Electron-hole transport in semiconductors: stochastic dynamics simulation

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Abstract. A random walk based stochastic simulation algorithm for solving a nonlinear system of transient drift-diffusion-Poisson equations for semiconductors with random doping profile is developed. The method is then applied to simulate and analyze the stochastic dynamics of the transport of electrons and holes in doped semiconductor material. This analysis has a theoretical but also a practical interest since an addition even of a small concentration of foreign atoms to the regular semiconductor material produces dramatic changes in the electrical properties. The nonlinear drift-diffusion-Poisson system is solved by the iteration procedure including alternating simulation of the drift-diffusion processes and solving the Poisson equation. Here, we extend the iteration algorithm to solve the drift-diffusion-Poisson system with additional term governing the random inputs in the system like the stochastic doping, random distribution of quantum dots, and an irregular family of defects. Impact of these random entries on the stochastic dynamics of the drift velocity and electron and hole concentrations is studied.

1. Introduction

Semiconductors and devices based on them are ubiquitous in every aspect of modern life. Electronic devices such as diodes, bipolar junction transistors, and field effect transistors drive modern electronic technology. Optoelectronic devices such as laser diodes, modulators, and detectors drive the optical networks [1]. To improve electronic and optoelectronic devices a deep study of the physical properties of semiconductors is needed. Mathematical modeling supports the physical experiments and contribute to modern device development.

The one of the basic approach for modeling electron-hole transport in semiconductors is the drift-diffusion-Poisson model [2] which was first presented by Van Roosbroeck in the year 1950 [3]. Monte Carlo methods are applied to solve the drift-diffusion-Poisson equations [1]. Monte Carlo approach was employed for simulation of transport in semiconductors by Kurosawa [5] in 1966. The transport problems are statistical in nature. Stochastic simulation methods allow to include in the model a randomness, such as, a noise, fluctuations in the coefficients and space inhomogeneity.

The drift-diffusion-Poisson system includes two drift-diffusion equations for electrons and holes coupled with a Poisson equation for the potential whose gradient forms the drift velocity. Standard approach to solve the drift-diffusion equation for a given point is the random walk on spheres [6] or on parallelepipeds methods [7]. To calculate the solution of the drift-diffusion-
Poisson system we need to compute solutions of the drift-diffusion equations for all points of the domain. For this purpose, we employ the discrete random walks implemented in the form of a cellular automaton (CA) algorithm described in [8]. The drift velocity is computed as the derivatives of the solution to Poisson equation calculated by Sabelfeld’s global random walk algorithm [9, 10, 11]. Thus, we use a hybrid Monte Carlo method with CA algorithm for solving the drift-diffusion-Poisson system. The drift-diffusion-Poisson equations are nonlinear where the right-hand side of the Poisson equation depends on the difference between electrons and holes concentrations, which, in its turn, depends on the drift velocity. Thus, the nonlinear drift-diffusion-Poisson system is solved by an iteration procedure including alternating simulation of the drift-diffusion and calculating the derivatives of the solution to Poisson equation. This iteration procedure is given in our recent paper [11]. In the present paper we introduce in the model doping impurities distributed at random in the semiconductor’s volume. The impurities influence the drift velocity. Thus, to simulate the doping corresponding changes are introduced to the right-hand side of the Poisson equation. Impact of the randomly allocated impurities on the dynamics of carrier distribution is studied.

The paper is organized as follows. In Section 2 the drift-diffusion-Poisson system describing the electron-hole transport in a semiconductor is given. In Section 3 a hybrid Monte Carlo and CA algorithm for solving the drift-diffusion-Poisson system is described. Section 4 presents the results of simulation of the transport of electrons and holes in the doped semiconductor.

2. Drift-diffusion-Poisson system

The drift-diffusion-Poisson system modeling the transport of the electrons and holes in semiconductors is given in the following form [2]:

\[
\frac{\partial n(r, t)}{\partial t} = \text{div}[D_n \nabla n(r, t) + n \nabla \psi(r, t)] + F_n(r, t) - R(n, p, r),
\]

\[
\frac{\partial p(r, t)}{\partial t} = \text{div}[D_p \nabla p(r, t) - p \nabla \psi(r, t)] + F_p(r, t) - R(n, p, r),
\]

\[
\Delta \psi(r, t) = -[n(r, t) - p(r, t) - C(r)].
\]

Here, \( r \) is a particle coordinate, \( t \) is a time, \( n(r, t) \) is a spatial distribution at time \( t \) of the electrons, negatively charged, and \( p(r, t) \) is a spatial distribution of the holes, positively charged. \( F_n(r, t) \) and \( F_p(r, t) \) are sources generating electrons and holes, respectively. \( R(n, p, r) \) is a function of electron-hole recombination. Here, we consider the case without the recombination, i.e. \( R(n, p, r) = 0 \). The function \( \psi(r, t) \) is a self-consistent electrostatic potential produced by the electrons and holes and by the doping profile \( C(r) \) of the semiconductor device.

The drift velocity is calculated as \( v(r, t) = \nabla \psi(r, t) \).

This system of equations is solved in a two-dimensional domain \( V \) with Dirichlet boundary conditions: for the electron and hole concentrations \( n|_\Gamma = 0, p|_\Gamma = 0 \), and for the Poisson equation \( \psi|_\Gamma = 0 \), and initial conditions \( n(r, 0) = n_0(r), p(r, 0) = p_0(r) \).

The drift-diffusion-Poisson system is solved by the hybrid Monte Carlo method with CA algorithm.

3. A hybrid Monte Carlo and cellular automata algorithm for solving the drift-diffusion-Poisson system

3.1. Cellular automata algorithm of simulation of the electron-hole drift and diffusion

The drift and diffusion of electrons and holes is simulated by the multi-particle CA algorithm described in [8]. CA is a discrete model consisting of a regular grid of cells [12]. Each cell has a state, which represents a simulated object. The states are changed according to rules imitating
rules of a simulated phenomenon. Time is discrete and consists of steps. For synchronous CA on each step all cell states are updated simultaneously. The algorithm implements actually a finite-difference approximation of the drift-diffusion equations.

The CA given in [8] simulates the motion of particles on a regular two-dimensional lattice. Cell states \( s \in \mathbb{N} \) are the number of particles in each cell. On each time step each particle in a cell can jump to the one of the four neighbor cells (left, right, up, and down) with a certain probability, or stay in the cell. The probabilities of jumping are calculated depending on the diffusion coefficients \( D_x, D_y \) and drift velocities \( V_x, V_y \) for horizontal and vertical directions:

\[
\begin{align*}
P_x &= \frac{\tau \cdot D_x}{h^2} + \frac{\tau \cdot v_x}{2h}, \\
P_y &= \frac{\tau \cdot D_y}{h^2} + \frac{\tau \cdot v_y}{2h}, \\
Q_x &= \frac{\tau \cdot D_x}{h^2} - \frac{\tau \cdot v_x}{2h}, \\
Q_y &= \frac{\tau \cdot D_y}{h^2} - \frac{\tau \cdot v_y}{2h},
\end{align*}
\]

where \( P_x \) and \( Q_x \) are probabilities that a particle jumps to the right and left neighbor cell, and \( P_y \) and \( Q_y \) are the probabilities that the particle jumps to the top and bottom neighbor cells, respectively, \( h \) is the size of the cell, and \( \tau \) is the time step. The time step should satisfy the Courant condition: \( \tau < \tau_c \), where \( \tau_c = \frac{h^2}{2 \max(D_x, D_y)} \).

Let us describe the algorithm of calculation of the particle concentration in all lattice cells based on this algorithm.

(i) On each time step \( t \), for all cells \((x, y)\) of the grid, for each particle in the cell \((x, y)\) one of five possible events is selected:

- With probability \( P_x \), the particle jumps to the right neighbor cell \((x+1, y)\), the number of particles in the cell \((x, y)\): \( N((x, y), t) = N((x, y), t) - 1 \) and the number of particles in the cell \((x+1, y)\): \( N((x+1, y), t) = N((x+1, y), t) + 1 \).
- With probability \( Q_x \), the particle jumps to the left neighbor cell \((x-1, y)\): \( N((x, y), t) = N((x, y), t) - 1, N((x-1, y), t) = N((x-1, y), t) + 1 \).
- With probability \( P_y \), the particle jumps to the top neighbor cell \((x, y+1)\): \( N((x, y), t) = N((x, y), t) - 1, N((x, y+1), t) = N((x, y+1), t) + 1 \).
- With probability \( Q_y \), the particle jumps to the bottom neighbor cell \((x, y-1)\): \( N((x, y), t) = N((x, y), t) - 1, N((x, y-1), t) = N((x, y-1), t) + 1 \).
- With probability \( 1 - P_x - Q_x - P_y - Q_y \), the particle remains in the current cell \((x, y)\), i.e., the number of particles in the cell \((x, y)\) does not change.

(ii) If any of the neighbor cells, \((x-1, y), (x+1, y), (x+1, y), (x+1, y+1)\), belongs to the boundary of the domain, then the particle that jumped into this cell disappears.

Thus, on each time step \( t \), we obtain the number of particles in each cell \( N((x, y), t) \). The particle concentration in each cell is computed by the formula: \( \rho((x, y), t) = N((x, y), t)/(h^2 \cdot N(0)) \), where \( N(0) \) is the total number of particles generated at the initial time.

The correctness of the CA algorithm has shown in [11] by comparison of the simulation results with the exact solution.

This CA algorithm is applied for simulation of the diffusion with drift of electrons and holes. Two different cell grids are employed for electrons and holes, and their concentrations are computed independently. The electron concentration in each cell is computed by the formula: \( n((x, y), t) = N_e((x, y), t)/(h^2 \cdot N(0)) \), where \( N_e((x, y), t) \) is the number of electrons in the cell \((x, y)\) at time \( t \), \( N(0) \) is the total number of electrons and holes generated at the initial time. Analogously, the hole concentration is computed as \( p((x, y), t) = N_p((x, y), t)/(h^2 \cdot N(0)) \).

To compute the electron-hole concentration in each cell of the grid the drift velocity values in these cells are needed. The drift velocity is a gradient of the solution to Poisson equation (4).
Sabelfeld’s global random walk method [10] allows to calculate the solution of the Poisson equation and its derivatives in a set of points at once.

3.2. The global Monte Carlo algorithm for the drift velocity calculation

The global random walk algorithm and a detailed derivation of the formulae are presented in [10]. Here, we give a brief description of the algorithm.

Let us consider the Poisson equation in a bounded domain $V$:

$$\Delta \psi (r) = -f(r), \quad r \in V, \quad (5)$$

with zero Dirichlet boundary conditions $\psi (r^*) = 0, \quad r^* \in \Gamma$.

Let us denote the arrays for the derivatives with respect to $x$ and $y$ by $v_x$ and $v_y$, respectively. The array sizes $\text{Size}$ coincide with the sizes of arrays for electron and hole concentrations. At the beginning, $v_x(r_i) = 0$, and $v_y(r_i) = 0$ for all grid cells.

According to [11], the algorithm of calculation of the drift velocity for all grid cells $r_i = (x_i, y_i), \; i = 1, \ldots, \text{Size}$, is as follows.

(i) Simulate a random point of exit of a particle from the point $\xi = (x_\xi, y_\xi)$ of the grid from the uniform distribution $\pi(r)$.

(ii) Simulate a random point of exit of a particle from the point $\xi$ to the boundary $\Gamma$. The exit point is simulated by the random walk on spheres (here, on circles) algorithm described in detail in [6]. Record the exit point $r^* = (x^*, y^*)$.

(iii) Calculate the random estimators for the partial derivatives with respect to $x$ and $y$ by the following formulae:

$$\frac{\partial \psi}{\partial x}(r_i) = \frac{f(\xi)}{\pi(\xi)} \left[ \frac{x_i - x^*}{|r_i - r^*|^2} - \frac{x_i - x_\xi}{|r_i - \xi|^2} \right], \quad i = 1, \ldots, \text{Size},$$

$$\frac{\partial \psi}{\partial y}(r_i) = \frac{f(\xi)}{\pi(\xi)} \left[ \frac{y_i - y^*}{|r_i - r^*|^2} - \frac{y_i - y_\xi}{|r_i - \xi|^2} \right], \quad i = 1, \ldots, \text{Size}. \quad (6)$$

Add the calculated values to the arrays $v_x$ and $v_y$.

(iv) Go to Step (i), and start the next random trajectory.

(v) Do the steps (ii)-(iv) $K$ times.

(vi) The derivatives $\psi_x(r_i)$ and $\psi_y(r_i)$ are calculated as averages over $K$ trajectories:

$$\psi_x(r_i) \approx v_x(r_i)/K, \quad \psi_y(r_i) \approx v_y(r_i)/K. \quad (7)$$

The correctness of the global random walk algorithm is shown in [11] by a comparison of the simulation results with the exact solution for a test task.

For the case of doped semiconductor, which is under study in this paper, the Poisson equation has the following right-hand side: $f(r,t) = -[n(r,t) - p(r,t) - C(r)]$, where $n(r,t)$ and $p(r,t)$ are the concentrations of electrons and holes in the cell $r$ at time $t$, obtained by the CA algorithm 3.1. The function $C(r)$ is a doping profile of the semiconductor.

3.3. Iterative algorithm for solving the drift-diffusion-Poisson system

The drift-diffusion-Poisson equations are nonlinear. To compute the electron and hole concentrations we need to calculate drift velocity values, which, in its turn, depend on the difference between the concentrations of electrons and holes. To solve the nonlinear system ([1]–[3]), we employ the following iterative procedure consisting of two steps:

(i) calculation of the electron $n(r,t)$ and hole $p(r,t)$ concentrations by the CA algorithm 3.1.
(ii) calculation of the drift velocity as derivatives with respect to $x$ and $y$ of the solution to Poisson equation by the global random walk algorithm 3.2.

In more detail, the iterative procedure is described as follows.

We employ a regular 2D grid presenting the domain in a discrete form.

(i) Generate the initial distribution of electrons $n(r,0)$ and holes $p(r,0)$ on the grid according to the given initial conditions.

Set a number of the iteration to $1$: $i = 1$.

(ii) Calculate the drift velocity values along $x$: $v_x(r, i)$, and $y$: $v_y(r, i)$, in each grid cell by the global random walk on circles algorithm 3.2 for the Poisson equation with the right-hand side $f(r, i) = -[n(r, i - 1) - p(r, i - 1) - C(r)]$.

(iii) For the computed velocity values $v_x(r, i)$ and $v_y(r, i)$ calculate the new values of the electrons and holes concentrations $n(r, i)$ and $p(r, i)$ in the each grid cell using the CA algorithm 3.1.

(iv) Increase the number of the iteration by $1$: $i = i + 1$.

(v) Calculate the current time $t = \tau \cdot i$, where $\tau$ is the time of a single iteration.

(vi) If the current time $t$ is greater than the desired time $T$, stop the simulation process.

(vii) If $t < T$, continue from Step (ii).

4. Results of simulation of the electron-hole transport in a doped semiconductor

To decrease the calculation time a parallel implementation of the iterative algorithm for solving the drift-diffusion-Poisson system is implemented, based on [13]. The calculations are performed on the “NKS-30T” cluster of the Siberian Supercomputer Center of the Siberian Branch of the Russian Academy of Sciences.

Let us consider the simulation results obtained by the parallel implementation of the iterative algorithm of solving the drift-diffusion-Poisson system for the following test. The electron-hole transport is simulated in a square domain $L \times L$, $L = 1$ nm. The cell size $h = 0.025$ nm. The diffusion coefficients for electrons and holes along $x$ and $y$ are equal: $D_{nx} = D_{ny} = D_{px} = D_{py} = 1$ nm$^2$/(ns)$^{-1}$. The time of a single iteration is $\tau = h^2/10 = 6.25 \cdot 10^{-5}$ ns. The doped centers are randomly uniformly distributed over the domain. The function $C(r)$ is taken as a constant for all centers: $C(r) = c$.

The source of the electrons and holes is placed in the center of the square. At the initial time instance, $t = 0$, the source generates $N_n((L/2, L/2),0) = 10^9$ electrons and $N_p((L/2, L/2),0) = 3 \cdot 10^8$ holes. We simulate a stationary source, therefore on each iteration $N_n((L/2, L/2), t) = 10^6$ electrons and $N_p((L/2, L/2), t) = 3 \cdot 10^6$ holes are additionally generated. The absorbing boundary is assumed. It means that the electrons and holes reaching the boundary disappear.

In the global random walk algorithm we run $K = 10^6$ trajectories. The random distribution of the doped centers introduces a stochasticity into the model. Therefore, we run $K_d = 200$ tasks with independent samples of the doped centers and average the obtained results.

The main difference of the current work from the our previous papers [11, 13] is an introduction to the model of doping impurities randomly distributed in the semiconductor. To study influence of the doping to the electron-hole transport we solve the drift-diffusion-Poisson equations for different values of the doping function $C(r)$. Figure 1 presents the drift velocity along $X$ and $Y$ directions for the horizontal cross-section $x \in [0; L]$ and fixed $y = L/2 = 0.5$ nm at time $t = 0.01$ ns for the different values of the function $C(r) = c$, $c \in \{0, 10000, 20000, 40000, 80000\}$. It is shown that an increasing of the value of $c$ leads to increasing of the drift velocity values. A sign of the velocity values indicates a drift direction. The maximum of electron and hole concentration is in the domain center, where the source is
Figure 1. The drift velocity (upper panels) and the electron and hole concentrations (lower panels) obtained at time instant $t = 0.01 \text{ ns}$ placed. The electron concentration grows at the domain center when the value of $c$ increases. However the hole concentration along the horizontal line $y = L/2 = 0.5 \text{ nm}$ behaves as follows: it first decreases with an increase of $c$ (for $c < 20000$), relative to the concentration for $c = 0$, and then increases (for $c \geq 20000$).

Two-dimensional fields of the drift velocity and concentrations for $c = 80000$ at time $t = 0.01 \text{ ns}$ are shown in Figure 2. The drift velocity direction of electrons and holes are opposite to each other. Therefore the electrons propagate mainly left and down, and the holes propagate mainly to the upper right corner and down. For the smaller values of the doping function $C(r)$ directions of charge movement are not so clearly expressed, the electrons and holes spread more uniformly around the source.

5. Conclusion
In this paper an iterative stochastic algorithm for solving the drift-diffusion-Poisson system of semiconductors with random doping profile is implemented. The transport of electrons and holes under the influence of the drift and diffusion is simulated by a CA model. The drift velocity is calculated as the gradient of the solution to Poisson equation which is computed by a global random walk algorithm for all grid points at once. Using a parallel implementation of the iterative algorithm for the drift-diffusion-Poisson equations we solved a test problem with zero boundary conditions and stationary electron and hole sources for different values of the doping function. The calculation experiments show that an increase of the doping function values causes an increase of the drift velocity which leads to highlighted directions of electron and hole movement.

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Figure 2. The drift velocity fields (upper panels) and the electron and hole concentration distributions (lower panels) obtained for $c = 80000$ at the time instant $t = 0.01$ ns.

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