Efficient Quantum Correction Model for Multi-dimensional CMOS Simulations

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Abstract

We present a new Quantum correction algorithm suitable for multi-dimensional CMOS simulations. The quantum effects are included using the Modified Local Density Approximation (MLDA). Physically accurate spatial distribution of quantized carriers can be predicted with only ten to twenty percents increased of computation time. The algorithm is also suitable to integrate into a device simulator. Simulation results are in good agreement with experimental data.

1. Introduction

Although surface quantization effects in semiconductor inversion and accumulation layers have been studied extensively using the self-consistent solutions of Schrödinger and Poisson equations [2,5,9], this approach is known to be too computationally expensive even in the three-subband model implemented by Hareland et al. [8]. Most previously proposed simple quantum mechanical (QM) correction models [3,6] were mainly focused on threshold voltage or capacitance shifts. They all failed to provide the spatial information of quantized carriers. A fast turnaround and physically accurate device simulator that accounts for the quantization effect is urgently called for to support our technology development. With this in mind, we have developed a computationally efficient algorithm based on the modified local density approximation (MLDA) proposed by Paasch and Ubensee [1]. This model can predict the spatial carrier distribution due to quantization [11] and is suitable to integrate into a device simulator such as FIELDAY [4]. With our algorithm, realistic quantized carrier and current distribution for 2d/3d device structures can be efficiently calculated. Very good agreement with experimental data has been achieved.

2. Model and Algorithm

According to Paasch and Ubensee, the effect of quantization on electron density near the Si/SiO2 interface can be approximated by [1],

$$n_{QM}(z) = N_c \cdot (\frac{2}{\sqrt{\pi}}) \int_0^\infty \{\frac{\sqrt{\xi}}{1+\exp[(\xi - E_F)/k_BT]} \cdot [1 - \sum_i J_o(2z\sqrt{\xi}/\lambda_n^i)]\}\, d\xi, \quad (1)$$

where $z, n_{QM}, N_c, E_F, J_o, \lambda_n^i$, is the distance from the interface, the QM corrected electron density, the conduction band effective density-of-states, the quasi-fermi level, the zeroth-order spherical Bessel function, and $\lambda_n^i = \sqrt{\frac{\hbar^2}{2m_n^* k_B T}}$ is the thermal wavelength, respectively. The lower bound in the above integration is referenced to the lowest bound state. A similar relation holds for the hole density. The summation of the Bessel function corresponds to the QM correction of the local density. For high-temperature or large z, Eq.(1) reduces to the Fermi-Dirac statistic for electron density. In order to ensure the zero-current condition under thermal-equilibrium, the extra gradient due to the QM corrected density must be considered in the current transport equation. Our algorithm works as follows: The QM corrected electron density is replaced by an equivalent quantum potential,ψ_{QM}, for electrons after each Newton iteration. The quantum potential at each nodal point is obtained by solving the following nonlinear equation,

$$\psi_{QM}(z) = -E_C(z) + E_F(z) - \frac{k_B T}{q} F_{1/2}^{-1}[n_{QM}/N_C(z)], \tag{2}$$

where n_{QM} is obtained from Eq.(1) and $F_{1/2}^{-1}$ is the inverse-Fermi function of order (1/2). A similar relationship exists for holes. The additional quantum potential for electrons and holes is then lumped into the band-structure parameters, θ_n, θ_p, commonly found in hetero-structure device equations [4]. In Fielday, the moment-based current density equation is expressed as,

$$\vec{j_n} = -q\mu_n n \nabla[\psi + \theta_n] + \mu_n n \nabla(k_B T_e) + k_B T_e \mu_n \nabla n, \tag{3}$$

with

$$\theta_n = \chi + \frac{k_B T}{q} \ln(N_C/N_{Co}) + \frac{k_B T}{q} \ln(\gamma_n) + \psi_{QM}. \tag{4}$$

The spatial variation of band structure, effective density of states, Fermi-Dirac statistics, and quantum potential are all accounted for by Eq.(4). The above procedure is repeated after each Newton iteration in the full-Newton loop until the solution update converges to a specified tolerance (default to less than 1.0^{-6} for relative update of potential, electron concentration and hole concentration).

3. Simulation Results and Discussions

In Fig.1, simulated MOS-capacitor C-V curve of varying oxide thickness, tox, agrees very well with experimental data. For comparison, the classical simulated C-V data for tox=4.5 nm is also shown. The model works well under all biasing conditions: inversion, depletion, and accumulation. The Ids-Vg characteristics for a 0.2 um gate length and 30 A oxide NMOSFET is given in Fig.2. Bear in mind that van Dort's model [6] only considered the integrated charge to modify threshold voltage and capacitance but not the spatial distribution of the charge density. The deficiency of van Dort's model has also been discussed by Ancona et al. [10]. The quantized electron distribution from the MLDA solution is clearly demonstrated in a two-dimensional contour shown in Fig.3. The asymmetry in the electron contour is due to the additional drain field from the applied drain voltage. The difference in the electron density distribution for the three models (Classical, van Dort, and MLDA) is highlighted in Fig.4. It is obvious that both the classical and van Dort's model failed to predict the charge depletion due to quantization. The algorithm is also very efficient as shown in Table 1. For a twelve thousand nodes NMOS mesh with two-carrier simulation,

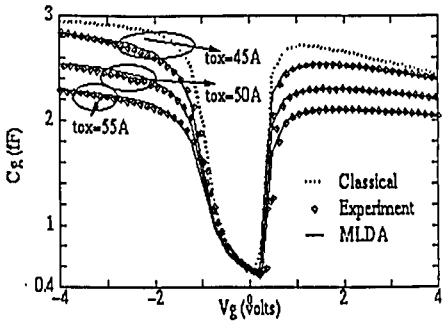

Figure 1: Simulated and experimental CV characteristics.

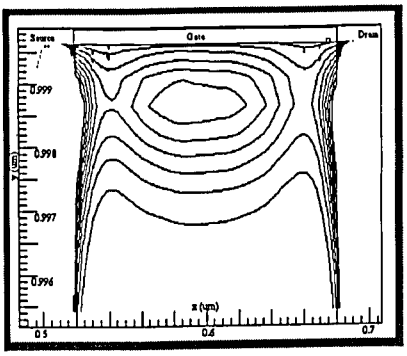

Figure 3: MLDA predicted electron concentration contour near the Si/SiO2 interface at Vg=Vt.

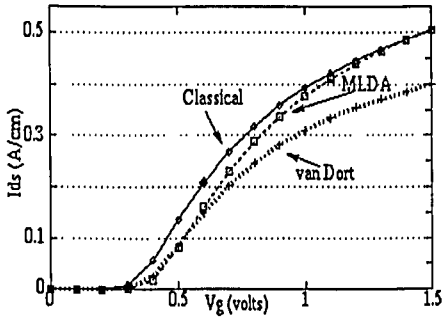

Figure 2: Vg-Ids Characteristics for different models.

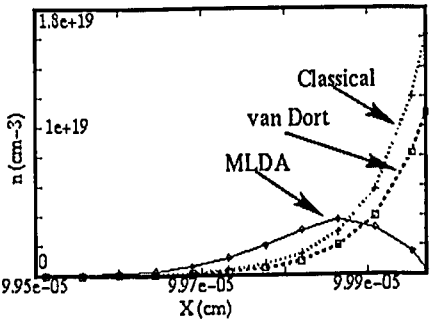

Figure 4: One Dimensional electron concentration near the oxide interface for different models at Vg=Vt.

Table 1: Comparison of required Newton iterations and CPU time for different models.

	MLDA # Newtons	Van Dort # Newtons	Classical # Newtons	MLDA CPU Time	Van Dort CPU Time	Classical CPU Time
vg=0	12	4	4	180 (s)	63(s)	59(s)
vg=0.7	6	6	4	90 (s)	94(s)	59(s)
vg=1.5	7	5	3	105 (s)	47(s)	44(s)
Total(16)	108	89	65	1,680 (s)	1,463(s)	1,022(s)

the required Newton iterations and CPU time is only fifteen percents longer than the model proposed by van Dort. It is worth mentioning that the current implementation automatically works for three-dimensional device structures. Our procedure also provides a framework for any QM correction to be included in charge transport equations. For higher accuracy, n_{QM} in Eq.(1) can be replaced by solution of Schrödinger equation. Moreover, our algorithm considered the QM correction effects on both the electron and hole current densities simultaneously. All previous QM correction algorithms [3,6,7,9,10] modified either the energy band gap or the intrinsic carrier concentrations. Therefore, quantization for both carriers under both inversion and accumulation cannot be treated simultaneously.

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