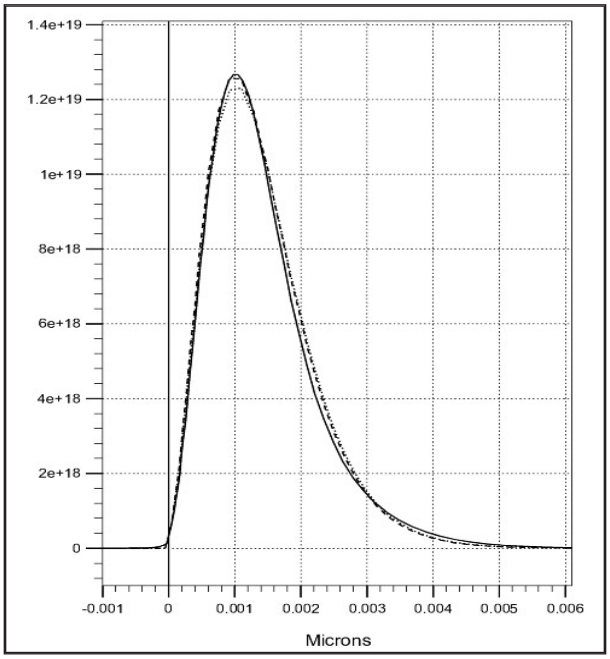

Figure 3. S-P (solid line) and DG (dashed and dotted lines) electron profiles.

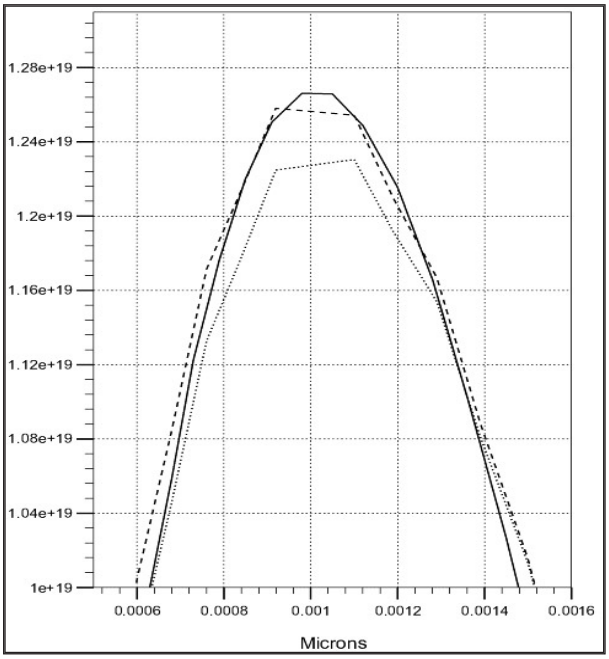

Figure 4. Electron profiles, zoom of Figure 3 around the peak, S-P in solid line, DG/_=3.4 in dashed line and DG/_=3.6 dotted lines.

The factor γ has been introduced to adjust the quantum correction which has been obtained after a few simplifications. Discussions about its introduction can be found in [7-9]. In this way it accounts the fact only one mass is used in DG model whereas three are used in S-P model. It could also be adjusted depending on the temperature of operation and the device (bulk, SOI, double gate).

Concerning the boundary conditions, they are the same as in a semi-classical scheme. The only boundary condition is that at contacts, the quantum correction is zero.

This model is compared to S-P model in Figure 3. The same device as described in section 2 has been used, the γ factor has been set to 3.6 (its default value as indicated in [8]) and 3.4 which fits better the S-P electron profile. The electron concentration is displayed in a linear scale and the x=0 coordinate corresponds to the interface. The Figure 4 is a zoom around the peak and it shows a difference between S-P and DG with γ=3.4 less than 1% at the peak. It confirms the DG model is suitable to capture quantum effects.

Then for each approach, semi-classical, Schrödinger-Poisson and Density-Gradient, we display in Figure 5 the C-V characteristics. The device used is the same as described in section 2 and γ =3.4 has been set for the DG model.

We clearly note the shift of the threshold voltage near 0.5 volt and the reduction of the quantum capacitance in inversion mode (Vg > 0.5 V). The difference observed between S-P approach and DG model in strong accumulation is explained by the fact the charge is treated in a full quantum scheme in S-P solver whereas a part of the charge should be treated semi-classically. However this small error is not really important because the more strongly doped the substrate, the less the carriers are confined [9], moreover the mode of operation of an actual MOSFET is in inversion mode, and Figure 5 shows the very good agreement between the DG model and the S-P approach in this case.

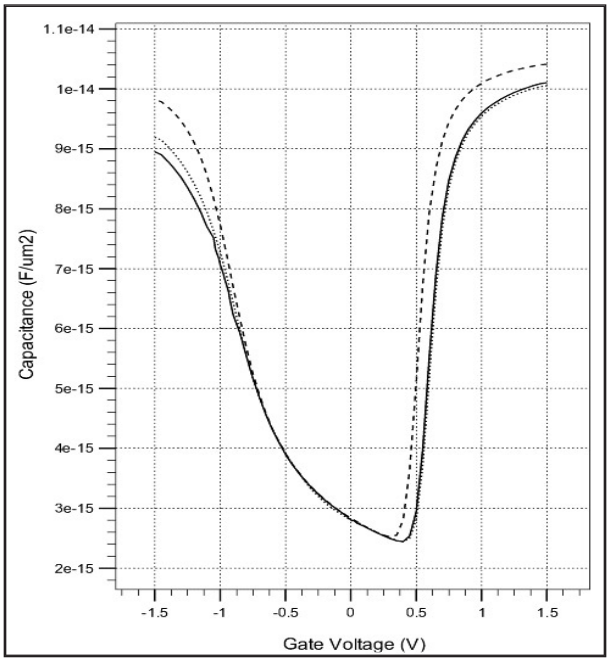

Figure 5. C-V curves, semi-classical in dashed line, S-P in dotted line and DG in solid line.

4. Conclusion

We have presented the different approaches to model quantum confinement in MOSFET implemented in the commercial device simulator ***ATLAS***. The Schrödinger-Poisson model is suitable for any kind of 1D or 2D devices (with planar or non-planar gate oxide) in which quantum effects are important and with bias conditions not to far from equilibrium (for instance, a small bias on the drain can be applied). This solver has been developed in collaboration with the University of Pisa, and has shown excellent agreement with their in-house code. Then a density gradient model has been described and its results, based on carriers'profiles and C-V curves, have proven its capability to model correctly the quantum confinement with an adjustment of the γ factor.

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