Mobility Modeling in Presence of Quantum Effects

K. Dragosits, V. Palankovski, and S. Selberherr
Institute for Microelectronics, TU Vienna, Gusshausstrasse 27–29, Vienna, Austria
Telephone: +43-1-58801/36018, Fax: +43-1-58801/36099, Email: Dragosits@iue.tuwien.ac.at

***Abstract*— CMOS oxide thicknesses in the nanometer range lead to the development of TCAD models which take care of the quantum mechanical effects at the semiconductor/insulator interface. It is obvious that the quantum distribution of carriers will not fit to existing mobility models which were empirically developed employing a classical profile. Especially the terms which account for surface scattering need modifications. By utilizing an optimization framework and comparison with measurements stemming from overall 30 devices from two different technology nodes, this subject was rigorously investigated. Finally, a model was developed, where only one material parameter (instead of three) is needed to describe the semiconductor/oxide interface.**

I. Introduction

CMOS oxide thicknesses in the nanometer range lead to the development of TCAD models which take care of the quantum mechanical effects at the semiconductor/insulator interface. Various approximation models for quantum mechanical (QM) effects exist and reasonable results were obtained for C/V characteristics, e.g. [1] [2] [3].

It is obvious that the quantum distribution of carriers will not fit to existing mobility models which were empirically developed employing a classical profile. Especially the terms which account for surface scattering are expected to need modifications. We present a suitable mobility model which extends the quantum approximation for the simulation of general device characteristics.

II. Methodology

For this work we used two series of conjugate CMOS devices from two different technology nodes, with channel lengths ranging from 130nm to 1μm. The key technology parameters such as gate length L_{G}, gate width W_{G}, gate oxide thickness T_{Ox}, and applied voltage V_{DD} are summarized in Table I.

TABLE I
KEY PARAMETERS FOR THE INVESTIGATED TECHNOLOGIES

Technology	L_{G}	W_{G}	T_{Ox}	V_{DD}
0.25 μm	0.2-1.0 μm	20 μm	4.7 nm	2.5 V
0.13 μm	0.115-0.7 μm	10 μm	2.3 nm	1.5 V

The underlying data set was already subject of a profound analysis with classical device models [5]. Transport was modeled by the drift diffusion equation set with a modest demand on computational resources. Remarkable agreement between measurement and simulation was obtained for the parameters in the Minimos mobility model [6]. This model reads as:

$$\mu = \frac{\mu_{\mathrm{ref}} + (\mu_{\mathrm{LI}} - \mu_{\mathrm{ref}}) \cdot (1 - F(y))}{[1 + F(y) \cdot (S/S_{\mathrm{ref}})^{\gamma}]}, \tag{1}$$

where μ is the overall mobility, μ_{LI} is the mobility inside the device, S is the pressing force at the surface, and $\mu_{\mathrm{ref}}, \gamma$ and S_{ref} are fitting parameters. The function $F(y)$ reads as:

$$F(y) = \frac{2 \cdot \exp\Big(-\left(y/y_{\mathrm{ref}}\right)^2\Big)}{1 + \exp\Big(-2 \cdot \left(y/y_{\mathrm{ref}}\right)^2\Big)}, \tag{2}$$

where y_{ref} is the distance from the interface up to which surface effects are taken into account.

These results were used as the starting point for the investigation of a suitable mobility model when the influence of the quantum confinement is considered.

III. Approximation of the Quantum Confinement

For an accurate approximation of the carrier concentration profile near the interface we utilize an approximation model which was recently developed [7] and implemented into the device simulator MINIMOS-NT. This model makes two modifications to the classical model: Firstly, the carrier density of states N near the interface is reduced with an exponential shape function proposed by Hänsch [1]:

$$N(y) = N \cdot \left(1 - \exp\left(-(y + y_0)^2/\lambda_{\mathrm{TH}}^2\right)\right). \tag{3}$$

Here y is the distance to the interface and y_0 is an offset to match the nonzero carrier concentration near the surface stemming from the finite barrier height. λ_{TH} is the thermal wavelength responsible for the reduction of the effect with increasing distance from the interface,

$$\lambda_{\mathrm{TH}} = \frac{\sqrt{2mkT}}{\hbar}. \tag{4}$$

Secondly, the band gap near the surface is replaced by the first discrete energy level (see Fig. 1). We set the band edge at the surface to

$$E_{\mathrm{g,Surf}}^{\mathrm{QM}} = E_{\mathrm{g,Surf}}^{\mathrm{Classical}} + \Delta E_{\mathrm{g}}, \tag{5}$$

here $E_{\mathrm{g,Surf}}^{\mathrm{QM}}$ is the modified bandgap energy which is used in the Boltzmann statistics, $E_{\mathrm{g}}^{\mathrm{Classical}}$ is the bandgap according to the material specification, and ΔE_{g} is the applied correction. Our model pins the band edge $E_{\mathrm{g}}^{\mathrm{QM}}(y)$ inside the device to the value of $E_{\mathrm{g,Surf}}^{\mathrm{QM}}$ as long as $E_{\mathrm{g,Surf}}^{\mathrm{QM}} > E_{\mathrm{g}}^{\mathrm{Classical}}(y)$.

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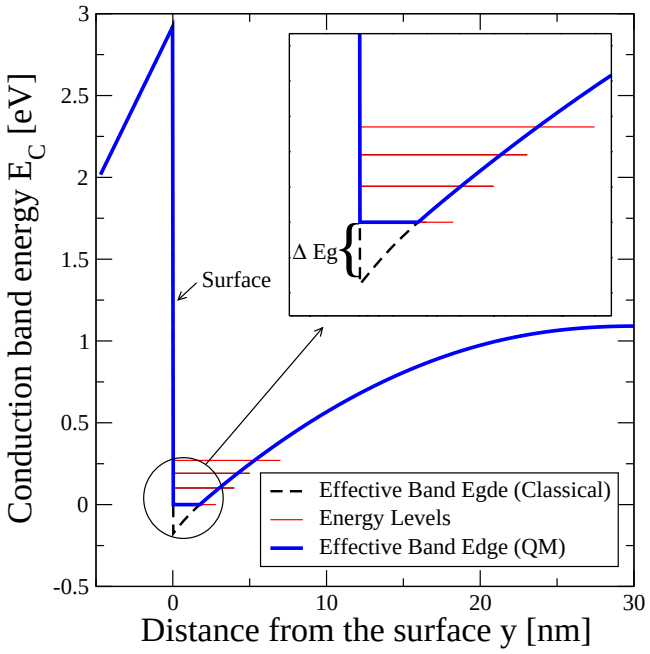

Fig. 1. Band structure near the surface and comparison between the conduction band edge of the classical and the new approach.

The offset ΔE_{g} of the first discrete energy level can be approximated by the following expression [3]:

$$\Delta E_{\mathrm{g}} = \frac{13}{9} \cdot \beta \cdot \left(\frac{\epsilon}{4qkT} \right)^{1/3} |E_{\mathrm{Surf}}|^{2/3}. \tag{6}$$

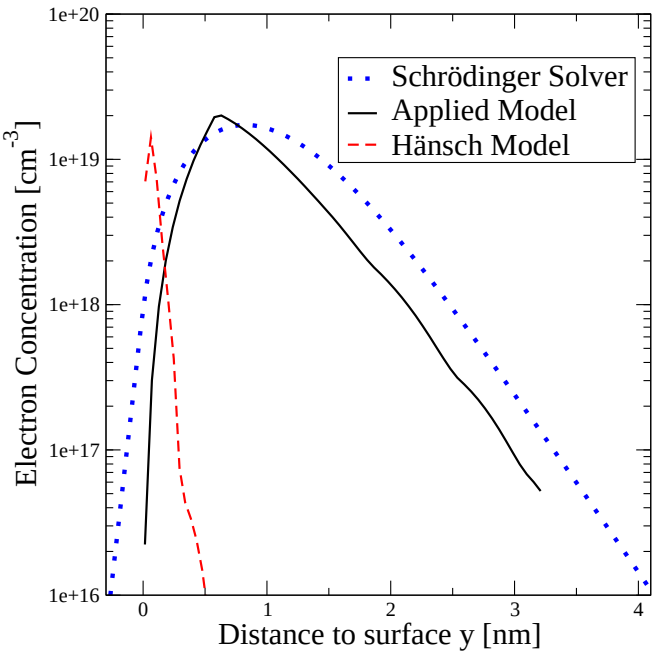

Fig. 2. Comparison of different QM correction models with the solution of a Schrödinger-Poisson solver.

Here $|E_{\mathrm{Surf}}|$ is the magnitude of the electric field at the interface, ϵ is the permittivity of the semiconductor, and the empirical constant $\beta = 4.1 \times 10^{-8}\mathrm{eVcm}$.

This model produces an excellent agreement to data obtained from simulations with a self consistent Schrödinger-Poisson solver with effective mass approach [8]. Fig. 2 gives a comparison of the carrier profiles from our approximation, the Hänsch model, and the Schrödinger-Poisson solver. This comparison shows that the Hänsch model is capable to move the carrier profile away from the interface and produces the correct maximum concentration, but fails to provide an accurate description of the actual concentration profile, whereas the approximation model offers decent properties.

IV. Simulations and Discussion

Our investigations were carried out with the optimization framework SIESTA [4] which allows the optimization of an arbitrary number of parameters in order to approach a specified target. Taking advantage of the accurate approximation of the carrier profile, the simulations were carried out with the respective physical oxide thicknesses given in Table I.

Running the optimization with the quantum approximation model led to remarkable results. Analysis of the extracted parameters show, that the term $(S/S_{\mathrm{ref}})^{\gamma}$ in the denominator of the mobility model, which accounts for the influence of the electric field at the surface, becomes negligible. Therefore two fitting parameters S_{ref} and γ are eliminated. The subsequent model reads as:

$$\mu = \mu_{\mathrm{ref}} + (\mu_{\mathrm{LI}} - \mu_{\mathrm{ref}}) \cdot (1 - F(y)), \tag{7}$$

where $F(y)$ is the function defined in (2). This leaves μ_{ref} as the only fitting parameter to account for the different properties of the interface in the new mobility model, and makes calibration to new technology nodes easy.

TABLE II
Mobility model parameters for the 0.25μm technology

Parameter	New Mobility Model NMOS	New Mobility Model PMOS	Minimos Mobility Model NMOS	Minimos Mobility Model PMOS
E_{w}[eV]	-0.39	0.576	-0.372	0.551
$\mu_{\mathrm{ref}}[\mathrm{cm}^2/\mathrm{Vs}]$	343	57.5	582	78
$S_{\mathrm{ref}}[\mathrm{V/cm}]$	-	-	5.4e5	6.6e5
γ	-	-	7.1	8.0

TABLE III
Mobility model parameters for the 0.13μm technology

Parameter	New Mobility Model NMOS	New Mobility Model PMOS	Minimos Mobility Model NMOS	Minimos Mobility Model PMOS
E_{w}[eV]	-0.482	0.435	-0.433	0.407
$\mu_{\mathrm{ref}}[\mathrm{cm}^2/\mathrm{Vs}]$	447.3	62.8	573	82
$S_{\mathrm{ref}}[\mathrm{V/cm}]$	-	-	6.3e5	6.2e5
γ	-	-	6.0	8.7

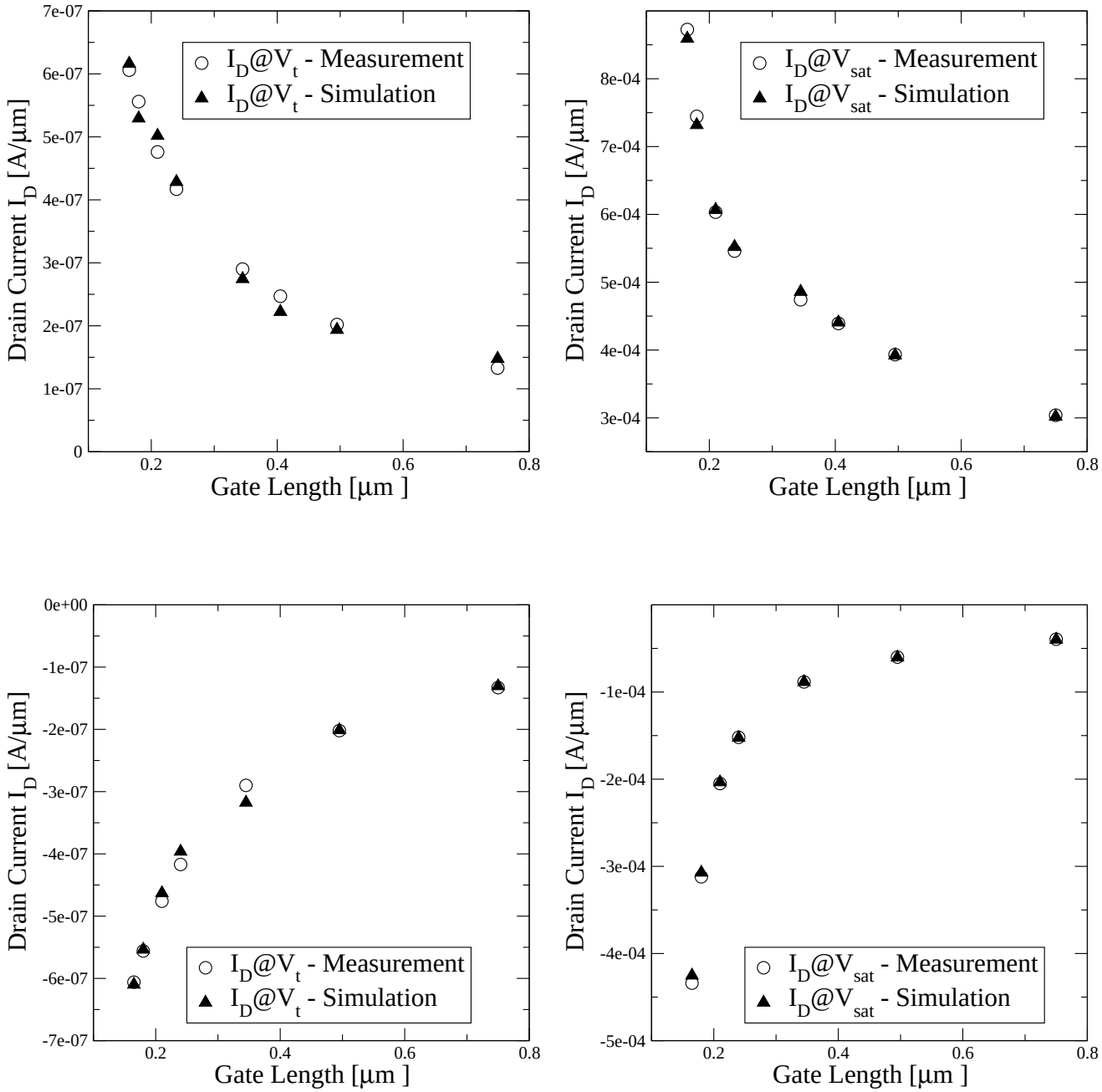

Fig. 3. Comparison simulation to measurement, 0.13μm technology, first row - NMOS, second row - PMOS, left - threshold, right - saturation.

As for the classical model, a very good agreement to the measured data is obtained, which is demonstrated in Fig. 3 and Fig. 4. A comparison of the parameters obtained with the new mobility model and the Minimos mobility model is given in Table II and Table III, where S_{ref} and γ are the additional fitting parameters needed by the Minimos mobility model.

V. Conclusion

A new mobility model which considers the presence of the quantum confinement at the semiconductor/insulator interface was presented. With this new model it has been possible to achieve a good match to two series of CMOS devices from two different technology nodes. Furthermore, with this new model, the number of necessary fitting parameters to cover the surface effects has been reduced to a minimum of one parameter. This parameter is a mobility and is sufficient to describe the properties of the semiconductor/insulator interface.

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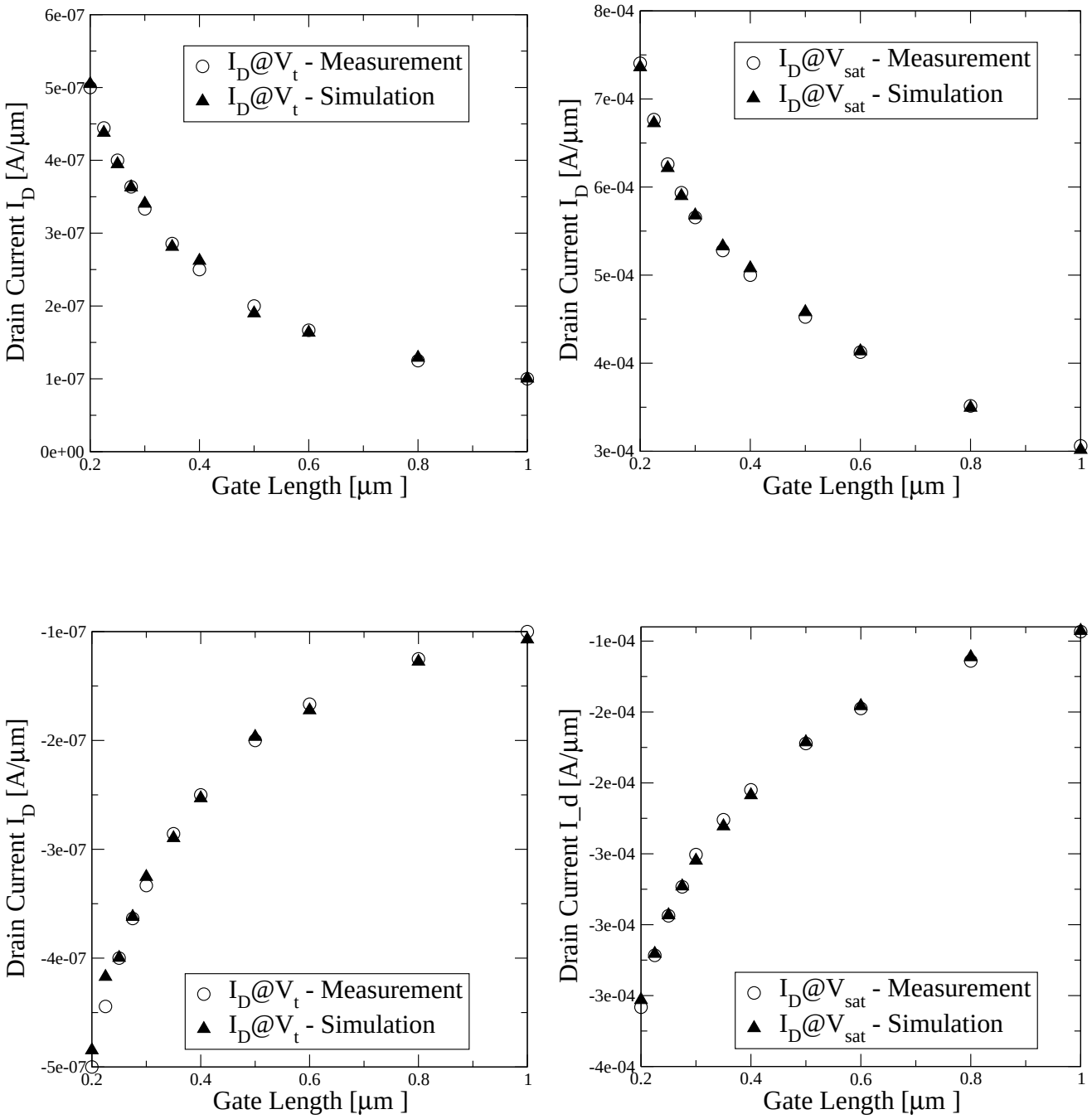

Fig. 4. Comparison simulation to measurement, 0.25μm technology, first row - NMOS, second row - PMOS, left - threshold, right - saturation.

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