Hybrid model for 2D quantum transport

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Introduction

Metal Oxide Semiconductor Field Effect Transistors have reached the scale of some nanometers per dimension.

Subband decomposition

At nanoscopic scale quantum phenomena become relevant and the energy levels become discrete, therefore the choice has been made of decomposing the probability density function into energy subbands.

Goal

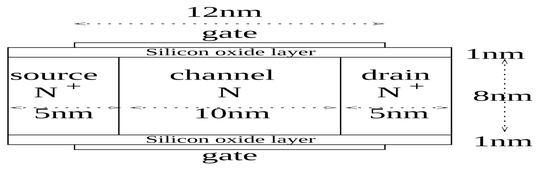
The goal of the project is the writing of subband models, the theoretical study of their well-posedness and their numerical simulation in 3D at both steady and transient states through microscopic or macroscopic models.

Here

Here a 2D simulation of two hybrid quantum-classical systems is shown : one is a steady-state macroscopic model and one is transient-state microscopic.

The device

The geometry of the device which is the object of our numerical study is drawn here :



The high doping is set $10^{20}\frac{1}{cm^3}$ while the low doping is set $10^{15}\frac{1}{cm^3}$. The built-in confining potential due to the SiO_2-layer is $3V$.

The model

Hybridity

• x-dimension is classical : electrons behave like ballistic particles, because 20 nm is large enough with respect to the Debye length

• z-dimension is quantum : particles behave like waves, because 8 nm is comparable with the Debye length.

Building blocks

Two main blocks are needed :

• the z-dimension uses the Schrödinger-Poisson equation for the subband decomposition (each eigenvalue and eigenfunction corresponds to an energy level) ; dimensions are coupled through Poisson equation :

$$-\frac{d}{dz}\left[\frac{1}{m_*(z)}\frac{d\chi^p}{dz}\right] - q(V+V_c)\chi^p = \epsilon^p\chi^p$$
$$-div_{x,z}\left[\varepsilon_R(x,z)\nabla_{x,z}V\right] = \frac{q}{\varepsilon_0}\left[N[V]-N_D\right].$$

• the x-dimension describes the motion of particles driven by the force field and subjected to collisions. Two possibilities :

– Drift-Diffusion, therefore an integration on the macroscopic variable $N_s(x)$ representing the surface density

$$-\mathrm{div}_x\left[\mathbb{D}\left(\nabla_x N_s(x) + \frac{1}{k_BT_L}N_s(x)\nabla_x U_s(x)\right)\right] = 0,$$

where $\mathbb{D} = \mu k_BT_L$ denotes the diffusion coefficient and U_s is the effective energy

$$U_s = -k_BT_L\log\left(\sum_p e^{-\frac{\epsilon_p}{k_BT_L}}\right).$$

– Boltzmann Transport Equation, therefore a microscopic description :

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\nabla_x\epsilon_p^{kin}\cdot\nabla_k f_p - \frac{1}{\hbar}\nabla_k\epsilon_p^{pot}\cdot\nabla_x f_p = Q_p[f_p].$$

For the scope of this work, we have used the simplest linear BGK approximation, a relaxation time operator (only intra-band scattering, not inter-band) :

$$Q_p[f_p] = \frac{1}{\tau}\left[\mathcal{M}(k)\rho_p - f_p(k)\right],$$

where τ is the relaxation time (given by the mobility μ through the relation $\tau = \frac{m_*\mu}{q}$), $\mathcal{M}_p(k)$ is the Maxwellian

$$\mathcal{M}_p(k) = \frac{\hbar^2|k|^2}{2\pi k_BT_Lm_*},$$

$\hbar$ the reduced Planck constant, k_B the Boltzmann constant, T_L the lattice temperature and m_* the effective mass.

Numerics for the BTE

Time discretization

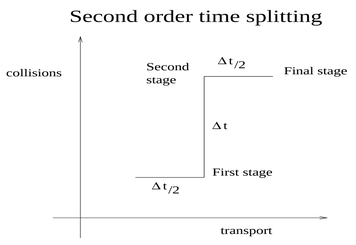
The time step Δt is fixed and the BTE is integrate in the slotboom variable $g_p(t,x,k)$ defined by

$$f_p(t,x,k) = g_p(t,x,k)\exp\left(-\frac{\epsilon_p[V](x)}{k_BT_L} - \frac{\hbar^2|k|^2}{2k_BT_Lm_*}\right)$$

(instead of the original $f_p(t,x,k)$) through a time splitting technique, allowing to solve for separate the transport part and the collision part

$$(\mathrm{tp}) : \frac{\partial g_p}{\partial t} + \frac{1}{\hbar}\nabla_x\epsilon_p^{kin}\cdot\nabla_k g_p - \frac{1}{\hbar}\nabla_k\epsilon_p^{pot}\cdot\nabla_x g_p - \frac{\partial\epsilon_p^{pot}}{\partial t}g_p = 0$$
$$(\mathrm{cp}) : \frac{\partial g_p}{\partial t} = \frac{1}{\tau}\left[\frac{\hbar^2}{2\pi k_BT_Lm_*}\int_{\mathbb{R}^2} g_p(k')\exp\left(-\frac{\hbar^2|k'|^2}{2k_BT_Lm_*}\right) - g_p(k)\right]$$

and then recombine them through a second order scheme which consists of three steps. The same technique also applies inside the transport part.



Border conditions

For the entering particles we impose inflow/outflow conditions, or Neumann for the outgoing ones : for instance at source contact we have

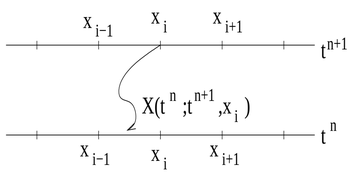
$$f_p^n(-x,k) = \frac{\rho_p^{eq}(0)}{\rho_p^n(0)}f_p^n(0,k) \quad \text{if } k_1 > 0$$
$$f_p^n(-x,k) = f_p^n(0,k) \text{ otherwise.}$$

Advection blocks

The advection stages are solved via characteristics, either using a pure semi-lagrangian scheme or a conservative scheme.

• Pure semi-lagrangian : just interpolate

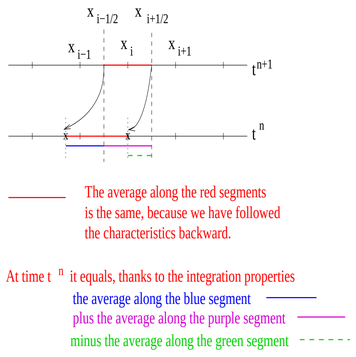
$$f(t^{n+1},x_i) = f(t^n, X(t^n;t^{n+1},x_i)).$$



This method is quite easy to implement, has a good control of spurious oscillations but the drawback is that it does not conserve mass.

• The conservative method is called Flux Balance Method :

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(t^{n+1},\xi)d\xi = \int_{x_{i-1/2}}^{x_{i+1/2}} f(t^n,\xi)d\xi + \frac{\Phi(t^n,x_{i-1/2}) - \Phi(t^n,x_{i+1/2})}{\Delta x}$$



Its drawback is that it does not avoid spurious oscillations as well as the SL.

Collision operator

The solution of a relaxation time collision operator is explicit.

Numerics for the SP block

The Schrödinger equation

The Schrödinger equation is approximated via standard finite differences, then the matrix is diagonalized by means of a LAPACK routine called DSTEQR. The equation being solved in H_0^1, so $\chi^p(z=0) = \chi^p(z=l_z) = 0$.

The Poisson equation

We need to solve 1D and 2D Poisson equation like

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right] + C\int\mathcal{A}(\zeta)V(\zeta)d\zeta = \mathcal{B}.$$

The Laplacian is approximated via finite differences, the integration via trapezoids and the linear system solved by means of a LAPACK routine called DGESV. At boundaries, Robin conditions are taken at contacts, Dirichlet at gates and homogeneous Neumann elsewhere.

The Newton iteration

Newton schemes are used to minimize functionals

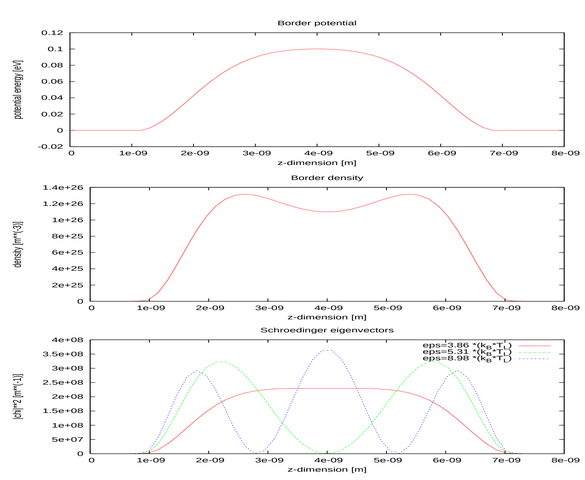
$$P[V] = -\mathrm{div}\left[\varepsilon_R\nabla V\right] - \frac{q}{\varepsilon_0}\left[N[V]-N_D\right].$$

• Technical point : the computation of the Gâteaux derivative of the functional, especially of the density $N[V]$ with respect to the potential.

Initial conditions : border potential

First of all we solve a 1D Schrödinger-Poisson problem for the border potential, because we need to compute the border configuration respecting the electrical neutrality conditions :

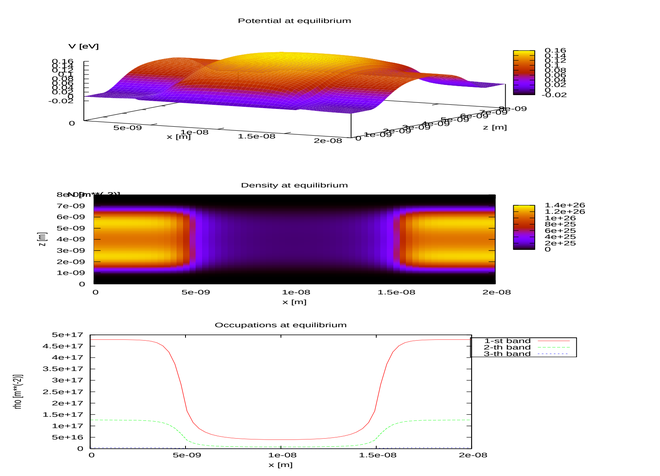
$$-\frac{d}{dz}\left[\frac{1}{m_*(z)}\frac{dV_b}{dz}\right] = \frac{q}{\varepsilon_0}\left[N[V_b]-N_D\right]$$
$$N[V_b] = \frac{\int N_D(\zeta)d\zeta}{\sum_q e^{-\epsilon_q[V_b]}}e^{-\epsilon_p[V_b]}|\chi_p(z)|^2.$$



Initial conditions : equilibrium state

In order to initialize the transient-state solver, we have first of all to compute a thermodynamical equilibrium for the system, which is already quite a complete problem. This is realized through solving a 2D Schrdinger-Poisson problem

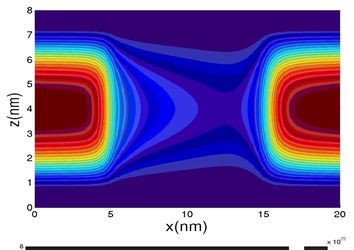
$$-\mathrm{div}_{x,z}\left[\frac{1}{m_*}\nabla_{x,z}V_{eq}\right] = \frac{q}{\varepsilon_0}\left[N[V_{eq}]-N_D\right]$$
$$N[V_{eq}] = \frac{\int N_D(0,\zeta)d\zeta}{\sum_q e^{-\epsilon_q[V_b]}}e^{-\epsilon_p[V_{eq}](x)}|\chi_p(x,z)|^2.$$



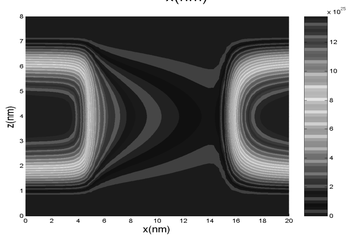
Long time behavior

We present here the stationary state computed by the drift-diffusion code.

Here we have the stationary state for an applied drain-source voltage of $V_{DS} = 0.2V$.



Here we have the stationary state for an applied drain-source voltage of $V_{DS} = 0.5V$.



Acknowledgments

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Références

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