A Drift-Diffusion subband model for the Double-Gate MOSFET

N. Ben Abdallah*, F. Méhats*, P. Pietra† and N. Vauchelet*
*Mathématiques pour l'Industrie et la Physique (UMR 5640), Université Paul Sabatier,
118 route de Narbonne, 31062 Toulouse cedex 4, France.
Email: naoufel@mip.ups-tlse.fr ; mehats@mip.ups-tlse.fr ; vauchel@mip.ups-tlse.fr
Telephone: (0033)561558314, Fax: (0033)561558385
† Istituto di Matematica Applicata e Tecnologie Informatiche del C.N.R.,
via Ferrata 1, I-27100 Pavia, Italy.
Email: pietra@imati.cnr.it

***Abstract*— A self-consistent model for charged particles, accounting for quantum confinement, diffusive transport and electrostatic interaction is considered. In this coupled quantum-classical system, the coupling occurs in the momentum variable : the electrons are like point particles in the direction parallel to the gas (classical transport) while they behave like waves in the transversal direction (quantum description). Numerical implementation of this model provides a simulation of the transport of charge carriers in a quasi bidimensional electron gas confined in a nanostructure.**

***Index Terms*— nanotransistor, Gummel iterations, Schrödinger equation, Fermi level, drift-diffusion system, Poisson equation, subband model, finite element method.**

I. Introduction

Nowadays, a great challenge consists in the downscaling at the nanometer scale of electronic components in order to improve speed and efficiency of semiconductor materials. In this task, modeling and numerical simulations play an important role in the determination of the limit size of the nanotransistors [14]. In nanoscale semiconductor devices like ultrashort channel double gate MOSFETs (DGMOS) [1], electrons might be extremely confined in one or several directions that we shall refer to as the confining directions. This leads to a partial quantization of the energy. In this work, we present a simulation of the transport in such a device. We consider a particle system which is partially quantized in one confined direction (denoted by z) and which, in the non-confined one, refered to as the transport direction and denoted by x, has a diffusive motion.

The subband model describes quantum systems at partial thermodynamic equilibrium as a statistical mixture of eigenstates of the Schrödinger operator in the transverse direction. The occupation number of each state is given by a thermodynamic equilibrium statistic function. Typically, it is given by $\exp(\frac{\epsilon_F-\epsilon}{k_BT})$ for Boltzmann statistics, or $1/(1+\exp(\frac{\epsilon-\epsilon_F}{k_BT}))$ for Fermi-Dirac statistics, where ϵ is the energy of the considered state, k_B is the Boltzmann constant, T is the temperature and ϵ_F is the so-called Fermi energy which, at zero temperature, represents the threshold between occupied and unoccupied states [13], [19].

In the transport direction, the motion of the charge carriers is governed by the drift-difusion equation. This equation is one of the most used models for charged particle transport in various areas such as gas discharges, plasmas or semiconductors. It consists in a conservation equation for the particle density, in which the current density is the sum of the diffusion current and the drift current which takes into account the electrostatic forces [10], [11], [17].

The system is at equilibrium in the confined direction with a local Fermi level ϵ_F which depends on the transport variable x. The variable x is assumed to lie in $(0,L) \in \mathbb{R}$ where L is the length of the device while z belongs to the interval $(0,\ell)$ with a width ℓ. At a time t and a position (x,z), the particle density $N(t,x,z)$ for Boltzmann statistics is given by

$$N(t,x,z) = \sum_{k=1}^{+\infty} e^{\beta(\epsilon_F(t,x)-\epsilon_k(t,x))}|\chi_k(t,x,z)|^2, \quad (1)$$

where $\beta = 1/(k_BT)$, ϵ_F is the Fermi Level and $(\chi_k,\epsilon_k)_{k\geq 1}$ is the complete set of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_*(z)}\frac{d}{dz}\chi_k\right) + (eV+U_c)\chi_k = \epsilon_k\chi_k. \quad (2)$$

In this equation $\hbar$ is the Planck constant, m_* the effective mass, e the elementary charge and U_c is a given potential barrier between the silicon and the oxyde in the nanotransistor. On the boundary we impose $\chi_k(t,x,0) = \chi_k(t,x,\ell) = 0$. The electrostatic potential V is a solution of the Poisson equation

$$-\mathrm{div}_{x,z}(\varepsilon_R\nabla_{x,z}V) = \frac{e}{\varepsilon_0}(N-N_D), \quad (3)$$

where ε_R is the relative permittivity, ε_0 the permittivity constant in vacuum and N_D is the doping density. We

define the repartition function $\mathcal{Z}$ by

$$\mathcal{Z}(t,x) = \sum_{k=1}^{+\infty} e^{-\beta\epsilon_k(t,x)}. \tag{4}$$

The surface density

$$N_s(t,x) = \int_0^\ell N(t,x,z)\,dz = e^{\beta\epsilon_F}\,\mathcal{Z}(t,x) \tag{5}$$

satisfies the drift-diffusion equation

$$\frac{d}{dt}N_s - \frac{d}{dx}\left(D\left(\frac{d}{dx}N_s + \beta N_s \frac{d}{dx}U_s\right)\right) = 0, \tag{6}$$

where D denotes the diffusion coefficient $D = \mu k_B T$ for a constant mobility μ and the effective energy U_s is given by

$$U_s = -k_B T \log\left(\sum_{k=1}^{+\infty} e^{-\beta\epsilon_k}\right). \tag{7}$$

The originality of this system is that the parameters of the drift-diffusion equation keep a trace of the quantum confinement in the transversal direction. Indeed, the expression of the effective potential (7) involves the diagonalization of the one dimensional Schrödinger operator (2). Remark that the density N satisfies :

$$N(t,x,z) = \frac{N_s(t,x)}{\mathcal{Z}(t,x)} \sum_k e^{-\beta\epsilon_k} |\chi_k(t,x,z)|^2. \tag{8}$$

The unknowns of the overall system are the surface density $N_s(t,x)$, the eigenenergies $\epsilon_k(t,x)$, the eigenfunctions $\chi_k(t,x,z)$ and the electrostatic potential $V(t,x,z)$. We say that the system is at the *thermal equilibrium* when the Fermi level ϵ_F is constant.

We present here a simulation of a Double-Gate MOSFET. The I-V characteristic is obtained by the drift-diffusion-Schrödinger-Poisson system (6)-(2)-(3). A mathematical study of this system has been done in [2]. Numerical simulations for nanotransistors which rely on the discretization of a Schrödinger-Poisson system are studied in [13] in particular to describe quantum ballistic transports [16]. In this work, this system is coupled with the drift-diffusion equation.

Let us end this introduction by referring to two other models which intend to incorporate quantum effects in the drift-diffusion equation. A full quantum drift-diffusion model (quantum in both directions) was derived in [7] and its numerical simulation was adressed in [8]. A quite similar model was introduced in [15] and used in [6] to simulate nanoscale MOSFETs.

II. Numerical simulation for a nanotransistor

A. Presentation of the modeled device

Our typical device of interest are very small Si/SiO_2 structures. Fig. 1 presents a scheme of the modeled double-gate MOSFET. The transport of the electrons takes place in the channel, which is the active region outside the reservoir.

TABLE I

Table of the main value used

Parameter	Value	Length	Value
N^+	$10^{20}cm^{-3}$	L_S	$15nm$
N	$10^{15}cm^{-3}$	L_C	$20nm$
U_c	$3\ eV$	L_D	$15nm$
$\varepsilon_R[Si]$	11.7	ℓ_{ox}	$2nm$
$\varepsilon_R[SiO_2]$	3.9	ℓ_{Si}	$8nm$

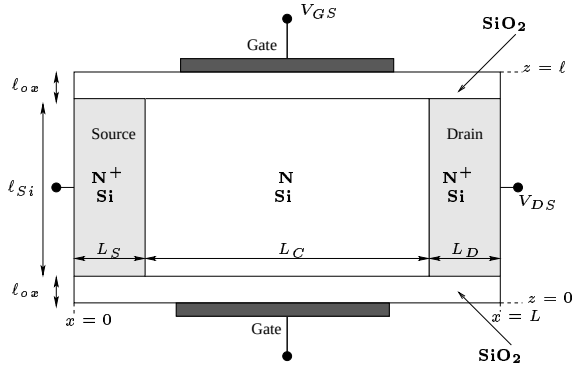

Fig. 1. Schematic representation of the modeled device

The transistor is assumed to be dopped by a large density N^+. These positive doping profile regions at the source and the drain contacts are equivalent to small electron reservoirs, in which we assume that the potential does not depend on the transport direction. The high barrier potential U_c which is of order $3eV$ forces the electrons to stay in the silicon zone.

Table I presents some numerical values used in the code.

B. The numerical method

In order to simulate the described device, we use finite elements method with Gummel iterations [9]. The Gummel method is well-known for the simulation of drift-diffusion models [4] and we apply it here with a self-consistent potential obtained by the resolution of a Schrödinger-Poisson system. More precisely our computation follows the next steps :

Step 1. First, we express the boundary conditions for the surface density N_s and the electrostatic potential V. Because of several ohmics contacts we have to choose mixed boundary conditions for the potential. At the contacts (drain, source and gates) the potential is fixed which implies Dirichlet-type boundary conditions, whereas the insulating frontier impose a Neumann-type condition.

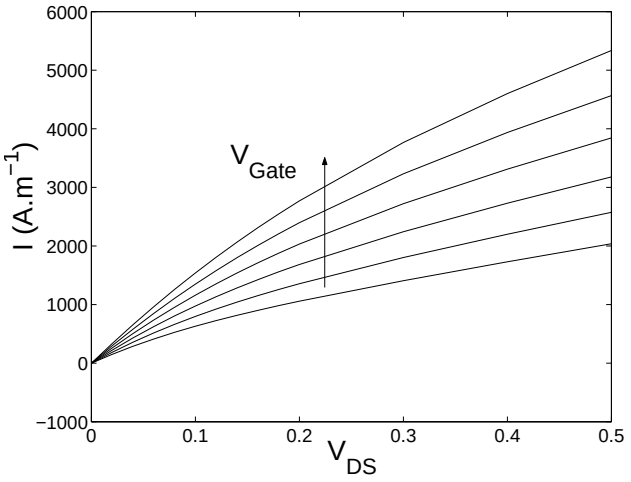

Fig. 2. $I-V$ characteristics for the device with differents gate-source voltage V_{GS}

Step 2. Next, we have to determine the density at the thermal equilibrium when there is no applied voltage. Since the Fermi level is constant, it is equal to its value at the boundary. We iterate a Gummel method for the resolution of the Schrödinger-Poisson system.

Step 3. In this last step we start from the equilibrium and apply a voltage at the contacts. Thus the whole coupled system (6)-(2)-(3) is considered. We implement again Gummel iterations. We point out the fact that the resolution of the Poisson equation needs a quasi-Newton method [5] in order to handle a well-conditionned system.

C. Numerical results

The main interest of this simulation is to obtain the I-V characteristics of the device, presented in Fig. 2, for different applied potential at the gates V_{GS}.

Fig. 3 and 4 present the potential and the density at the equilibrium obtained at the end of the second step.

Fig. 5 shows the value of the density of electrons when there is an applied drain-source voltage and no applied voltage at the gate. We constat an accumulation in the channel. In the Fig. 6 the applied voltage V_{GS} keeps the same value but the gate-source voltage is equal to $0.3V$. We notice that the maximum value is smaller and is moved in the transversal direction.

All these results are presented in the context of Boltzmann statistics and the same ideas can be extended for Fermi-Dirac statistics. This kind of implementation can be used for a one-valley silicon as well as for a three-valley silicon when the transverse effective mass differs from the longitudinal one due to anisotropic effects. The model presented is justified in particular for large the doping zones of the nanotransistor. In a future work, we will study

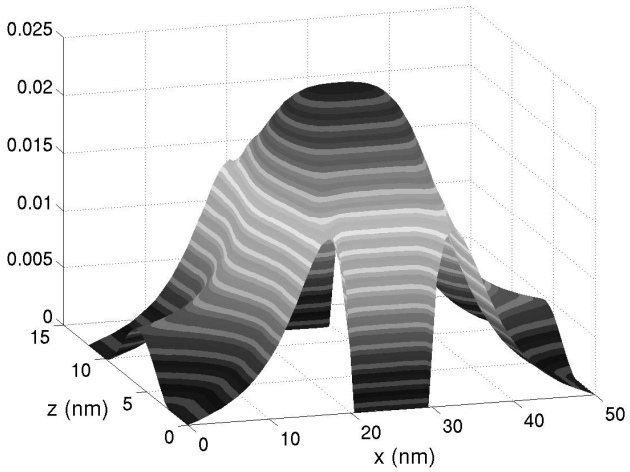

Fig. 3. Electrostatic potential at the equilibrium (V)

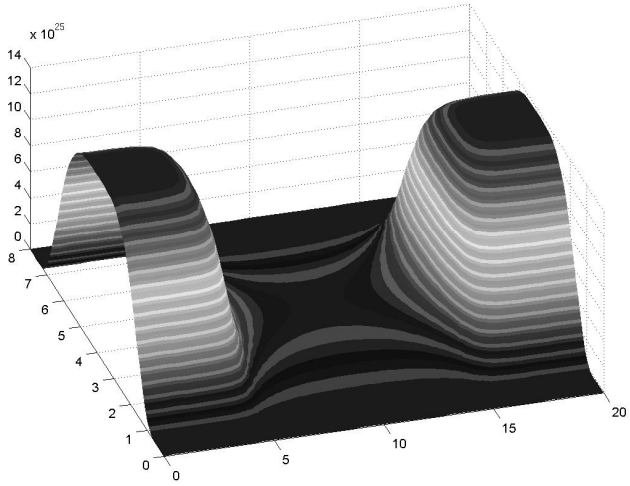

Fig. 4. Density at the equilibrium (m^{-3})

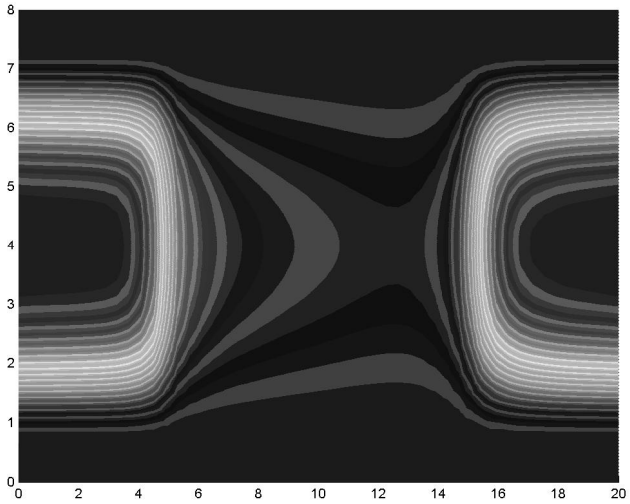

Fig. 5. Density of charge carriers for a applied drain-source voltage $V_{DS}=0.2V$ and for $V_{GS}=0V$

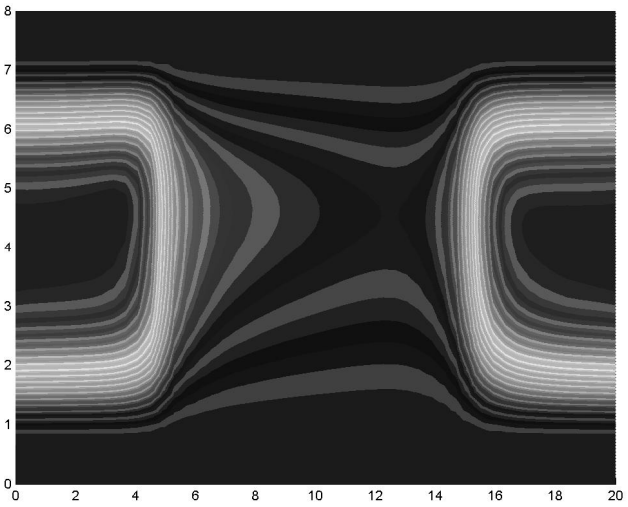

Fig. 6. Density of charge carriers for a applied drain-source voltage $V_{DS} = 0.2V$ and for $V_{GS} = 0.2V$

its coupling with a purely balistic model of Schrödinger type [3], [12].

ACKNOWLEDGMENT

The authors acknowledge support by the European IHP network No. RNT2 2001 349 entitled "Hyperbolic and kinetic equation : asymptotics, numerics, applications", by the ACI Nouvelles Interfaces des Mathématiques No. ACINIM 176-2004 entitled "MOQUA" and funded by the French ministry of research as well as the ACI Jeunes chercheurs no. JC1035 "Modèles dispersifs vectoriels pour le transport à l'échelle nanométrique".

References

[1] F. Balestra, S. Cristoloveanu, M. Benachir, J. Brini, T. Elewa, *Double-gate silicon-on-insulator transistor with volume inversion: A new device with greatly enhanced performance*, IEEE Electron Device Lett., vol. EDL-8, pp 410-412, Sept. 1987.

[2] N. Ben Abdallah, F. Méhats, N. Vauchelet, *Analysis of a Drift-Diffusion-Schrödinger-Poisson model*, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 1007-1012.

[3] N.Ben Abdallah, E. Polizzi, M. Mouis, F. Méhats, *Simulation of 2D quantum transport in ultrashort DG-Mosfets : a fast algorithm using subbands*, Proceedings of the SISPAD conference 2003, IEEE product TH8679-TBR, 267–270 (2003).

[4] F. Brezzi, L.D. Marini, P. Pietra, *Méthodes d'éléments finis mixtes et schéma de Scharfetter-Gummel*, C.R. Acad. Sci. Paris Sér. I, 305 (1987), 599-604.

[5] Ph. Caussignac, B. Zimmermann, R. Ferro, *Finite element approximation of electrostatic potential in one dimensional multilayer structures with quantized electronic charge*, Computing 45, (1990) 251-264.

[6] C. De Falco, E. Gatti, A. L. Lacaita and R. Sacco, *Quantum-corrected drift-diffusion models for transport in semiconductor devices*, to appear in J. Comp. Phys.

[7] P. Degond, F. Méhats, C. Ringhofer, *Quantum Energy-Transport and Drift-Diffusion models*, J. Stat. Phys. **118** (2005), no. 3-4, 625–665.

[8] S. Gallego, F. Méhats, *Numerical approximation of a quantum drift-diffusion model*, C. R. Acad. Sci. Paris, Ser. I **339** (2004), 519–524.

[9] H.K. Gummel, *A self-consistent iterative scheme for one-dimensional steady state transistor calculations*, IEEE Trans. on Elec Dev., 11 (10) 455, 1964.

[10] P. A. Markowich, C. A. Ringhofer, C. Schmeiser, *Semiconductor equations*, Springer-Verlag, Vienna, 1990.

[11] M. S. Mock, *Analysis of mathematical models of semiconductor devices*, Advances in Numerical Computation Series 3, Boole Press, 1983.

[12] C. Negulescu, N. Ben Abdallah, E. Polizzi, M. Mouis, *Simulation Schemes in 2D nanoscale MOSFETs: a WKB based method*, to appear in J. Comp. electronics special issue for the ICWE 10.

[13] F. Nier, *A stationary Schrödinger-Poisson system arising from the modelling of electronic devices*, Forum Math. **2** (1990), no. 5, 489–510.

[14] F.G. Pikus, K. Likharev, Appl. Phys. Lett. 71 (1997) 3661.

[15] A. Pirovano, A. Lacaita, A. Spinelli, *Two dimensional Quantum Effects in Nanoscale MOSFETs*, IEEE Trans. Electron. Dev. **49** (2002), no. 1, 25–31.

[16] E. Polizzi, N. Ben Abdallah, *Subband decomposition approach for the simulation of quantum electron transport in nanostructures*, J. Comp. Phys. 202 (2005) 150-180.

[17] K. Seeger, *Semiconductor Physics. An Introduction*, 6th edition, Springer, Berlin, 1997.

[18] S. Selberherr, *Analysis and Simulation of Semiconductors Devices*, Springer-Verlag, 1984.

[19] B. Vinter, C. Weisbuch, *Quantum Semiconductor Structures*, Academic Press, 1991.