Stochastic algorithm for solving transient diffusion equations with a precise accounting of reflection boundary conditions on a substrate surface

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A R T I C L E   I N F O

A B S T R A C T

A new random walk based stochastic algorithm for solving transient diffusion equations in domains where a reflection boundary condition is imposed on a plane part of the boundary is suggested. The motivation comes from the field of exciton transport and recombination in semiconductors where the reflecting boundary is the substrate plane surface while on the defects and dislocations an absorption boundary condition is prescribed. The idea of the method is based on the exact representations of the first passage time and position distributions on a parallelepiped (or a cube) with a reflection condition on its bed face lying on the substrate. The algorithm is meshfree both in space and time, the particle trajectories are moving inside the domain in accordance with the Random Walk on Spheres (RWS) process but when approaching the reflecting surface they switch to move on parallelepipeds (or cubes). The efficiency of the method is drastically increased compared with the standard RWS method. For illustration, we present an example of exciton flux calculations in the cathodoluminescence imaging method in semiconductors with a set of threading dislocations.

1. Introduction

Stochastic methods for solving boundary value problems for parabolic and elliptic differential equations are based on probabilistic representations in the form of mathematical expectations in the space of diffusion processes [1]. The most popular stochastic method, the Random Walk on Spheres (RWS) algorithm (e.g., see [2–4]) is extensively used in practical simulations when solving the diffusion [5], drift–diffusion–reaction

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equations, both for steady-state and transient Dirichlet boundary value problems [6–8], systems of diffusion–reaction equations [9], and some higher order elliptic equations [3]. Extensions to other type of random walks, e.g., random walk on half-spheres [10], rectangles and parallelepipeds [11–14], cylinders [15], etc. have been developed. The Dirichlet (absorbing) boundary conditions cause no problems for the random walk on spheres process: the trajectory is stopped as it hits a small layer near the boundary, $\Gamma_\varepsilon = \{\mathbf{x} : |\mathbf{x} - \mathbf{y}| < \varepsilon\}$ where $\mathbf{y}$ is a boundary point closest to the point $\mathbf{x}$. It is known [3] that the random walk on spheres process converges to the boundary very fast: the mean number of steps N to reach the boundary Γ_ε behaves as $N \sim |\log(\varepsilon)|$. This type of random walk methods are meshfree, and calculate the solution in arbitrary points without calculating the whole solution field in the domain. However the efficiency of the method drops considerably if on a part of the boundary a reflection boundary condition is prescribed. The difficulty comes from the fact that generally, it is not possible to exactly simulate the behavior of the trajectory of the diffusion process in the vicinity of the reflecting boundary. Usually one introduces an approximation by expanding the solution near the boundary which results in a new arbitrary parameter, h, a small distance on which the diffusing particle is reflecting inside the domain when reaching the Γ_ε boundary [4]. This approach introduces an addition error, which is of order h, usually one takes $h \sim \sqrt{\varepsilon}$. But worse still, the length of the simulated diffusion trajectory may be very long since it may be many times reflecting and entering again the layer Γ_ε. This may drastically increase the computer time.

In this paper we suggest a different approach which is based on an explicit simulation of the reflecting diffusion process. The developed method does not use any approximation, it is meshfree and highly efficient since the random walking particles are moving in accordance with the exact distributions which we derive from the Green function for an arbitrary rectangular parallelepiped (or a cube) with a reflection condition on its bed face and absorbing conditions on its other five faces. Our motivation to develop an efficient random walk algorithm for solving diffusion problems with reflecting boundaries comes from the cathodoluminescence imaging problems we studied by simulation of exciton trajectories [16] and some nonlinear coagulation problems [17]. In this paper we present simulations of transient cathodoluminescence signals (e.g., see [18]) for a domain bounded by a plane (a semiconductor substrate) and a set of cylinders (dislocation surfaces). Finally we note that the suggested algorithm can be easily extended to drift–diffusion–reaction problems with a reflection condition on a plane part of the boundary by following the approach we used in [6,7].

2. Formulation of the mixed boundary value problem

Important practical case in semiconductor transport problems deals with domains where a part of the boundary is a plane or a part of a plane while other parts are composed by dislocation surfaces [16,18,19]. The approach we suggest in this paper is that in this case, it is convenient to use near the plane surface a random walk on cubes or rectangular parallelepipeds with one reflecting face while other five faces are absorbing. The starting point of the particle is taken in the center of the cube or the parallelepiped. We deal in this paper with the general anisotropic diffusion case. We mention by passing that in the anisotropic diffusion, the Green function for a ball is not known in the literature, so it seems that the choice of the random walking cubes or parallelepipeds is the only one possible for anisotropic equations.

Let us consider a three-dimensional nonstationary anisotropic diffusion equation:

$$\frac{\partial w(\mathbf{x}, t)}{\partial t} = \sum_{k=1}^{3} a_k \frac{\partial^2 w}{\partial x_k^2}, \qquad \mathbf{x} = (x_1, x_2, x_3) \in V, \quad t \in [0, T] \tag{1}$$

where a_k, $k = 1, 2, 3$ are diffusion coefficients in the relevant directions.

The domain V is assumed to be bounded or unbounded, in the latter case it is supposed that $w \to 0$ as $|\mathbf{x}| \to \infty$. Denote by Γ the boundary of V. We assume that a part of Γ, say, Γ_1, is a plane or a part of a plane, and let $\Gamma_2 = \Gamma \setminus \Gamma_1$.

We consider the following mixed boundary value problem for Eq. (1): zero initial condition, $w(\mathbf{x}, 0) = 0$, the reflection condition on Γ_1, and absorption condition on Γ_2 are posed. According to the reciprocity theorem [7] the function $w(\mathbf{x}, t)$ equals the flux to the boundary Γ_2 if we prescribe the boundary conditions as follows: $w(\mathbf{y}, t) = 1$ for $\mathbf{y} \in \Gamma_2$, and $\frac{\partial w}{\partial \boldsymbol{\nu}} = 0$ for $\mathbf{y} \in \Gamma_1$ where $\boldsymbol{\nu}$ is a normal unit vector on Γ_1.

3. The transient Green function for a rectangular parallelepiped with a reflection condition on the bed face and absorption condition on the other faces

Let us denote by Π a rectangular parallelepiped lying inside the domain V: $\Pi = \{0 \leq x_k \leq l_k; k = 1, 2, 3\}$. We need a Green function $G(\mathbf{x}, \mathbf{y}, \tau)$ with zero initial conditions and the following boundary conditions: zero normal derivative of G on Γ_1, and $G = 0$ on Γ_2. Here Γ_1 is the bed face of Π with $x_3 = 0$, and Γ_2 consists of other five faces of Π. The point $\mathbf{y}$ is the position of the unit point source. This Green function can be found by solving the relevant spectral problem. We present the result:

The Green function of this problem reads $G(\mathbf{x}, \mathbf{y}, \tau) = \prod_{k=1}^{3} G_k(x_k, y_k, \tau)$ where the G_k are the Green functions of the relevant 1D boundary value problems. In our case, the Green functions G_1 and G_2 are the same as for the Dirichlet conditions

$$G_k(x_k, y_k, \tau) = \frac{2}{l_k} \sum_{m=1}^{\infty} \sin\left(\frac{m\pi x_k}{l_k}\right) \sin\left(\frac{m\pi y_k}{l_k}\right) \exp\left[-\frac{m^2\pi^2 a_k}{l_k^2} \tau\right], \qquad k = 1, 2,$$

and the Green function G_3 obtained from the spectral expansion has the form

$$G_3 = \frac{2}{l_3} \sum_{m=1}^{\infty} \cos\left(\frac{(2m-1)\pi y_3}{2l_3}\right) \cos\left(\frac{(2m-1)\pi x_3}{2l_3}\right) \exp\left[-\frac{(2m-1)^2\pi^2 a_3}{4l_3^2} \tau\right].$$

Note that these series diverge as the time τ tends to zero, or, more exactly, as the dimensionless parameters $a_k\tau/l_k^2$ tend to zero. Therefore, for very small values of $a_k\tau/l_k^2$ we can use the following representations obtained by the Poisson series transformation (e.g., see [12,13]):

$$G_k(x_k, y_k, \tau) = \frac{1}{2\sqrt{\pi a_k\tau}} \sum_{m=-\infty}^{\infty} \left\{ \exp\left[-\frac{(x_k - y_k + 2ml_k)^2}{4a_k\tau}\right] - \exp\left[-\frac{(x_k + y_k + 2ml_k)^2}{4a_k\tau}\right]\right\}, \quad k = 1, 2, \quad (2)$$

and

$$G_3(x_3, y_3, \tau) = \frac{1}{2\sqrt{\pi a_k\tau}} \sum_{m=-\infty}^{\infty} (-1)^m \left\{ \exp\left[-\frac{(x_k - y_k + 2ml_k)^2}{4a_k\tau}\right] + \exp\left[-\frac{(x_k + y_k + 2ml_k)^2}{4a_k\tau}\right]\right\}. \quad (3)$$

In what follows we consider the case when $a_k\tau/l_k^2$ is not very small. The case when this parameter is small can be treated analogously using the expansions (2), (3).

For the sake of random walk efficient implementation we choose always the starting point in the center of the parallelepiped, then ($k = 1, 2$)

$$G_k = \frac{2}{l_k} \sum_{m=1}^{\infty} (-1)^{m+1} \sin\left(\frac{(2m-1)\pi\, y_k}{l_k}\right) \exp\left[-\frac{(2m-1)^2\pi^2 a_k}{l_k^2} \tau\right], \quad (4)$$

and

$$G_3 = \frac{\sqrt{2}}{l_3} \sum_{m=1}^{\infty} \gamma_m \cos\left(\frac{(2m-1)\pi y_3}{2l_3}\right) \exp\left[-\frac{(2m-1)^2\pi^2 a_3}{4l_3^2} \tau\right] \quad (5)$$

where $\gamma_m = \cos\left(\frac{(2m-1)\pi}{4}\right)$ is a sequence of ± 1 values: $\gamma_1 = 1$, $\gamma_{4m-2} = \gamma_{4m-1} = -1$, and $\gamma_{4m} = \gamma_{4m+1} = 1$, $m = 1, 2, \ldots,$.

Integrating the normal derivatives of the Green function over the five absorbing faces we obtain the probability density of the first passage time:

$$p(\tau) = \frac{32\sqrt{2}}{\pi} \Big[\frac{a_1}{l_1^2} F_1(a_1, \tau) F_2(a_2, \tau) \hat{F}_2(a_3, \tau) + \frac{a_2}{l_2^2} F_1(a_2, \tau) F_2(a_1, \tau) \hat{F}_2(a_3, \tau)$$
$$+ \frac{a_3}{4l_3^3} \hat{F}_1(a_3, \tau) F_2(a_1, \tau) F_2(a_2, \tau) \Big]$$

where

$$F_1(a_i, \tau) = \sum_{m=1}^{\infty} (-1)^{m+1} (2m - 1) \exp\Big[-\frac{(2m-1)^2 \pi^2 a_i}{l_i^2} \tau \Big], \qquad i = 1, 2,$$

$$F_2(a_i, \tau) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{2k-1} \exp\Big[-\frac{(2k-1)^2 \pi^2 a_i}{l_i^2} \tau \Big], \qquad i = 1, 2,$$

$$\hat{F}_1(a_3, \tau) = \sum_{m=1}^{\infty} \hat{\gamma}_m (2m - 1) \exp\Big[-\frac{(2m-1)^2 \pi^2 a_3}{4l_3^2} \tau \Big],$$

$$\hat{F}_2(a_3, \tau) = \sum_{k=1}^{\infty} \hat{\gamma}_m \frac{1}{2k-1} \exp\Big[-\frac{(2k-1)^2 \pi^2 a_3}{4l_3^2} \tau \Big].$$

Here $\hat{\gamma}_{2m-1} = \gamma_{2m-1}$, and $\hat{\gamma}_{2m} = -\gamma_{2m}$, $m = 1, 2, \ldots$. Now we find the distribution densities of the exit point on the five absorbing faces of the parallelepiped. First we note that the 1D probability densities on the horizontal coordinates x_1 and x_2 are derived by taking the normal derivatives on the relevant faces. This yields

$$p_{a_1}(y_1, \tau) = \frac{1}{F_2(a_1, \tau)} \frac{\pi}{2l_1} \sum_{k=1}^{\infty} (-1)^{k+1} \sin\Big[\frac{(2k-1)\pi y_1}{l_1} \Big] \exp\Big[-\frac{(2k-1)^2 \pi^2 a_1}{l_1^2} \tau \Big],$$

$$p_{a_2}(y_2, \tau) = \frac{1}{F_2(a_2, \tau)} \frac{\pi}{2l_2} \sum_{k=1}^{\infty} (-1)^{k+1} \sin\Big[\frac{(2k-1)\pi y_2}{l_2} \Big] \exp\Big[-\frac{(2k-1)^2 \pi^2 a_2}{l_2^2} \tau \Big].$$

Analogously we find the probability density function

$$p_{a_3}(y_3, \tau) = \frac{1}{\hat{F}_2(a_3, \tau)} \frac{\pi}{2l_3} \sum_{k=1}^{\infty} \gamma_k \cos\Big[\frac{(2k-1)\pi y_3}{2l_3} \Big] \exp\Big[-\frac{(2k-1)^2 \pi^2 a_3}{4l_3^3} \tau \Big].$$

The conditional probability density on the five absorbing faces under the condition that the time is fixed is represented as a weighted sum of independent 2D distribution densities:

$$p(y_1, y_2, y_3 | \tau) = \frac{1}{p(\tau)} \Big\{ \frac{16\sqrt{2}}{\pi} \frac{a_1}{l_1^2} F_1(a_1, \tau) F_2(a_2, \tau) \hat{F}_2(a_3, \tau) p_{a_2}(y_2, \tau) p_{a_3}(y_3, \tau)$$

$$+ \frac{16\sqrt{2}}{\pi} \frac{a_2}{l_2^2} F_1(a_2, \tau) F_2(a_1, \tau) \hat{F}_2(a_3, \tau) p_{a_1}(y_1, \tau) p_{a_3}(y_3, \tau)$$

$$+ \frac{8\sqrt{2}}{\pi} \frac{a_3}{l_3^2} \hat{F}_1(a_3, \tau) F_2(a_1, \tau) F_2(a_2, \tau) p_{a_1}(y_1, \tau) p_{a_2}(y_2, \tau) \Big\}.$$

From this representation we can construct the sampling algorithm from the distribution density on the five absorbing faces of the parallelepiped: first we choose the face from the weight probabilities, and then sample the point from the relevant independent one-dimensional probability densities. Indeed, with probability

$$P_1 = \frac{1}{p(\tau)} \frac{16\sqrt{2}}{\pi} \frac{a_1}{l_1^2} F_1(a_1, \tau) F_2(a_2, \tau) \hat{F}_2(a_3)$$

we sample from the density $p_{a_2}(y_2, \tau) p_{a_3}(y_3, \tau)$ a random point $(0, y_2, y_3)$ or (l_1, y_2, y_3) on the faces $x_1 = 0$ or $x_1 = l_1$ with probability $1/2$. With probability

$$P_2 = \frac{1}{p(\tau)} \frac{16\sqrt{2}}{\pi} \frac{a_2}{l_2^2} F_1(a_2, \tau) F_2(a_1, \tau) \hat{F}_2(a_3)$$

we sample from the density $p_{a_1}(y_1, \tau) p_{a_3}(y_3, \tau)$ a random point $(y_1, 0, y_3)$ or (y_1, l_2, y_3) on the faces $x_2 = 0$ or $x_2 = l_2$ with probability $1/2$. Finally, on the face $x_3 = l_3$ we sample with probability $P_3 = 1 - P_1 - P_2$ a random point (y_1, y_2, l_3) from the density $p_{a_1}(y_1, \tau) p_{a_2}(y_2, \tau)$.

In conclusion we note that the sampling random variables from the densities presented in this paper in the form of alternating series can be efficiently carried out by Devroye's method [20] as described in detail in our recent paper [7]. Another even more efficient technique is to use a tabulation of the probability densities and apply the alias Walker's algorithm [20]. More details are given in the next section.

4. Algorithm

For clarity, we describe the random walk algorithm for solving the mixed boundary value problem (1) under the reflection boundary condition on Γ_1 and absorption conditions on Γ_2 for the isotropic diffusion case when $a_1 = a_2 = a_3$. Or more generally, the Dirichlet boundary condition on Γ_2 is assumed: $w(\mathbf{y}, t) = g(\mathbf{y}, t)$, $\mathbf{y} \in \Gamma$ where $g(\mathbf{y}, t)$ is an arbitrary given function. The anisotropic case is treated analogously.

Before we present the algorithm, let us shortly describe the algorithm of sampling from $p(\tau)$, the first passage time for a sphere and the same for the parallelepiped. Here different approaches can be used, e.g., see [11–13]. For instance, in [12] it is suggested to numerically invert the distribution function which is quite time consuming. In [7] we applied the Devroye method for densities represented in the form of alternating series. This method converges very rapidly. However our simulations have shown that the most efficient algorithm is constructed as follows: first precalculate discrete tables for the densities, and then it remains to apply the Walker alias method which is extremely efficient: the cost does not depend on the size of the approximating array. For instance, in the case of a sphere of radius R, and diffusion coefficient D, first we approximate the first passage time density for a sphere of unit radius and $D = 1$:

$$p(\tau) = 2 \sum_{m=1}^{\infty} (-1)^{n+1} \pi^2 n^2 \exp\left(-\pi^2 n^2 \tau\right) \tag{6}$$

by a discrete approximation, and generate the random time t using Walker's algorithm. Then calculate the desired sample time τ as $\tau = R^2 t / D$. Note that in the small time region instead of (6) we can use the well known approximation [12] $p(\tau) = -F'(\tau)$ where $F(\tau) = 2 \exp[1/(4\tau)] \frac{1}{\sqrt{\pi\tau}}$. The same approach is used for generating the first passage time for parallelepipeds since all we need here is to precalculate the values of the first passage time density in the nodes of a one-dimensional grid.

To calculate the solution $w(\mathbf{x}, t)$ in a fixed point $\mathbf{x}_0$, for $t \in [0, T]$, we simulate N independent trajectories all starting from the point $\mathbf{x}_0$.

The general simulation procedure is organized as follows: as long as the random position of the random walk is far from the reflecting boundary Γ_1, we use the random walk on spheres process. But when the random walk enters a layer Γ_H of depth H near the boundary Γ_1, we switch to simulate the random walk on parallelepipeds (or cubes) whose bed faces are lying on Γ_1. Due to the reflection condition the random walk after only a few steps comes out of the layer Γ_H and proceeds till it hits the boundary $\Gamma_{2,\varepsilon}$ where a value of 1 is scored at the relevant first passage time. By $\Gamma_{2,\varepsilon}$ we denote here the ε-layer along the absorbing boundary Γ_2. In more detail the algorithm can be described as follows.

We introduce a layer of depth H near the reflecting boundary Γ_1 such that when entering H, the particle switches to the random walk on parallelepipeds (or cubes). The value H is arbitrarily chosen but large enough.

1. A sphere $S(\mathbf{x}_0, R_0)$ centered at $\mathbf{x}_0$, and with a radius R_0 equal to the shortest distance between $\mathbf{x}_0$ and the boundary Γ is constructed.

2. Sample a random point $\mathbf{x}_1$ from the uniform distribution on the surface of the sphere $S(\mathbf{x}_0, R_0)$. The first passage time τ_0 is sampled from the density $p(\tau)$. Thus the time at which the particle arrives at its new position $\mathbf{x}_1$ on the sphere is $\tau_1 = t - \tau_0$ where τ_0 is simulated according to the density $p(\tau)$ in this sphere.

3. If the point $\mathbf{x}_1$ is still in the domain $V \setminus H$, then with $\mathbf{x}_1$ as a new center, we inscribe the next sphere, $S(\mathbf{x}_1, R_1)$, the random point uniformly distributed on this sphere is sampled, and the random time τ_1 spent inside the sphere is simulated, etc.

4. If however the randomly walking point hits, say, on a step k, the layer H, then the next step is simulated as follows. Inscribe a parallelepiped (or a cube) centered in the point $\mathbf{x}_k$, with its bed face lying on Γ_1, simulate the next point, $\mathbf{x}_{k+1}$ on the five absorbing faces, and generate the random first passage time τ_k as described in Section 3.

5. If the next point, $\mathbf{x}_{k+1}$, is still inside the layer H, we simulate the next step as the random point distributed on the parallelepiped (a cube) centered at $\mathbf{x}_{k+1}$, etc. If however the point $\mathbf{x}_{k+1}$ jumps outside the layer, we switch again to the issue 3 and proceed to simulate the random walk on spheres process till the particle comes back to the layer, etc.

6. If a particle is continuing to move randomly within the region $G_\varepsilon = G \setminus \Gamma_{2\varepsilon}$ until $t - \sum_i \tau_i \leq 0$, then a value of zero is scored. If the particle hits the set $\Gamma_{2\varepsilon}$ (say, at a point $\mathbf{x}_\varepsilon$), at a time $t_1 = t - \sum_i \tau_i \geq 0$, then the value $g(\mathbf{y}, t_1)$ is scored, where $\mathbf{y}$ is a boundary point closest to the point $\mathbf{x}_\varepsilon$.

We have described the simulation of one trajectory which is terminated with a calculated score S_1 equal to zero or to $g(\mathbf{y}, t_1)$. After simulation of N trajectories one calculates the arithmetic mean of all the scores. This mean value is close to the exact solution to within a bias of order ε, and a statistical error of order of $C N^{-1/2}$ where the constant C depends on the variation of the function g on the boundary and the time interval $(0, T)$. The cost of this algorithm is of order of $\log(\varepsilon)/\varepsilon^2$.

5. Simulation of the exciton transport and recombination in a semiconductor with a set of dislocations

The governing equation includes now an absorption term:

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = D \Delta u(\mathbf{x}, t) - \frac{1}{\bar{\tau}} u(\mathbf{x}, t) \tag{7}$$

where $\bar{\tau}$ is the mean life time of the exciton before it recombines and gives rise to a photon emission [16,18]. The domain V representing a semiconductor with a set of threading dislocations is considered as a half-space $\{z \geq 0\}$ with imbedded right semi-cylinders with their bases lying on the plane $z = 0$. The positions of the dislocations are sampled at random uniformly distributed on the substrate. The surface $z = 0$ (excluding the dislocation bases) is our reflecting boundary Γ_1, and the union of the cylinders' surfaces is the absorbing boundary Γ_2.

Using the relation $u(\mathbf{x}, t) = \exp[-t/\bar{\tau}] w(\mathbf{x}, t)$ between w, the solution of the heat equation, and u, the solution of (7), we conclude that our problem to find u is reduced to solve the heat equation for the function w with zero initial condition, reflection condition on Γ_1, and transformed boundary condition $w(\mathbf{y}, t) = \exp[t/\bar{\tau}] g(\mathbf{y}, t)$ on the absorbing boundary Γ_2, i.e., on the dislocations' surfaces.

The domain V representing a semiconductor is taken as a semi-infinite rectangular parallelepiped defined by its base $X_{\mathrm{s}} \times Y_{\mathrm{s}} = 100 \times 100$ nm^2 lying on the plane $z = 0$, and z-coordinate on $[0, \infty)$. A unit instantaneous exciton source is distributed in the domain V as follows: the coordinates x, y are uniformly distributed while the vertical coordinate z is distributed on $(0, \infty)$ with the probability density $f(\xi, \eta, \zeta, t) = \delta(t) \frac{1}{100} \exp(-\zeta/100)$.

In our simulations we calculated the following functions: (1) the total flux of excitons to the dislocations' surfaces, (2) the cathodoluminescence intensity $CL(t)$ which is the concentration of excitons absorbed
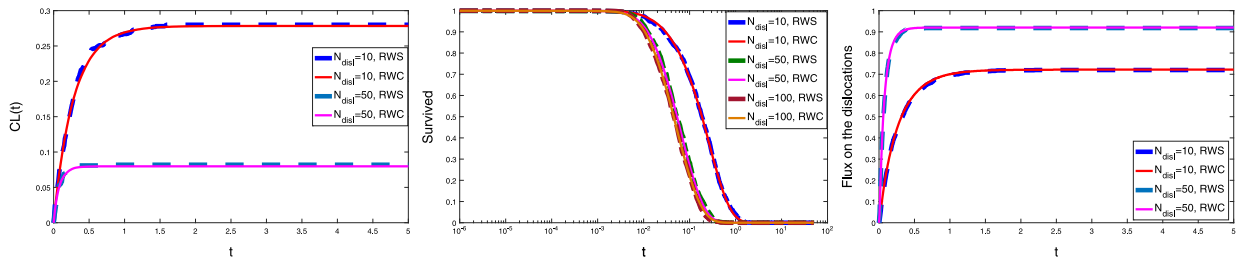
Fig. 1. Comparison of RWC and RWS algorithms: the solid lines present the results obtained by RWC, and the dashed lines are obtained by the RWS algorithm. The presented curves are the transients of the intensity of cathodoluminescence, CL(t) (left panel), the concentration of survived excitons (middle panel), and the total flux to the dislocation surfaces (right panel), depending on the number of dislocations $N_{dis} = 10, 50, 100$.

(recombined) inside the domain V due to their finite life time, and (3) the concentration of survived excitons, i.e., the part of excitons which still are diffusing inside the domain V. The following modeling parameters were taken in the computer simulations: the diffusion coefficient $D = 900 \, \text{nm}^2/\text{ns}$, the lifetime $\bar{\tau} = 1$ ns, the diffusion length $L = \sqrt{D\bar{\tau}} = 30$ nm, the dislocation radius $R_{dis} = 3$ nm, the number of exciton trajectories $N = 10^6$.

The results of simulation presented in Fig. 1 are the transients of the intensity of cathodoluminescence, CL(t) (left panel), the concentration of survived excitons (middle panel), and the total flux to the dislocations surfaces (right panel), depending on the number of dislocations $N_{dis} = 10, 50, 100$. The solid curves are the results obtained by the method developed in this paper, where the random walk on cubes (RWC) were used when approaching the plane boundary, and the dashed curves are obtained by the RWS method described in [7]. The results agree with an accuracy of 0.1%, while the computer time of the method based on the random walk on cubes was 15 times less compared with that of RWS. We mention here one interesting result of the simulations: the concentration of the survived excitons is considerably different for the number of excitons 10 and 50. However with the increase of the number of excitons from 50 to 100 the transients of these concentrations almost coincide.

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