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IMPACT OF THE DISLOCATION DENSITY ON THE TRANSIENT PHOTOLUMINESCENCE INTENSITY IN GaN SEMICONDUCTOR

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Abstract: The time-resolved photoluminescence in a layer of GaN with an embedded array of threading dislocations is studied. An instantaneous spatially uniform source of excitons is considered. The transport and recombination of excitons is governed by a 3D transient drift-diffusion-recombination equation with mixed Dirichlet and Robin boundary conditions on the plane surface and the cylindrical boundaries of the dislocations. We develop a stochastic simulation algorithm which solves this problem by tracking exciton trajectories. The drift of the excitions is affected by the piezoelectric fields around the dislocations. The parameters of the piezoelectric field, the exciton's diffusion length and its mean life time are taken from the experimental study published recently in our triple article in Physical Review Applied of 2022. The main finding in the present paper concerns the relation between the photoluminescence

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intensity and the dislocation density. It is shown that from a transient photoluminescence curve it is possible to extract the dislocation density with high resolution.

Keywords: photoluminescence, threading dislocations, piezoelectric field, radiative recombination, exciton's lifetime, random walk on spheres, transient drift-diffusion-recombination equation

1 Introduction

In this paper, we study a time-resolved photoluminescence in GaN in the presence of a family of threading dislocations. The first experimental study that analyzed the exciton dynamics at a single dislocation in GaN probed by picosecond time-resolved cathodoluminescence is reported in Ref.[8]. In our paper we suggest a transport model in the form of a transient drift-diffusion-recombination partial differential equation governing the exciton motion in GaN in the presence of a family of threading dislocations distributed randomly with a prescribed density. We develop a stochastic simulation method for solving this equation and establish a relation between the photoluminescence intensity and the dislocation density in GaN.

Let us consider a nonstationary drift-diffusion-recombination equation, a counterpart of the stationary formulation of the exciton transport problem studied in our recent papers [5], [6],[2],[4], [7]. The nonstationary problem is to be solved in the infinite domain G which is a half space $z \geq 0$ with an embedded array of threading dislocations. The dislocations are assumed to be circular semi-cylinders with axes perpendicular to the plane $z = 0$. The boundary of the domain Γ is thus composed by Γ_1, the plane $z = 0$, and Γ_2, the union of surfaces of the semi-cylinders.

The excitons are injected instantaneously at the time $t = 0$ with a spatial distribution $q(\mathbf{x})$, hence the source of excitons reads $f(\mathbf{x}, t) = q(\mathbf{x})\delta(t)$. The concentration of excitons in the domain $u(\mathbf{x}, t)$ is governed in the time interval $0 \leq t \leq T$ by the equation

$$\frac{\partial u}{\partial t} = D\Delta u(\mathbf{x}, t) + \nabla \cdot (\mathbf{v}(\mathbf{x})u) - \lambda^2(\mathbf{x})u + f(\mathbf{x}, t) \tag{1}$$

under the initial and boundary conditions

$$u(\mathbf{x}, 0)\big|_G = 0, \tag{2}$$

$$u(\mathbf{y}, t)\big|_{\Gamma_2} = 0, \tag{3}$$

$$\nabla u \cdot \boldsymbol{\nu} + Su\big|_{\Gamma_1} = 0, \tag{4}$$

and $u \to 0$ as $|\mathbf{x}| \to \infty$. Here $\boldsymbol{\nu}$ is the outward surface normal unit vector, and S is the surface recombination velocity. In Eq. (1), D is the diffusion coefficient, $\mathbf{v}$ is the drift velocity caused by the piezoelectric field, and $\lambda^2(\mathbf{x}) = 1/\tau(\mathbf{x})$, where $\tau(\mathbf{x})$ is the lifetime of the exciton. The lifetime depends on the distance from the dislocation outcrop due to the piezoelectric field of the dislocation [6]. The cylinders around dislocation lines are assumed to absorb excitons nonradiatively, which is described by the Dirichlet condition (3). This simplification is not essential, and the general case of the partial reflection/absorption, assumed in the Robin boundary condition (4) at the planar surface, can be applied at the dislocations as well.

To solve numerically this problem, we apply a stochastic simulation method which is based on a probabilistic interpretation of the drift-diffusion process and the relevant Monte Carlo method, a Random Walk on Spheres algorithm (RWS). For the stationary case, the details of RWS are described in Refs. [5] and [10], the nonstationary problem is considered in Refs. [11] and [12].

In the present paper, we apply the RWS algorithm to calculate transient PL intensity in the crystal with dislocations. In contrast to Refs. [11] and [12], we develop the RWS algorithm to calculate integral characteristics, particularly, volume integral of the solution of the drift-diffusion equation which governs the CL intensity. To this end, we derive a Reciprocity relation which drastically simplifies calculation of this integral.

The Monte Carlo algorithm works by tracking trajectories of the excitons inside the domain, and recombining on the boundaries in accordance with the boundary conditions prescribed. Simulation of the exciton trajectories is carried out as follows. The trajectory starts at a position $\mathbf{x}_0$ inside the domain, taken with a probability obtained from the initial spatial distribution of excitons $q(\mathbf{x})$.

The point $\mathbf{x}_0$ is taken as the center of a sphere of a radius R_1 which lies inside the domain. The choice of the radius depends on the gradients of the coefficients λ^2 and the velocity $\mathbf{v}$. The radius has to be chosen small enough to ensure that these quantities can be approximated by constants within the sphere. If these coefficients are constants, the radius can be taken maximal among spheres centered at $\mathbf{x}_0$ and inscribed in G.

To make a step, one calculates the probability Q_{R_1} that the exciton survives and reaches the surface of the sphere. Calculation of this probability is presented in section 2.3. If the exciton survives, one calculates the random exciton's exit position on the sphere and the respective random time when this event happens. The exit time and position are sampled as described in Ref. [11]. Then, a second sphere is inscribed with its center at the exciton's exit position on the first sphere, the survival probability Q_{R_2}, the exit position and the exit time for the second sphere are calculated, etc. If the exciton is not survived in a sphere, the trajectory terminates, one calculates the random position inside the sphere where the trajectory stops and the relevant random time when it happens (see Sec. 2.3.)

To describe the trajectories at the boundaries, we introduce a shell Γ_ε of the boundary defined such that the minimal distance from any point in the shell to the boundary Γ is smaller than ε. The parameter ε can be taken arbitrarily small. Practically, we take $\varepsilon = 10^{-3} d_0$, where d_0 is the diameter of the cylinder around the dislocations. If the exciton position $\mathbf{x}_2$ occurs in the Γ_ε shell of the absorbing boundary, the trajectory is terminated. If the surface is partially reflecting with the surface recombination velocity S, one calculates the recombination probability

$$P_h = \frac{hS}{D + hS}, \tag{5}$$

where h is a step of the reflection from Γ. The value of h is taken proportional to $\sqrt{\varepsilon}$ to have an ε error of the solution. With the probability P_h, the trajectory is terminated. A new exciton is generated and its trajectory is calculated by the algorithm described above. With probability $1 - P_h$, the random walk trajectory is reflected in the direction opposite to the normal direction $\boldsymbol{\nu}$ to the point $\mathbf{x}_2 - h\boldsymbol{\nu}$. In case of the reflection boundary condition, $S = 0$, the trajectory is always reflected.

2 Integral relations for the solution of drift-diffusion equations

We call the equation Eq. (1) with its boundary conditions the direct drift-diffusion problem. Below we formulate the adjoint drift-diffusion equation and give a relation between these two problems known as the Reciprocity relation [11]. We need for our applications not the whole solution field $u(\mathbf{x}, t)$, but its integral characteristic, namely, the total concentration of excitons survived to a time instant t, i.e., the spatial integral $I(t) = \int\limits_G u(\mathbf{x}, t)\, d\mathbf{x}$, and the total flux of excitons to the boundary Γ or on certain parts of the boundary Γ_k:

$$I_k(\mathbf{x}_0, t) = -\int\limits_0^t dt' \int\limits_{\Gamma_k} \mathbf{J} \cdot \nu_k \, d\sigma_k, \tag{6}$$

where the flux $\mathbf{J}$ includes both diffusion and drift fluxes, $\mathbf{J} = D\nabla u + \mathbf{v}n$, and $\mathbf{x}_0$ is a position of the point source.

A straightforward way to calculate these integral characteristics is to find the solution $u(\mathbf{x}, t)$ and then take the time and spatial integrals. This complicated calculation can be avoided by deriving adjoint drift-diffusion equations, directly governing these two integral characteristics.

In what follows we consider a point source located at $\mathbf{x}_0$. The direct problem is governed by the equation

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = D\Delta u + \nabla \cdot (\mathbf{v}u) - \lambda^2 u + \delta(t)\delta(\mathbf{x} - \mathbf{x}_0) \tag{7}$$

for the time interval $0 \le t < T$ with zero initial conditions, $u(\mathbf{x}, 0) = 0$, and relevant homogeneous boundary conditions. We consider here a general case, the Robin boundary conditions

$$(\mathbf{J} \cdot \boldsymbol{\nu}_k + S_k u)\big|_{\Gamma_k} = 0, \tag{8}$$

where $\boldsymbol{\nu}_k$ are outward surface normal unit vectors, S_k stand for the surface recombination velocities, and $k = 1, \ldots m$.

2.1. Reciprocity relation 1. *Assume we are given the direct problem (7), (8) and adjoint one written in the backward time $\tilde{t} = T - t$ in the form*

$$\frac{\partial w}{\partial \tilde{t}} = D\Delta w - \mathbf{v} \cdot \nabla w - \lambda^2 w + g(\mathbf{x})\delta(\tilde{t}), \quad \tilde{t} \in [0, T] \tag{9}$$

with the initial condition $w(\mathbf{x}, 0) = 0$ and boundary condition

$$\left(D\nabla w \cdot \boldsymbol{\nu}_k + S_k w\right)\Big|_{\Gamma_k} = 0, \tag{10}$$

where $g(\mathbf{x})$ is an arbitrary bounded function defined in G. Then,

$$w(\mathbf{x}_0, t) = \int\limits_G g(\mathbf{x}) u(\mathbf{x}, t)\, d\mathbf{x}. \tag{11}$$

Proof. Multiply the direct equation by w, the adjoint equation by u, and subtract. This yields

$$\begin{aligned} \frac{\partial(uw)}{\partial t} &= \nabla \cdot \left[D\big(w\nabla u - u\nabla w\big) + \mathbf{v}uw\right] \\ &\quad -ug\delta(t) + w\delta(t)\delta(\mathbf{x} - \mathbf{x}_0). \end{aligned} \tag{12}$$

Here, the relation $w\, \partial u/\partial t = \partial(wu)/\partial t - u(\partial w/\partial \tilde{t})\, (d\tilde{t}/dt)$ is used. Integrate now this equality over time and domain G, apply the Green formula to transform the volume integral to surface integrals, and use the initial and boundary conditions for the direct and adjoint equations. This yields

$$\begin{aligned} w(\mathbf{x}_0, t) = -\int\limits_0^t dt' \Big\{ \sum_{k=1}^m \int\limits_{\Gamma_k} \left[D\big(w\nabla u - u\nabla w\big) + \mathbf{v}uw\right] \cdot \boldsymbol{\nu}_k\, d\sigma_k \Big\} \\ + \int\limits_G g(\mathbf{x}) u(\mathbf{x}, t)\, d\mathbf{x}\ . \end{aligned}$$

The first integral in the right-hand side of this equation vanish due to zero boundary conditions (8) and (10) for u and w, respectively. This completes the proof.

Taking the function $g(\mathbf{x})$ identically equal to 1, we obtain from Eq. (11) the total concentration of survived excitons.

A similar reciprocity relation can be obtained for the flux to the boundary. The adjoint problem in this case is governed by a homogeneous equation also in the backward time $\tilde{t} = T - t$, so that $d\tilde{t}/dt = -1$.

$$\frac{\partial w}{\partial \tilde{t}} = D\Delta w - \mathbf{v} \cdot \nabla w - \lambda^2 w, \quad \tilde{t} \in [0, T] \tag{13}$$

with the initial condition $w(\mathbf{x}, 0) = 0$, and boundary conditions

$$\left(D\nabla w \cdot \boldsymbol{\nu}_k + S_k w\right)\Big|_{\Gamma_k} = S_k \delta_{ik}, \tag{14}$$

where δ_{ik} is the Kronecker symbol. Note that the Dirichlet (absorbing) boundary condition corresponds to $S_k = \infty$, while the Neumann (reflection) condition to $S_k = 0$.

The fluxes $I_k(\mathbf{x}_0, t)$ defined by Eq. (6) are functions of the point $\mathbf{x}_0$, the position where the instantaneous point source is placed, and time t measured from the time instant $t = 0$ when the exciton was released. The next reciprocity relation states that the flux $I_k(\mathbf{x}_0, t)$ coincides with $w(\mathbf{x}_0, t)$, the solution of the adjoint problem at the time $\tilde{t} = T$ which is the time where the initial conditions for the direct equation are posed.

2.2. Reciprocity relation 2. *Assume we are given the direct (7),(8) and adjoint (13),(14) problems, as formulated above. Then,*

$$w(\mathbf{x}_0, t) = -\int\limits_0^t d\tau \int\limits_{\Gamma_k} \mathbf{J} \cdot \boldsymbol{\nu}_k \, d\sigma_k, \tag{15}$$

where $\mathbf{J} = D\nabla u + \mathbf{v}u$.

Proof. Multiply the direct equation by w, the adjoint equation by u, and subtract. This yields

$$\frac{\partial(uw)}{\partial t} = \nabla \cdot \big[D\big(w\nabla u - u\nabla w\big) + \mathbf{v}uw\big] + w\delta(t)\delta(\mathbf{x} - \mathbf{x}_0). \tag{16}$$

Here the relation $w\,\partial u/\partial t = \partial(wu)/\partial t - u(\partial w/\partial \tilde{t})\,(d\tilde{t}/dt)$ is used. Integrate now this equality over time and domain G, apply the Green formula to transform the volume integral to surface integrals, and use the initial and boundary conditions for the direct and adjoint equations. This yields

$$\begin{aligned} w(\mathbf{x}_0, t) \quad = \quad & -\int\limits_0^t dt' \Big\{ \sum_{k=1}^{m} \int\limits_{\Gamma_k} \big[D\big(w\nabla u - u\nabla w\big) \\ & \qquad\qquad + \mathbf{v}uw\big] \cdot \boldsymbol{\nu}_k \, d\sigma_k \Big\}. \end{aligned} \tag{17}$$

The terms with $k \neq i$ in the right-hand side of this equation vanish, which immediately follows from the homogeneous boundary conditions for w and u. Due to the non-zero term S_i in the right-hand side of the boundary condition (14) at the i-th boundary, we come, after simple transformations of the integrand in (17), to the desired result (15).

Thus, the first reciprocity relation states that the total concentration of survived excitons at time t from a unit instantaneous point source located at a point $\mathbf{x}_0$ is the solution $w(\mathbf{x}_0, t)$ of the adjoint boundary value problem (9), (10). Similarly, the second reciprocity relation states that the total transient flux at time t to a part of the boundary Γ_k from a unit instantaneous point source located at a point $\mathbf{x}_0$ is the solution $w(\mathbf{x}_0, t)$ of the adjoint boundary value problem (13), (14).

The adjoint equation (9) admits a probabilistic interpretation. To formulate this interpretation, we derive a spherical integral relation, which is a transient counterpart of the stationary spherical integral relation presented in Ref. [10]. This integral property relates the solution of the drift-diffusion equation in the center of a sphere with the integral of the solution over the surface of the sphere.

2.3. Spherical integral relation. *Any solution $w(\mathbf{x}, t)$ of the drift-diffusion equation (13) with constant diffusion coefficient, velocity and the parameter λ satisfies the following spherical integral relation for any sphere inscribed in G:*

$$\begin{aligned} w(\mathbf{x}_0, t) \quad &= \quad Q_R \int_0^t \int_0^\pi \int_0^{2\pi} w(\mathbf{x}_0 + R\,\boldsymbol{\zeta}, t - t') \\ &\qquad \times p_\kappa(\theta, \varphi; \gamma, \beta)\ p_t(t')\, d\varphi\, d\theta\, dt', \end{aligned} \tag{18}$$

where $Q_R = Q_1\, Q_2$,

$$Q_1 \quad = \quad \frac{\mu}{\sinh\big(\mu\big)}, \quad \mu = \frac{R}{\sqrt{D}}\sqrt{\lambda^2 + \frac{|\mathbf{v}|^2}{4D}}, \tag{19}$$

$$Q_2 \quad = \quad \frac{\sinh(\kappa)}{\kappa}, \quad \kappa = \frac{|\mathbf{v}|R}{2D}. \tag{20}$$

The probability density of the exit time $p_t(\tau)$ and the probability density of the exit point on the sphere $p_\kappa(\theta, \varphi; \gamma, \beta)$ are given by the following explicit expressions:

$$p_t(t) = \frac{2}{Q_1} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\pi^2 n^2 D}{R^2}\ \exp\Big\{ - \Big(\frac{\pi^2 n^2 D}{R^2} + \frac{|\mathbf{v}|^2}{4D} \Big) t \Big\}, \tag{21}$$

$$p_\kappa(\theta, \varphi; \gamma, \beta) = \frac{1}{4\pi Q_2}\ \exp\big\{ \kappa [\sin\theta \sin\gamma \cos(\varphi - \beta) + \cos\theta \cos\gamma] \big\} \sin\theta. \tag{22}$$

Here γ, β are the zenith and azimuthal angles of the velocity vector $\mathbf{v}$, and θ, φ are the zenith and azimuthal angles of the exit point on the sphere. In the coordinate system where the z-axis coincides with the direction of the velocity,

$$\begin{aligned} p_\kappa(\theta, \varphi) \quad &= \quad \frac{1}{4\pi Q_2} \sin\theta\ \exp\big\{ \kappa \cos\theta \big\}, \\ &\qquad 0 \le \theta \le \pi,\ 0 \le \varphi \le 2\pi. \end{aligned} \tag{23}$$

The proof is obtained by reasoning analogous to that used in the stationary case [10], and can be found in Ref. [11].

In the algorithm description, we need to simulate a random time when the exciton's trajectory terminates in a sphere. The distribution density of this time can be obtained as follows. First take the volume integral of the Green function over the interior of the sphere, then normalize the result to unity.

This yields

$$p(t) = \frac{\lambda^2}{1-Q_1}\frac{\sinh(\kappa)}{\kappa}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{2\,n^2\pi^2}{\kappa^2+n^2\pi^2} \times \exp\left\{-\left[\frac{n^2\pi^2 D}{R^2}+\lambda^2+\frac{|\mathbf{v}|^2}{4D}\right]t\right\}. \quad (24)$$

The spherical integral relation admits a clear probabilistic interpretation: a particle starting from the center of the sphere survives with the probability Q_R and hits the surface of the sphere at a random exit point, the distribution density of which is $p_\kappa(\theta,\varphi)$, at the random exit time distributed with the probability density $p_t(\tau)$. Note that the spatial distribution of the exit point coincides with that obtained for the stationary case. Simulation of the exit point from this distribution is given in Ref. [10]. The random exit time can be efficiently simulated by Devroye's method [3].

It remains to describe the behavior of the excitons when they approach the boundary. The case of the Dirichlet condition is obvious: the trajectory terminates if the exciton hits Γ_ε. The case of Robin boundary condition is more complicated. The Robin boundary conditions can be approximated in a small distance h from the boundary to within an accuracy of $O(h)$ if the boundary is smooth. Let us write a finite-difference approximation of the boundary condition

$$h^{-1}D[w(\mathbf{r},t)-w(\mathbf{r}-h\boldsymbol{\nu}_k,t)]+S_k w(\mathbf{r},t)=S_i\delta_{ik}, \quad (25)$$

and rewrite (25) in the form

$$w(\mathbf{r},t)=(1-p_h)w(\mathbf{r}-h\boldsymbol{\nu}_k,t)+p_h\delta_{ik}, \quad (26)$$

where

$$p_h=\frac{hS_k}{D+hS_k}. \quad (27)$$

The representation (26) has a clear probabilistic interpretation as a total probability formula: with probability $1-p_h$ a random walk trajectory is reflected at the point first entering Γ_ε in the direction opposite to the normal direction $\boldsymbol{\nu}_k$ to the point $\mathbf{r}-h\boldsymbol{\nu}_k$. With the probability p_h, the trajectory is terminated, the counter is scored with 1 if $k=i$, and 0 otherwise. The case of the Neumann boundary condition corresponds to $S=0$ in the Robin condition, hence, $p_h=0$, which implies that the exciton is always reflected in this case. In practice, we recommend to choose the value of h proportional to $\sqrt{\varepsilon}$ while the value ε which defines the Γ_ε is taken proportional to the desired accuracy in calculation of w.

3 The transient CL intensity problem in a dislocation free crystal

The aim of this section is to find an analytical solution of the diffusion problem in half-space in the absence of dislocations, with a finite surface recombination velocity S at the planar surface. We obtain the solution for two cases, with reabsorption of excitons and without the reabsorption. The solution for the latter case is given by Ahrenkiel [1].

The problem is formulated as follows: find the solution $n(z,t)$ of the diffusion equation in the halfspace $0 \le z < \infty$

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial z^2} - \frac{n}{\tau} \tag{28}$$

with the initial condition

$$n(z,0) = \exp(-\alpha z) \tag{29}$$

and the boundary condition

$$\left(-D\frac{\partial n}{\partial z} + Sn\right)\bigg|_{z=0} = 0. \tag{30}$$

The quantities of interest are the fraction of excitons at time t, if the light is not absorbed on the way out:

$$I_{\text{noabs}}(t) = \alpha \int_0^\infty n(z,t)\,dz, \tag{31}$$

and the intensity when the light is absorbed on the way out:

$$I_{\text{abs}}(t) = \alpha \int_0^\infty n(z,t)\exp(-\alpha z)\,dz. \tag{32}$$

Solution of the problem (28)–(30) is (see [9], Sec. 1.1.3-6)

$$n(z,t) = \int_0^\infty G(z,\xi,t)\exp(-\alpha\xi)\,d\xi, \tag{33}$$

where

$$G(z,\xi,t) = \frac{e^{-t/\tau}}{2\sqrt{\pi D t}}\Big\{\exp\Big[-\frac{(z-\xi)^2}{4Dt}\Big] + \exp\Big[-\frac{(z+\xi)^2}{4Dt}\Big] \\ -2\frac{S}{D}\int_0^\infty \exp\Big[-\frac{(z+\xi+\eta)^2}{4Dt} - \frac{S}{D}\eta\Big]\,d\eta\Big\}. \tag{34}$$

Calculation of the integrals (31) and (32) gives

$$I_{\text{noabs}}(t) = \frac{\exp(-t/\tau)}{1 - S/\alpha D}\Big\{e^{S^2 t/D}\text{erfc}\Big(S\sqrt{t/D}\Big) - \frac{S}{\alpha D}e^{\alpha^2 Dt}\text{erfc}\Big(\alpha\sqrt{Dt}\Big)\Big\} \tag{35}$$

and

$$I_{\text{abs}}(t) = \\ \alpha\exp(-t/\tau)\Big\{\frac{\alpha D + S}{\alpha D - S}\sqrt{Dt/\pi} - \frac{DS}{(\alpha D - S)^2}e^{S^2 t/D}\text{erfc}\Big(S\sqrt{t/D}\Big) \\ +\Big[\frac{1}{2\alpha} - \alpha Dt - \frac{2\alpha SDt}{\alpha D - S} + \frac{DS}{(\alpha D - S)^2}\Big]e^{\alpha^2 Dt}\text{erfc}\Big(\alpha\sqrt{Dt}\Big)\Big\}. \tag{36}$$

At $t = 0$, the solutions are

$$I_{\mathrm{noabs}}(t)|_{t=0} = 1, \quad I_{\mathrm{abs}}(t)|_{t=0} = 1/2. \tag{37}$$

Note that the asymptotics at $t \to \infty$ are

$$I_{\mathrm{noabs}}(t) \propto t^{-1/2} \exp(-t/\tau), \quad I_{\mathrm{abs}}(t) \propto t^{-3/2} \exp(-t/\tau). \tag{38}$$

4 Simulation results

In this section we present simulation results. The computer simulations are based on the Monte Carlo algorithm described above. They were performed on the resources of the Siberian Supercomputer Center of the Siberian Branch of Russian Academy of Sciences [13].

The first test is for the case of a half-space with surface recombination velocity $S = 0$. The instantaneous source of excitons has a uniform distribution along the axes X, Y and an exponential distribution along the axis Z: $Q(\xi, \eta, \zeta) = \frac{1}{a} \exp(-\zeta/a)$. The computer experiment uses the following modeling parameters in nanoscales: the diffusion coefficient $D = 200000$ $\mathrm{nm}^2/\mathrm{ns}$, the absorption rate $1/\tau = 2.23\,\mathrm{ns}^{-1}$, $a = 1/\alpha = 100$, the number of trajectories $N = 10^6$. The size of the ε-boundary was chosen as $\varepsilon = 10^{-3}$ nm.

Formulas (35) and (36) at $S = 0$ take the following form:

$$I_{\mathrm{noabs}}(t) = \exp(-t/\tau), \tag{39}$$

$$I_{\mathrm{abs}}(t) = \frac{\exp(-t/\tau)}{a} \Big[\sqrt{\frac{Dt}{\pi}} + \Big(\frac{a}{2} - \frac{Dt}{a}\Big) \exp\Big(\frac{Dt}{a^2}\Big) \mathrm{erfc}\Big(\frac{\sqrt{Dt}}{a}\Big) \Big]. \tag{40}$$

The Figure 1 presents the concentration of survived excitons (survived concentration) to the time t calculated by the formulas (39), (40) and obtained by the simulation. The plots are shown in the logarithmic scale, the time is measured in nanoseconds.

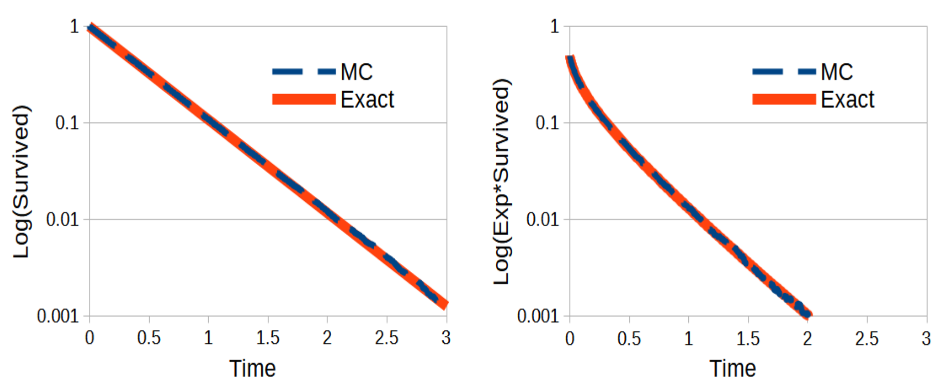

Рис. 1. Comparison of the simulation results and the exact solution for a half-space with $S = 0$ on the plane $z = 0$, and an instantaneous source with exponential distribution $Q(\xi, \eta, \zeta) = \frac{1}{a} \exp(-\zeta/a)$.

The plot "Survived"differs from the plot "ExpSurvived"in that the plot "ExpSurvived"shows concentrations weighted by $\exp(-\alpha z)$. The plot "Survived"corresponds to the case when the light is not absorbed on the way out ($I_{\rm noabs}(t)$). The plot "ExpSurvived"corresponds to the case when the light is absorbed on the way out ($I_{\rm abs}(t)$). The plots are shown in the logarithmic scale, the time is measured in nanoseconds. As shown in the figure, the results of the computer simulations are in a perfect agreement with the exact solutions.

The second test is for the case of a half-space $z \geq 0$ with an embedded array of threading dislocations. The dislocations are assumed to be circular semi-cylinders of radius R_{dis} with Dirichlet boundary conditions on their surfaces. On the plane $z = 0$ the reflecting boundary conditions are prescribed.

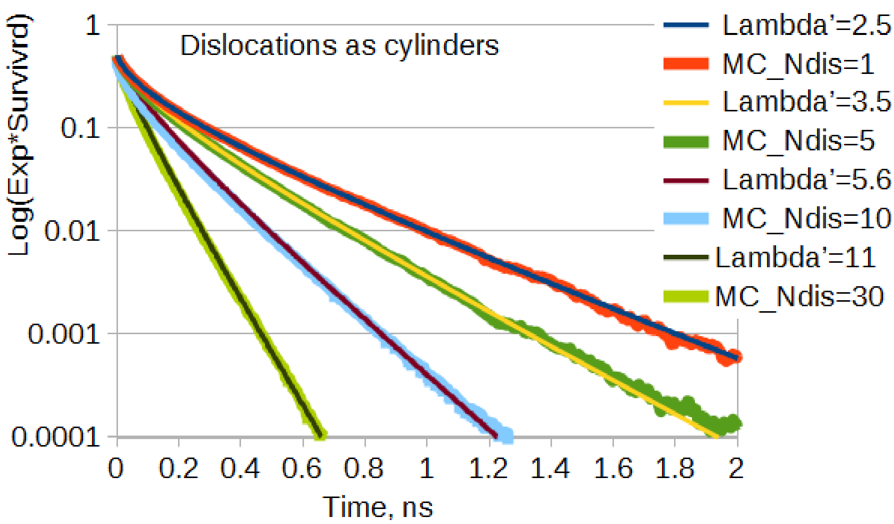

Рис. 2. Survived concentration obtained by the computer simulation for different number of dislocations: "MC_Ndis=1 "MC_Ndis=5 "MC_Ndis=10 "MC_Ndis=30"for 1, 5, 10, 30 dislocations, respectively. The curves present the comparison of the simulation results with the exact solution calculated by the formula (36) for various values of $\lambda = 1/\tau$: "Lambda=2.5 "Lambda=3.5 "Lambda=5.6 "Lambda=11".

The following modeling parameters are taken in the computer simulations: the diffusion coefficient $D = 200000\,\mathrm{nm}^2/\mathrm{ns}$, the absorption rate $1/\tau = 2.23\,\mathrm{ns}^{-1}$, the diffusion length $L = 300$ nm, the recombination rate on the plane $z = 0$: $S = 0\,\mathrm{nm}/\mathrm{ns}$, the dislocation radius $R_{dis} = 3$ nm, the number of trajectories $N = 10^6$. The source of excitons is uniformly distributed in the XY plane and has the exponential distribution along the axis Z: $Q(\xi, \eta, \zeta) = \frac{1}{100}\exp\left(-\zeta/100\right)$. The size of the domain representing a semiconductor is taken equal to $X_{\rm s} \times Y_{\rm s} = 1000 \times 1000$ nm^2 along the axes X and Y and unbounded along the axis Z. Periodic boundary conditions along the axes X and Y are prescribed. The dislocation centers are randomly distributed on the XY plain.

The Figure 2 shows the survived concentration weighted by $exp(-\alpha z)$ obtained by the simulation for different number of dislocations $Ndis$.

These curves can be calculated using the formula (36) for different values of $\lambda = 1/\tau$. For example, in Figure 2, the survived concentration obtained by the computer simulation for one dislocation (which corresponds to the dislocation density 10^{-6} per nm^2) agrees with the exact solution calculated by the formula (36) for $\lambda = 2.5$. The simulation results for 5, 10, 30 dislocations agree with the exact solutions for $\lambda = 3.5,\ 5.6,\ 11$, respectively.

The next test differs from the previous one only in the way how the dislocations are modeled. According to [6], the lifetime τ depends on the distance from the dislocation outcrop due to the piezoelectric field of the dislocation. This dependence is taken into account, and dislocation is modeled not by cylinder, but by a field with specified lifetime values.

In this case the survived concentration agrees with the exact solution calculated using the formula (36) for various values of surface recombination velocity S at the planar surface.

The Figure 3 shows the survived concentration weighted by $exp(-\alpha z)$ obtained by the simulation for different number of dislocations $Ndis$, where dislocations are modeled as a field.

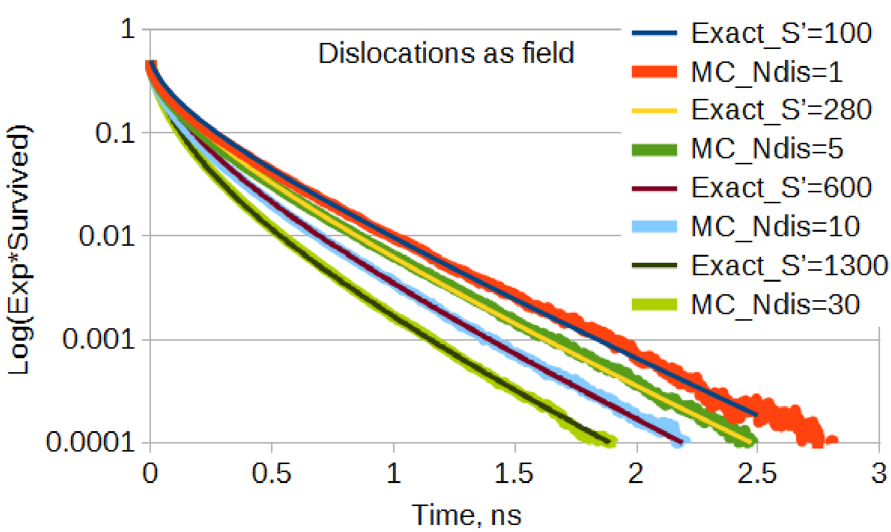

Рис. 3. Survived concentration obtained by the computer simulation for different number of dislocations $Ndis$, where dislocations are modeled as a field. Comparison of the simulation results with the exact solution calculated by the formula (36) for various values of S.

As shown in the figure, the results of the computer simulations are in a perfect agreement with the exact solutions for various values of S. For example, the survived concentration obtained by the computer simulation for one dislocation agrees with the exact solution calculated by the formula (36) for $S = 100$. The simulation results for 5, 10, 30 dislocations agree with the exact solutions for $S = 280,\ 600,\ 1300$, respectively.

Conclusion

The time-resolved photoluminescence in a layer of GaN with an embedded array of threading dislocations is studied by computer simulations. We develop an exciton transport model in the form of a 3D transient drift-diffusion-recombination equation with mixed Dirichlet and Robin boundary conditions on the plane surface and the cylindrical boundaries of the dislocations. A stochastic simulation algorithm is constructed which solves this problem by tracking exciton trajectories. The drift of the excitions is affected by the piezoelectric fields around the dislocations. The parameters of the piezoelectric field, the exciton's diffusion length and its mean life time are taken from the experimental study published recently in our triple article (Phys. Rev. Applied, v.17 (2023)). By a series of computer simulations we have established a relation between the photoluminescence intensity and the dislocation density. As a byproduct, we have shown that from a transient photoluminescence curve it is possible to extract the dislocation density with high resolution.

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