Schrödinger Approach and Density Gradient Model for Quantum Effects Modeling

A. Ferron¹, B. Cottle¹, G. Curatola³, G. Fiori³, E. Guichard¹
¹ Silvaco Data Systems, 55 rue Blaise Pascal, 38330 Montbonnot Saint-Martin, France
² Silvaco International, 4701 Patrick Henry Dr., Santa Clara, CA 95054, USA
³ University of Pisa, Via Diotsaleti 2, I-56122, Pisa, Italy

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 SiO₂/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:

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

where \( x \) is the position along a vertical slice (normal to the gate oxide), \( \Psi_{li}, E_{li} \) (resp. \( \Psi_{ti}, E_{t1i}, E_{t2i} \)) are the i-th longitudinal (resp. transverse) eigenvector and eigenvalue, \( k_B \) is the Boltzmann constant.

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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 (V\(_{\text{gate}}\)=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:

\[
\tilde{J}_n = qD_n \nabla n - qn\mu_n \nabla (\Psi - \Lambda) - \mu_n nk T \nabla \ln n_p
\]

with:

\[
\Lambda = \frac{\gamma h^2}{6m} \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}
\]

where:

\[
D_n = \frac{k_B T}{q} \mu_v
\]

(if Boltzmann statistics is assumed), 
\(\mu_v\) is the electron mobility,
\(\Psi\) is the electrostatic potential,
\(n_p\) is the intrinsic carrier concentration,
\(m\) is the electron effective mass,
\(\gamma\) is a fit factor.
The factor $\gamma$ 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 $\gamma$ 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 $\gamma=3.4$ 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 $\gamma=3.4$ 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 ($V_g > 0.5$ 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.
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 \( \gamma \) factor.

References