On the qualitative characteristics of a two-dimensional mathematical model of diffusion of minority charge carriers generated by a low-energy electron beam in a homogeneous semiconductor material

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Abstract. The problem of two-dimensional diffusion of excitons generated by a pulsating sharply focused low-energy electron beam in a single-crystal gallium nitride was considered by mathematical modeling methods. For the describing the energy loss by electrons in a semiconductor target, a mathematical model is used, based on a separate description of the energy loss by electrons that have experienced small-angle scattering and are absorbed by the target and electrons that have been reflected at large angles and left the target. The main attention is paid to the solution of the differential equations of heat and mass transfer and to the problems of their correctness and stability.

1. Introduction
A quantitative description of the diffusion of minority charge carriers (MCC) is largely crucial for the correct identification of the parameters of a semiconductor material by time-of-flight measurements. The essence of time-of-flight cathodoluminescent (CL) measurements [1, 2] is as follows. On the surface of the investigated semiconductor mask is applied, impermeable to CL radiation – see figure 1. The mask has a round hole of a known radius. CL radiation is excited at the center of the hole by means of a focused pulsed electron beam (electron probe) and the radiation arising in a semiconductor is recorded in the spectral region characteristic for recombination of generated particles, for example, free excitons in gallium nitride, a promising material for optoelectronics and microwave technology. After the balance between generation and recombination processes is established in the sample, the excitation stops: the electron beam is deflected by the blanking system onto the mask, the electrons do not fall on the semiconductor, the MCC does not appear in the semiconductor, and CL radiation is not excited. The nature of the following decrease in the intensity of the CL depends in general only on the known hole radius, the exciton lifetime, which can be obtained from the CL measurements of the semiconductor under study before the mask is applied, and the diffusion coefficient characterizing the motion of the excitons under the mask.
Figure 1. Scheme of the experiment.

Mathematical model describing the decrease in the intensity of CL, will let us to obtain estimates of the diffusion coefficient of excitons in the materials under study [3] based on the analysis of experimental data, by solving the corresponding inverse problem. In mathematical modeling of the lateral transport of excitons (a process realized in the thin surface region of a semiconductor), this problem was considered as two-dimensional – the use of such a model was justified at low electron energies of the probe.

2. Statement of the problem
The need for a mathematical study is due to the following. Previously, the problem of simulating the diffusion of excitons and their subsequent radiative recombination with the release of CL radiation from a semiconductor for the process in question was solved only by using the model of energy loss by primary electrons in the target (and, consequently, exciton generation) in the form of a two-dimensional normal Gaussian distribution, which is a rather rough approximation, describing the available experimental data on energy loss in a condensed substance only qualitatively [2-4]. Quantitative agreement with experiment is achieved using a mathematical model based on the separate description of energy loss by electrons that have experienced small-angle scattering and are absorbed by the target and electrons that have been reflected at large angles and left the target [5, 6]. The construction of a mathematical model of time-of-flight CL, which takes into account the peculiarities of the energy loss in a condensed substance and the evaluation of the effect of such an account on the results of a computational experiment, is the subject of this paper. In this case, the main attention is paid to the first stage of construction and research of the CL model: the solution of the differential equations of heat and mass transfer, the problems of their correctness and stability [4]. Note that physical processes (in particular, diffusion processes) are reduced to mathematical models that are described by initial or boundary-value problems for partial differential equations, therefore, the study requires solving a number of the following tasks: 1) establishing the existence of a solution; 2) proof of the uniqueness of the solution; 3) justification of the continuous dependence of the solution on the data of the problem (initial and boundary data, the free term, the coefficients of the operator equation).

Tasks that satisfy the requirements of 1)-3) are called correctly posed.

The study of this issue is very important, since the initial data and the parameters of the task have measurement error, and, as the classical example of J. Hadamard (see, for example, [7]) shows, with minor changes in the initial data, the solution of the problem can differ dramatically. The problem of the correctness of such models is rarely studied because of the great difficulties of a logical and technical nature, which also makes the present study very important.

3. Mathematical model of the process
The proposed mathematical model of the exciton diffusion in a round hole, as in [2-4], is described using the partial differential equation
\[ c_t = D \Delta c - c/\tau \]  

(1)

with initial condition

\[ c(x, y, 0) = n(x, y), \]

(2)

where \( c(x, y, t) \) is the exciton concentration at a point with coordinates \((x, y)\) at the time \( t \) instant, \( \Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2 \) is the two-dimensional Laplace operator, \( D \) is the diffusion coefficient and \( \tau \) is the life time of the excitons, and the function \( n(x, y) \) satisfies the stationary differential equation describing the two-dimensional diffusion of excitons in the quasi-equilibrium state:

\[ \Delta n - n/\lambda^2 = -\Phi(x, y), \]

(3)

where \( \lambda = \sqrt{D\tau} \) is the diffusion length of free excitons, and the function of the source of exciton generation \( \Phi(x, y) \), in contrast to \([2-4]\), is described not by the density function of a two-dimensional normal Gauss distribution, but more approximate to real conditions \([5, 6]\).

For the considered mathematical model, a solution is found, its uniqueness is proved, and continuous dependence on the initial data of the problem is established. Before formulating the main results, we introduce the following notation:

\[ \Pi_{xy} = \{(x, y): -\infty < x < +\infty, -\infty < y < +\infty\}, \quad \Pi = \{(t, x, y): t > 0, (x, y) \in \Pi_{xy}\}. \]

Note that in \([3, 4]\) the solution of problem (3) is given, which in the polar coordinate system is described by the formula

\[ n(r) = I_0(\chi r) \int_0^r K_0(\chi \eta) n_0 d\eta + K_0(\chi r) \int_0^r I_0(\chi \eta) n_0 d\eta, \]

(4)

where \( I_0(x), K_0(x) \) is the modified Bessel function of the first and second kind of zero order, respectively.

Using the formula for solving the heat equation \([3-5]\), a solution was obtained for problem (1)-(2)

\[ c(x, y, t) = \exp(-t/\tau) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} n(\xi, \eta) \exp \left\{ -\frac{r^2(\xi^2 + \eta^2)}{4Dt} \right\} d\xi d\eta \]  

(5)

4. Qualitative characteristics of the mathematical model

The following theorems establish the uniqueness of problems (1)-(2) and (3) in the plane, and, consequently, the general problem (1)-(3).

**Theorem 1.** The solution of problem (3) in the plane is unique.

**Proof.** Suppose the contrary. Let \( n_1 \) and \( n_2 \) be two different solutions of problem (3) in the plane. Consider a function \( u = n_2 - n_1 \) that satisfies the following differential equation
\[ \Delta u - u/\lambda^2 = 0 \]

and tends to zero at infinity.

Applying formula (4) with \( \Phi(x, y) = 0 \) to obtained problem, we get from where \( u = 0 \). The obtained contradiction proves the uniqueness of the solution of the problem (3) in the plane.

**Theorem 2.** The solution to problem (1)-(2) is unique.

**Proof.** Making in equation (1) and the initial condition (2) a replacement \( (x, y) = 0 \), we get for the function \( \Phi(x, y) = 0 \). The obtained contradiction proves the uniqueness of the solution of the problem (1)-(2).

Following V.S. Vladimirov [7], the continuous dependence of the solution \( u \) on the data \( D \) of the problem means the following: let the sequence of data, \( D_k \), \( k \to \infty \) and, \( u_k, k = 1, 2, ... \) be the corresponding solutions of the problem; then it must be \( u_k \to u, k \to \infty \) in the sense of a properly chosen convergence.

The following theorems establish the continuous dependence of the solution of problem (1)-(3) on the term on the right-hand side. The proof of these theorems is based on the uniqueness of problem (1)-(3), as well as on formulas for solutions (4) and (5).

**Theorem 3.** Let \( n_1(x, y) \) be the solution of the equation \( \Delta n - n/\lambda^2 = -\Phi_1(x, y) \), \( n_2(x, y) \) be the solution of the equation \( \Delta n - n/\lambda^2 = -\Phi_2(x, y) \) and for all \((x, y) \in \Pi_{xy}\)

\[ |\Phi_2(x, y) - \Phi_1(x, y)| \leq \epsilon. \] (8)

Then for all \((t, x, y) \in \Pi\) fair assessment \[ |n_2(x, y) - n_1(x, y)| \leq \lambda^2 \cdot \epsilon. \]

**Proof.** By alternately applying formula (4) for the functions \( n_1 \) and \( n_2 \), we obtain

\[ n_1(r) = I_0(\chi r)\int_0^r \Phi_1(\theta)K_0(\chi r_0)\theta d\theta + K_0(\chi r)\int_0^r \Phi_1(\theta)I_0(\chi r_0)\theta d\theta, \]

\[ n_2(r) = I_0(\chi r)\int_0^r \Phi_2(\theta)K_0(\chi r_0)\theta d\theta + K_0(\chi r)\int_0^r \Phi_2(\theta)I_0(\chi r_0)\theta d\theta. \]

Subtracting the second equality from the first and taking into account the estimate (8), we have

\[ |n_2(r) - n_1(r)| \leq \epsilon I_0(\chi r)\int_0^r K_0(\chi r_0)\theta d\theta + \epsilon K_0(\chi r)\int_0^r I_0(\chi r_0)\theta d\theta. \] (9)

Applying to (9) the formulas

\[ \int_a^\infty xK_0(x)dx = aK_1(a), \int_0^a xI_0(x)dx = aI_1(a), I_v(z)K_{v+1}(z) + I_{v+1}(z)K_v(z) = 1/z, \]

will get
\[ |n_2(r) - n_1(r)| \leq \varepsilon \left( \frac{1}{\varepsilon^2} \int r r_0(\varepsilon r) K_1(\varepsilon r) + \frac{1}{\varepsilon^2} \int r r_1(\varepsilon r) K_0(\varepsilon r) \right) = e\lambda^2. \]

**Theorem 4.** Let \( c_1(x, y) \) the solution of equation (1) with the initial condition \( c_1(x, y, 0) = n_1(x, y) \), and \( c_2(x, y) \) be the solution of equation (1) with the initial condition \( c_2(x, y, 0) = n_2(x, y) \) and for all \( (x, y) \in \Pi_{xy} \)

\[ |n_2(x, y) - n_1(x, y)| \leq \delta. \] \hspace{1cm} (10)

Then for all \( (t, x, y) \in \Pi \) fair assessment \( |c_2(x, y, t) - c_1(x, y, t)| \leq \delta. \)

**Proof.** Applying alternately formula (5) to the tasks for the functions \( c_1 \) and \( c_2 \), we get

\[ c_1(x, y, t) = \frac{\exp(-t / \tau)}{4\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} n_1(\xi, \eta) \exp \left\{ -\frac{r^2(\xi, \eta)}{4\tau t} \right\} d\xi d\eta, \]

\[ c_2(x, y, z, t) = \frac{\exp(-t / \tau)}{4\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} n_2(\xi, \eta) \exp \left\{ -\frac{r^2(\xi, \eta)}{4\tau t} \right\} d\xi d\eta. \]

Subtracting the second equality from the first and taking into account the estimation (10), we have

\[ |c_2(x, y, t) - c_1(x, y, t)| \leq \delta \exp(-t / \tau) \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} n_2(\xi, \eta) \exp \left\{ -\frac{r^2(\xi, \eta)}{4\tau t} \right\} d\xi d\eta. \] \hspace{1cm} (11)

Using the Fubini theorem and the Poisson integral, we rewrite the estimation (11) as

\[ |c_2(x, y, t) - c_1(x, y, t)| \leq \delta \exp(-t / \tau) \]

and therefore, for all \( (t, x, y) \in \Pi \) fair assessment

\[ |c_2(x, y, t) - c_1(x, y, t)| \leq \delta. \]

**Theorem 5.** Let \( c_1(x, y) \) be the solution of equation (1) with the initial condition \( c_1(x, y, 0) = n_1(x, y) \), \( c_2(x, y, 0) = n_2(x, y) \) be the solution of equation (1) with the initial condition \( c_2(x, y, 0) = n_2(x, y) \) and for all \( (x, y) \in \Pi_{xy} \) functions \( n_1(x, y) \) and \( n_2(x, y) \) satisfy the conditions of Theorem 3. Then for all \( (t, x, y) \in \Pi \) fair assessment

\[ |c_2(x, y, t) - c_1(x, y, t)| \leq \lambda^2 \cdot \varepsilon. \]

The proof of Theorem 5 immediately follows from Theorems 3 and 4.

**5. Evaluation of the solution of the mathematical model**

Let us estimate the solution of the problem (3). As was shown above, this solution is described by the formula (4).

Denote

\[ c_0 = \frac{1.085(1 - \eta)P_0}{\pi^2 \alpha^2 z_m \left( 1 - \eta + \eta \frac{z_m}{z_m} \right)} \left\{ 1 + \frac{\eta a^2}{(1 - \eta) a^2} \right\}. \]
\[ A_1(r) = I_0(\chi r) \int r \Phi(r_0) K_0(\chi r_0) r_0^2 dr_0, \quad A_2(r) = K_0(\chi r) \int r \Phi(r_0) I_0(\chi r_0) r_0^2 dr_0. \]

Notice, that
\[ \Phi(x,y) \leq c_\phi \text{ for all } (x,y) \in \Pi_{xy}. \quad (12) \]

Applying to \( A_1(r) \) the estimate (12) and the formula \( \int_a^\infty x K_0(x) dx = a K_1(a) \), we get
\[ A_1(r) \leq c_\phi I_0(\chi r) \int r K_0(\chi r_0) r_0^2 dr_0 - \frac{c_\phi F}{\chi} I_0(\chi r) K_1(\chi r). \quad (13) \]

Similarly, taking into account the formula \( \int_0^a x I_0(x) dx = a I_1(a) \) for \( A_2(r) \), we get the estimation
\[ A_2(r) \leq c_\phi r K_0(\chi r) I_1(\chi r) / \chi. \quad (14) \]

Applying to (4) successively estimates (13), (14) and the formula \( I_{\nu}(z) K_{\nu+1}(z) + I_{\nu+1}(z) K_{\nu}(z) = 1/2 \), we conclude
\[ n(r) \leq c_\phi / \chi^2 = c_\phi \lambda^2. \quad (15) \]

Note that for large values \( r \) in formula (4), the main contribution comes from the expression \( c_\phi \lambda^2 \), the following terms are infinitesimal, i.e. the asymptotic formula \( n(r) = c_\phi \lambda^2 (1 + o(1)) \) is valid. We also note that in [3-5] the right-hand side of equation (3) was given by a function \( \Psi(x,y) = G_0 \varphi(x,y) / \lambda^2 \), \( G_0 \) is the frequency of generation of the excitons, and \( \varphi(x,y) = \exp \left\{ -\left[ (x-m_x)^2 / \sigma_x^2 + (y-m_y)^2 / \sigma_y^2 \right] / 2 \pi \sigma_x \sigma_y \right\} \) is the density of the two-dimensional normal Gaussian distribution.

Carrying out similar reasoning for the model in [3-5], we get
\[ n(r) \leq c_\psi \lambda^2, \quad c_\psi = G_0 \pi \left( 2 \pi \sigma_x \sigma_y \lambda^2 \right). \quad (16) \]

Note that due to the estimates (15) and (16) and the similarity of the right-hand sides \( \Phi \) and \( \Psi \) in equation (3), the graphs for the functions of the corresponding values \( n \) and \( c \) do not practically differ (there are stretches and shifts that do not exceed in absolute value \( |c_\phi - c_\psi| \)).

6. Results of mathematical modeling

Mathematical modeling of exciton diffusion was carried out for semiconductor parameters characteristic of gallium nitride, which is a promising material for creating opto-, micro-, and nanoelectronic devices capable of operating at high voltages as well as in adverse environmental conditions. The frequency of exciton generation was taken to be \( G_0 = 10^{13} \text{ c}^{-1} \), and the energy distribution profile of electrons in the beam was specified by a Gaussian function with zero expectation and dispersion of 60 nm, which corresponds to the conditions of real experimental CL measurements.

Figure 2 shows the results of mathematical modeling of the obtained solution (4) of the stationary equation of lateral diffusion of excitons (3) for different values of the diffusion coefficient \( D \). The
lifetime of excitons here was assumed to be equal to $\tau = 271$ ps. The results obtained in the calculations were normalized to their maximum value.

![Figure 2](image2.png)

**Figure 2.** The normalized density of excitons for various values of the diffusion coefficient $D$: 1 – 0.2, 2 – 0.55, 3 – 0.9, 4 – 1.6 cm$^2$/s. The calculations were performed by formula (4) for the material parameters characteristic of a homogeneous GaN. Lifetime excitons is $\tau = 271$ ps.

The profiles of the dependence of the density of excitons on the coordinates have a Gaussian shape. The larger profiles $D$ decrease more hollowly, which corresponds to the following physical interpretation of the problem: with increasing excitons diffuse into more and more distant points from the origin of coordinates (center of the electron beam). In this case, for $r > 0.6$ mkm, the exciton density is less than 0.1 of the maximum for all the presented dependences, which can give the first rough estimate for the upper limit for the radius of the hole in the mask, which can be used to obtain correct results in experimental measurements.

![Figure 3](image3.png)

**Figure 3.** Exciton density for various values of the time $t$ elapsed since the electron beam was turned off: 1 – 0 ns, 2 – 0.01 ns, 3 – 0.14 ns, 4 – 0.27 ns, 5 – 0.4 ns. Diffusion coefficient $D = 1.2$ cm$^2$/s. Calculations are performed by formula (5) for material parameters characteristic of GaN. Exciton lifetime $\tau = 271$ ps.
Figure 3 presents the results of mathematical modeling of the obtained solution (5) of the nonstationary equation of lateral diffusion of excitons (1) for various values of time \( t \) elapsed since the electron beam deviated from the sample. The results obtained in the calculations were normalized to the maximum value at \( t = 0 \). The lifetime of excitons was assumed to be equal to \( \tau = 271 \text{ ps} \), the diffusion coefficient of excitons \( D = 1.2 \text{ cm}^2/\text{s} \).

Analysis of curves of figure 3 shows that with an increase in time, the density of excitons decreases very rapidly and reaches rather small values already after an interval of less than \( 2\tau \) s. The exciton density profiles for large values \( t \) are gentler as a result of the exciton diffusion. In this case, the most part of the excitons are concentrated in the region of \( |x| < 0.5 \text{ mkm} \); therefore, when conducting an experiment, in order to obtain correct results for estimating the diffusion coefficient, it is desirable to choose an orifice even smaller than the radius than this value.

7. Conclusions
The qualitative properties of the constructed two-dimensional mathematical model of diffusion of particles generated by a low-energy electron beam in a semiconductor material based on a separate description of energy loss by electrons that have experienced small-angle scattering and are absorbed by the target and electrons that have been reflected at large angles and left the target have been studied. For the model under study, the uniqueness of the solution is proved, the continuous dependence of the solution (output data) on the input data is established, the solution is estimated. The results can be used when planning an experiment in electron probe technology.

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