Self-consistent Monte Carlo Solution of Wigner and Poisson Equations Using an Efficient Multigrid Approach

Majid Benam[1(✉)], Maciej Wołoszyn[2], and Siegfried Selberherr[1]

[1] Institute for Microelectronics, TU Wien, Gußhausstraße 27, 1040 Vienna, Austria
{benam,selberherr}@iue.tuwien.ac.at
[2] Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Krakow, Poland
woloszyn@agh.edu.pl

Abstract. An accurate self-consistent solution of the coupled Wigner and Poisson equations is of high importance in the analysis of semiconductor devices. The proposed solver has two main components: a Wigner equation solver which treats the Wigner potential as a generating mechanism and is responsible for the generation and annihilation of signed particles used in the Monte Carlo method, and a Poisson equation solver which uses an efficient multigrid approach to take the electron distribution into account, and update the value of the potential in each time step. Results for the electron distribution, the electrostatic potential, and the electrostatic force calculated as the gradient of the potential energy are presented for a Cartesian xy-region which is not charged by any external doping or other sources of fixed charge in the beginning of the simulation. However, wavepackets representing electrons are constantly injected from one edge every femtosecond. Comparing the electron distribution in two cases, namely, obtained without taking the Poisson equation into account and with self-consistently solving the Poisson equation with the Wigner equation, demonstrates the repulsion of the injected wavepackets in the latter using the vector visualization of the force.

1 Introduction

Although some level of understanding can be achieved by considering independent carriers while analyzing nano-scale transport, a more accurate description requires the use of self-consistent models, where carrier-carrier interactions are also taken into account [1].

In this work, the Poisson equation is self-consistently solved with the Wigner equation. The solver provides the possibility of calculating physical quantities such as carrier concentration and current. Initial and boundary conditions are carefully analyzed so that a consistent and compatible set is used in order to obtain accurate and reliable results. There is also the option to select a position-dependent relative permittivity in the Poisson equation, which enables the simulation of devices consisting of materials with different properties.

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A simulation using the self-consistent solver starts with an initialization step in which geometrical aspects and physical quantities such as initial concentration and potential are given by input files or external functions, see Fig. 1. Some additional simulation parameters as well as the boundary conditions are set and the properties of the particles to be injected in the region are decided. The particles are then injected through the use of an injection zone at the bottom of the actual region. The Wigner potential is calculated, which in turn determines the statistics of the generation mechanisms in the actual time step. The Poisson equation solver is then called with the obtained value of the carrier concentration in order to update the value of the electrostatic potential for the next time step.

A charge redistribution scheme is used after the Poisson solution step to map charges among the neighboring cells in a more efficient way for the next iteration. The evolution of the particles is then performed using the signed-particle Monte Carlo approach, explained in Sect. 2. This loop is repeated at each time step.

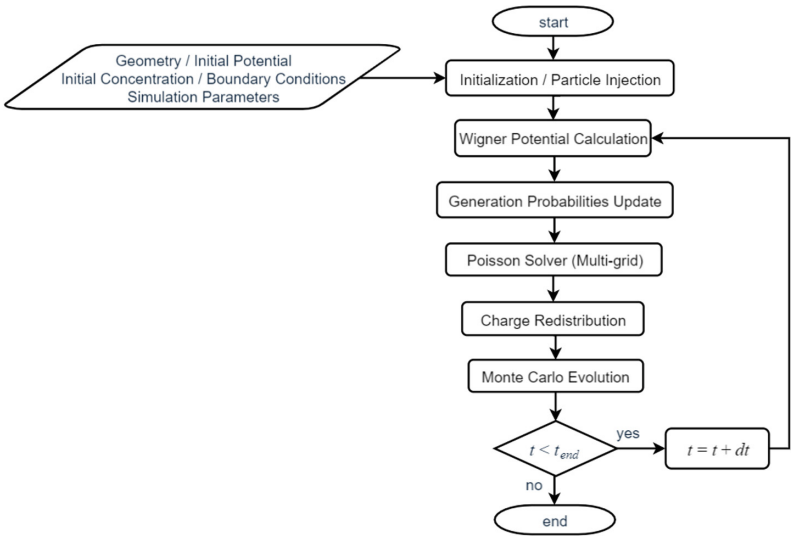

Fig. 1. Flowchart for the self-consistent solution of Poisson and Wigner equations

The solver for the Poisson equation, presented in more details in Sect. 3, receives the updated value of the carrier distribution in each time step and utilizes a multigrid approach to compute the updated value of the electrostatic potential, which is then used to calculate the new Wigner potential, and hence the new statistics for the generation of new pairs of particles [2].

2 Wigner Monte Carlo Solver

For an accurate description of carrier transport processes in nanometer sized electronic devices, the effects of quantum mechanics have to be taken into account [3]. In order to maintain the closest resemblence to the classical concepts, the Wigner formalism presents a well-established choice as it bridges the gap between purely quantum (ballistic) evolution and the classical (diffusive) transport by the relatively convenient use of functions and variables defined in the phase space.

The Wigner equation, which is the governing equation in the Wigner formalism, is written in the semi-discrete form as:

$$\left(\frac{\partial}{\partial t} + \frac{\hbar \mathbf{q} \Delta k}{m^*} \nabla_{\mathbf{r}}\right) f_w(\mathbf{r}, \mathbf{q}, t) = \sum_{\mathbf{q}} V_W(\mathbf{r}, \mathbf{q} - \mathbf{q}') f_w(\mathbf{r}, \mathbf{q}', t), \tag{1}$$

where $\mathbf{r}$ and $\mathbf{q}\Delta k$ are the discrete vectors for position and momentum, respectively, and f_w is the Wigner function. The semi-discrete Wigner potential, which appears on the RHS of Eq. (1) and plays a central role in the signed-particle method as it dictates the particle generation statistics, is defined as:

$$V_W(\mathbf{r}, \mathbf{q}) \equiv \frac{1}{i\hbar \mathbf{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} d\mathbf{s} e^{-i\mathbf{q}\Delta k.\mathbf{s}} \left[V(\mathbf{r} + \frac{\mathbf{s}}{2}) - V(\mathbf{r} - \frac{\mathbf{s}}{2})\right] \tag{2}$$

Interpreting the Wigner Potential in the semi-discrete form as a generation mechanism, from each original particle, two additional particles can be created with wavevector $\pm k_0$ and signs ± 1, through an algorithm to propagate numerical particles along trajectories and scatter them to different wavevectors [4].

The Monte Carlo procedure in Fig. 1 consists of evolution and annihilation steps. In the evolution step, classical drift and consecutive generation/scattering processes are repeated iteratively for all particles in the (growing) ensemble, until the end of the time-step is reached. However, since all the particles within a given cell of the phase space have the same probabilistic future and thus contribute in a similar fashion in the averaging process used to calculate physical quantities, two particles of opposite sign within a cell cancel out (annihilate) each other and cease to exist. Therefore the annihilation step is utilized to control the particle ensemble growth.

3 Poisson Equation Solver (Multigrid Approach)

Starting from the differential form of Gauss's law, $\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon}$ and using $\mathbf{E} = -\nabla V$, we obtain:

$$\nabla \cdot \mathbf{E} = -\nabla \cdot (\nabla V) = -\nabla^2 V, \tag{3}$$

where $\mathbf{E}$ and V are the electric field vector and the scalar electrostatic potential, respectively. Following from Eq. (3), in a homogeneous dielectric domain, the Poisson equation can be written in its general form in three dimensions as:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon}, \tag{4}$$

with ρ being the space charge density:

$$\rho = q(p - n + C),$$

where q is the elementary charge of an electron, p and n are the hole and electron concentrations, respectively, and C is the concentration of additional fixed charges. Note that in Eq. (4), $\epsilon = \epsilon_r \epsilon_0$, where ϵ_r is the relative permittivity (dielectric) for the material, and it is considered to be constant ($\epsilon_r = \epsilon_{\mathrm{Si}} = 11.7$) in the simulations discussed in this paper. However, the Poisson equation solver can treat also a position-dependent ϵ_r to model materials with different properties.

The Poisson equation accounts for Coulomb carrier-carrier interactions and therefore has to be frequently solved during the simulation in order to properly model the electric field driving the carriers. There are many ways to numerically solve this equation, ranging from direct methods like Gaussian elimination to iterative ones, such as the Jacobi, Gauss-Seidel, or successive over-relaxation method (SOR). The method utilized in this paper is a matrix method known as Multigrid (MG).

After pre-smoothing Gauss-Seidel iteration steps, a fine-to-coarse relaxation process is used to initialize the correction potential on a coarser grid. As illustrated in the example in Fig. 2, from all the nodes on the initial fine grid on the left, a coarser mesh (only the blue dots) are chosen in the first round, and then an even coarser grid (only the red dots), and so on. For the prolongation scheme, however, a coarse-to-fine approach is used to transfer the calculated error from a coarser grid to the corresponding finer grid using interpolation [5].

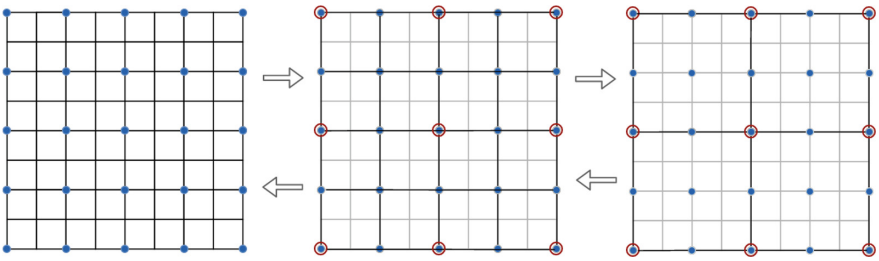

Fig. 2. Multigrid fine-to-coarse relaxation (left to right) and coarse-to-fine prolongation (right to left) schemes

The criteria for convergence is that on all the nodes in the initial fine grid, the absolute value of the potential update is smaller than a selected threshold value.

4 Boundary Conditions

Boundary conditions are of crucial importance whenever solving a partial differential equation. In the case of incorporating a Poisson equation solver into our main Wigner Ensemble Monte Carlo (WEMC) approach, we must make sure that the boundary conditions for both equations are compatible and consistent.

For the Wigner equation solver we can basically assign *absorbing* or *reflecting* boundary conditions to any of the edges of the simulation domain. Referring to a boundary as *absorbing* means it is reflection-less and all particles leave and cease to exist at the boundary, which does not influence the evolution of the particles and corresponds to a Neumann boundary condition for the Poisson equation. A *reflecting* boundary, on the other hand, represents the case where the particles are reflected from the boundary, and no particles are injected from the boundary, which approximates it to an infinite potential step. Such a boundary, which corresponds to a Dirichlet boundary condition in the Poisson equation, is useful to approximate interfaces between semiconductors and oxide, where the wavefunction rapidly decays towards zero [4].

The self-consistent solver provides the option to incorporate any combination of Dirichlet (a boundary condition on the potential) and Neumann (a boundary condition on the derivative of the potential, i.e. the electric field) conditions on each side of the simulation domain, provided that there is at least one segment with a Dirichlet boundary condition specified on it.

5 Results

In this section the results of the simulations for two scenarios are presented, namely without solving the Poisson equation, and with self-consistently solving the Poisson equation with the Wigner equation. The results are obtained for a Cartesian xy-region of 64 nm $\times$64 nm, where the x and y dimensions are of numerical importance and all physical quantities remain constant in z-direction, and it basically contributes only in calculating the cell volume and the carrier concentration. It is important to note that the simulation region is very small, and even small values of charge result in high values of density on the RHS of Poisson equation.

The simulation region is not charged by any external doping or other sources of fixed charge in the beginning of the simulation. However, wavepackets representing electrons are constantly injected into the region every femtosecond. The wavepackets are distributed in a Gaussian shape in space, but all have the same initial momentum. The x-component of momentum is set to zero in order to make the analysis of the spreading of particles more straightforward. Each wavepacket represents one electron and thus carries the charge $-e$, where e is the elementary charge.

The top and bottom boundary conditions are set to “reflecting” in the Wigner equation which is compatible with the zero Dirichlet boundary condition in the Poisson equation. The left and right boundaries are set to “absorbing”, which corresponds to a Neumann boundary condition in the Poisson equation.

As illustrated in Fig. 3, when the Poisson equation is not solved and the initial potential is not updated, the injected particles do not repulse each other and continue their evolution with their initial momentum. Without solving the Poisson equation, the initial potential is zero, and as it is not updated, the electrostatic potential and the electric field remain zero throughout the whole simulation.

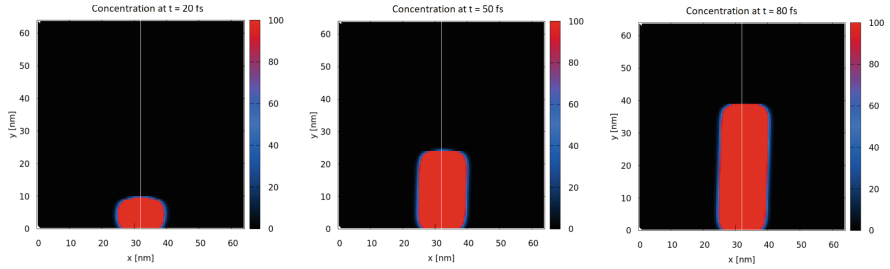

Fig. 3. The electron distribution (in $10^{19} \times \mathrm{m}^{-3}$) for three different time steps ($t = 20\,\mathrm{fs}$ left, $t = 50\,\mathrm{fs}$ middle, $t = 80\,\mathrm{fs}$ right) without solving the Poisson equation

However, when the Poisson equation is solved in each time step, see Fig. 4, the electron concentration and thus the potential values are updated and the expected repulsion between the particles occurs. The spreading increases as more particles are injected into the region and the repulsive forces between particles become more dominant.

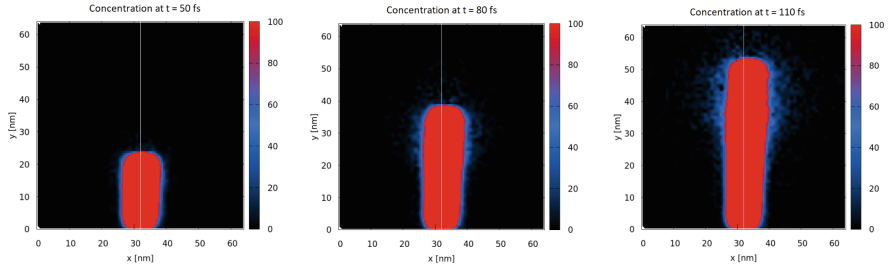

Fig. 4. The electron distribution (in $10^{19} \times \mathrm{m}^{-3}$) for three different time steps ($t = 50\,\mathrm{fs}$ left, $t = 80\,\mathrm{fs}$ middle, $t = 110\,\mathrm{fs}$ right) with solving the Poisson equation every femtosecond

The corresponding results for the electrostatic potential are shown in Fig. 5:

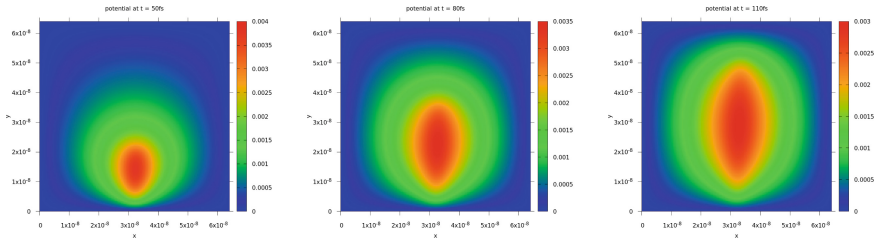

Fig. 5. The potential values (in eV) for three different time steps ($t = 50\,\text{fs}$ left, $t = 80\,\text{fs}$ middle, $t = 110\,\text{fs}$ right)

The corresponding values for the force are shown in Fig. 6:

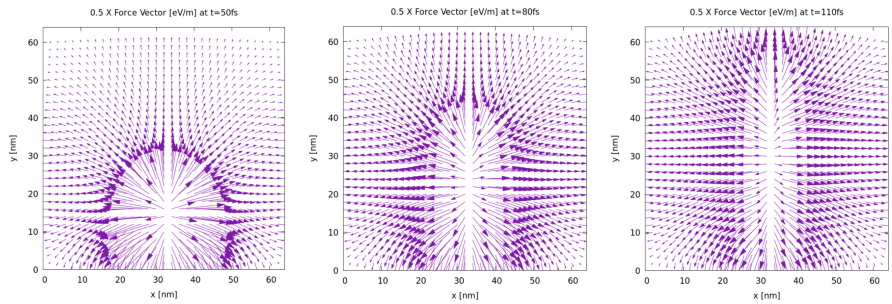

Fig. 6. The force vector field for three different time steps ($t = 50\,\text{fs}$ left, $t = 80\,\text{fs}$ middle, $t = 110\,\text{fs}$ right). For better visualization purposes, the force vectors are half the actual size in $\frac{\text{eV}}{\text{m}}$.

The general shape of the electrostatic potential remains the same, as the particles are mainly accumulated in the central line. In each time step, the distribution of the electrons changes due to the injection of the new wavepackets and also the interactions between the already present particles. The ensemble of particles moves from bottom to top, and similarly evolves the electrostatic potential and the resulting force vector. The particles reflected from the top and bottom boundaries also contribute in the calculation of the electrostatic potential.

6 Conclusion

A self-consistent solution of the coupled Wigner and Poisson equation has been presented. A multigrid approach is used to solve the Poisson equation, which

results in an updated value of the electrostatic potential, and hence new particle generation statistics in each time step. Results for the electron distribution, the electrostatic potential, and the electrostatic force were illustrated for a Cartesian xy-region. Comparing the electron distribution, when the Poisson equation is solved and when it is not solved, shows the expected repulsion of the injected wavepackets (representing particles) in the former case.

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