Infocommunications and Radio Technologies, 2021, vol. 4, no. 2, pp. 85–94.
Инфокоммуникационные и радиоэлектронные технологии. 2021. Т. 4, № 2. С. 85—94.
ISSN: 2587-9936

On some problems of modeling the processes of interaction of wide electron beams with planar microwave structures based on gallium nitride

M. A. Stepovich [1], V. V. Kalmanovich [1], and M. N. Filippov [2]

[1] *Department of Physics and Mathematics, Tsiolkovsky Kaluga State University*
Kaluga, 248023, Russian Federation
m.stepovich@rambler.ru, v572264@yandex.ru
[2] *Chemical Analysis Laboratory,*
Kurnakov Institute of General and Inorganic Chemistry RAS
Moscow, 119071, Russian Federation
fil@igic.ras.ru

Received: May 19, 2021
Peer-reviewed: September 16, 2021
Accepted: September 16, 2021

Abstract: *The problem of mathematical modeling of the diffusion of nonequilibrium minority charge carriers generated by kilovolt electrons in semiconductor targets is considered. Models are considered that make it possible to perform calculations in homogeneous targets and multilayer planar semiconductor structures. In carrying out the calculations, the matrix method was used, which makes it possible to solve the differential equations of heat and mass transfer in multilayer planar structures with an arbitrary number of layers. Some results of mathematical modeling of the processes of interaction of wide electron beams with planar structures for GaN and substrate materials (SiC and Si) are presented.*

Keywords: *mathematical modeling, semiconductors, wide electron beam, minority charge carrier, diffusion.*

For citation (IEEE): M. A. Stepovich, V. V. Kalmanovich, and M. N. Filippov, “On some problems of modeling the processes of interaction of wide electron beams with planar microwave structures based on gallium nitride”, *Infocommunications and Radio Technologies*, 2021, vol. 4, no. 2, pp. 85–94.

УДК 621.396.67(075.8) + 621.397.6(075.8)

О некоторых проблемах моделирования процессов взаимодействия широких электронных пучков с планарными микроволновыми структурами на основе нитрида галлия

[1] Степович М. А., [1] Калманович В. В., [2] Филиппов М. Н.

[1] *Физико-математический факультет,*
Калужский государственный университет им. Циолковского
Калуга, 248023, Российская Федерация
m.stepovich@rambler.ru, v572264@yandex.ru
[2] *Лаборатория химического анализа,*
Институт общей и неорганической химии им. Курнакова РАН
Москва, 119071, Российская Федерация
fil@igic.ras.ru

Получено: 19 мая 2021 г.
Отрецензировано: 16 сентября 2021 г.
Принято к публикации: 16 сентября 2021 г.

Аннотация: *Рассмотрена проблема математического моделирования диффузии неравновесных неосновных носителей заряда, генерируемых киловольтными электронами, в полупроводниковых мишенях. Рассмотрены модели, позволяющие проводить расчеты в однородных мишенях и многослойных планарных полупроводниковых структурах. При проведении расчетов использовался матричный метод, позволяющий решать дифференциальные уравнения тепломассопереноса в многослойных планарных структурах с произвольным числом слоев. Приведены некоторые результаты математического моделирования процессов взаимодействия широких электронных пучков с планарными структурами для GaN и материалов подложки (SiC и Si).*

Ключевые слова: *математическое моделирование, полупроводники, широкий электронный пучок, неосновные носители заряда, диффузия.*

Для цитирования (ГОСТ 7.0.5—2008): Степович М. А., Калманович В. В., Филиппов М. Н. О некоторых проблемах моделирования процессов взаимодействия широких электронных пучков с планарными микроволновыми структурами на основе нитрида галлия // Инфокоммуникационные и радиоэлектронные технологии. 2021. Т. 4, № 2. С. 85—94.

Для цитирования (ГОСТ 7.0.11—2011): Степович, М. А. О некоторых проблемах моделирования процессов взаимодействия широких электронных пучков с планарными микроволновыми структурами на основе нитрида галлия / М. А. Степович, В. В. Калманович, М. Н. Филиппов // Инфокоммуникационные и радиоэлектронные технологии. — 2021. — Т. 4, № 2. — С. 17—94.

1. Introduction

Gallium, indium and aluminum nitrides are promising materials for micro-, opto- and microwave electronics [1, 2]. The properties of these materials [3] are such that semiconductor devices based on them can operate at high voltages, temperatures and in adverse environmental conditions, for example, under radiation exposure – in nuclear reactors or in space. Because of this, the problem of studying the process of heat and mass transfer in these semiconductor materials and structures based on them is of interest both from a theoretical point of view of describing physical processes and from a practical point of view of technology for creating, improving and using semiconductor devices.

One of the few methods that allow non-contact non-destructive diagnostics of such objects are electron probe methods based on the use of beams of kilovolt electrons. Registration of informative signals excited in the target and comparison of experimental data with the mathematical model of the phenomenon under study allow us to identify target parameters that are very difficult or even impossible to determine using other methods [4, 5].

This paper discusses some of the problems of modeling the processes of interaction of wide electron beams with homogeneous materials and planar microwave structures based on gallium nitride.

2. Homogeneous materials

2.1. Collective diffusion model

In this case, the differential equation for the diffusion of nonequilibrium minority charge carriers (MCCs) generated by a wide electron beam in a semi-infinite homogeneous semiconductor target has the classical form [6, 7]:

$$D\frac{\mathrm{d}^2\Delta p(z)}{\mathrm{d}z^2}-\frac{\Delta p(z)}{\tau}=-\rho(z) \tag{1}$$

with boundary conditions

$$D\frac{\mathrm{d}\Delta p(z)}{\mathrm{d}z}\bigg|_{z=0}=\upsilon_s\Delta p(0),\ \Delta p(\infty)=0. \tag{2}$$

Here D, L, τ are electrophysical parameters: diffusion coefficient, diffusion length and lifetime of the MCC, respectively, while $L=\sqrt{D\tau}$, and ν_s is the rate of surface recombination of the MCC. The function $\Delta p(z)$ describes the depth distribution of non-equilibrium MCCs generated by an external energy impact

after their diffusion in the semiconductor. Function $\rho(z)$ is the dependence on the coordinate of the density of MCCs generated by an electron beam in a semiconductor target prior to their diffusion. The solution to problem (1), (2) is given in [6, 7] For a wide electron beam $\rho(z)$ can be found from the expression for the energy density of the electron beam released in the target per unit time before the start of the diffusion process [8].

2.2. Independent sources model

The diffusion of MCCs generated in a semiconductor target by an electron beam is modeled using the model, according to which the diffusion of nonequilibrium MCCs generated by an electron beam from any microvolume of the semiconductor is not affected by other electrons or holes from other microregions of the material. In this case, for one-dimensional diffusion in a semi-infinite semiconductor, the depth distribution of excess MCCs is given by the expression

$$\Delta p(z) = \int_0^\infty \Delta p(z, z_0)\, dz_0.$$

The function $\Delta p(z, z_0)$ describes the distribution over the depth of the MCCs generated by a plane infinitely thin source located at a depth z_0, $z_0 \in [0, \infty)$; z is the coordinate measured from the flat surface into the interior of the semiconductor.

The distribution $\Delta p(z, z_0)$ is found as a solution to the differential equation

$$D\frac{\mathrm{d}^2 \Delta p(z, z_0)}{\mathrm{d}z^2} - \frac{\Delta p(z, z_0)}{\tau} = -\rho(z)\delta(z - z_0) \qquad (3)$$

with boundary conditions

$$D\frac{\mathrm{d}\Delta p(z, z_0)}{\mathrm{d}z}\bigg|_{z=0} = \upsilon_s \Delta p(0, z_0),\ \Delta p(\infty, z_0) = 0. \qquad (4)$$

From the solution (3), (4) we find the required distribution of MCCs after their diffusion.

Note that model (3), (4), in principle, allows modeling layered structures with different material parameters in each layer.

3. Inhomogeneous materials

3.1. Model for a semi-infinite multilayer planar semiconductor structure based on the model of independent sources

Initially, to solve this problem for a multilayer semiconductor structure, standard methods of mathematical analysis were used. Using these methods (see

(3), (4)), we have obtained a solution only for two-layer and three-layer structures [9, 10]. An attempt to obtain an analytical solution for an arbitrary number of layers of a multilayer structure was unsuccessful. This problem was solved using the matrix method (see below).

3.2. Model of diffusion of non-equilibrium minority charge carriers generated by wide electron beam in a multilayer semiconductor target with final thickness

In the case of one-dimensional diffusion into the final semiconductor along the OZ axis, perpendicular to the surface of the n-layer semiconductor structure $\left(z \in [0, l]\right)$, the depth distribution of the MCC is found as a solution to the differential equation:

$$D^{(i)}(z)\frac{\mathrm{d}^2\Delta p^{(i)}(z)}{\mathrm{d}z^2} - \frac{\Delta p^{(i)}(z)}{\tau^{(i)}(z)} = -\rho^{(i)}(z),\ i = \overline{1,n}, \tag{5}$$

with boundary conditions

$$D^{(1)}\left.\frac{\mathrm{d}\Delta p^{(1)}(z)}{\mathrm{d}z}\right|_{z=0} = \nu_s^{(1)}\Delta p^{(1)}(0),$$

$$D^{(n)}\left.\frac{\mathrm{d}\Delta p^{(n)}(z)}{\mathrm{d}z}\right|_{z=l} = -\nu_s^{(n)}\Delta p^{(n)}(l). \tag{6}$$

The superscript in parentheses indicates the layer number. For a multilayer structure, we denote: $z_1 = 0$, $z_{n+1} = l$ - the outer boundaries of the semiconductor, z_2, z_3, ..., z_n - the coordinates of the interfaces of the layers; $D^{(i)}$, $L^{(i)}$, $\tau^{(i)}$ are parameters: diffusion coefficient, diffusion length and lifetime of the MCC in the i-th layer, respectively, while $L^{(i)} = \sqrt{D^{(i)}\tau^{(i)}}$, $i = \overline{1,n}$. At the boundaries of the semiconductor (at $z = 0$ and at $z = l$) the reduced rates of surface recombination $S^{(1)} = L^{(1)}\nu_s^{(1)}/D^{(1)}$, $S^{(n)} = L^{(n)}\nu_s^{(n)}/D^{(n)}$, where $\nu_s^{(1)}$ and $\nu_s^{(n)}$ are the rates of surface recombination of the MCC in the first and n-th layers, respectively. The function $\Delta p^{(i)}(z)$ describes the depth distribution in the i-th layer of non-equilibrium MCCs generated by an external energy impact after their diffusion in the semiconductor. Function $\rho^{(i)}(z)$ is the dependence on the coordinate of the density of MCCs generated by an electron beam in a semiconductor target prior to their diffusion. For a wide electron beam, it can be found from the expression for the energy density of the electron beam released in the target per unit time before the start of the diffusion process [8]. The solution to problem (5), (6) can be obtained by the matrix method [11, 12].

4. Results of mathematical modeling

Some results of mathematical modeling of the processes of interaction of wide electron beams with planar structures for GaN and substrate material SiC and Si are shown in fig. 1 and fig. 2.

Fig. 1 shows the distributions of the MCC $\Delta p(z)$ generated by the electron beam in the semiconductor structure "GaN film-GaN substrate" for various thicknesses and beam electron energies: 5, 10, 15, 20, 25 and 30 keV. The following parameter values were used: for a GaN film $L = 35\ \mu\text{m}$, $\tau = 10^{-6}$ s, $S = 30$, $v_s = 1.05 \cdot 10^9\ \mu\text{m/s}$, $D = 1.22 \cdot 10^9\ \mu\text{m}^2/\text{s}$; similar values for a GaN substrate are $L = 30\ \mu\text{m}$, $\tau = 10^{-5}$ s, $S = 30$, $v_s = 9 \cdot 10^7\ \mu\text{m/s}$ and $D = 9 \cdot 10^7\ \text{mkm}^2/\text{s}$. The layer thicknesses are as follows: a – 0.5 μm thick (0.1 μm GaN film and 0.4 μm GaN substrate); b – 1.9 μm thick (0.1 μm GaN film and 1.8 μm GaN substrate); c – 3.6 μm thick (0.1 μm GaN film and 3.5 μm GaN substrate). The parameters of the film and substrate are selected so as to show the influence of the thickness of the structure and the energy of primary electrons on the MCCs distributions.

The curves shown in fig. 2 illustrate the influence of the electron beam energy and electrophysical parameters of GaN on the results of diffusion of MCCs. At an electron beam energy of 10 keV, almost all of their energy is released in a 0.5 mkm thick target – see figure 1a. An increase in the beam energy for a film of this thickness leads to a decrease in the energy lost in the target (figure 1a) and, as a consequence, to a decrease in the generated MCCs. The smaller value for 10 keV, as compared to the distribution at 20 keV, may be associated with stronger influence of surface MCC recombination. Note that the value of the reduced rate of surface recombination is quite large, and the value corresponds to an almost infinite rate of surface recombination.

Analysis of the parameters of various multilayer planar structures and processes for various electron energies [11, 12] suggests that for films with a relatively small thickness, model (5) can be used with the right-hand side $\rho(z)$, which is characteristic of the substrate material.

Otherwise, the calculations should use the parameters characteristic of the film material.

In such cases, on the right-hand side of equation (5), it is necessary to use one $\rho(z)$ that depends only on the parameters of the substrate or film, and this equation will have the following form:

$$D^{(i)}(z)\frac{\mathrm{d}^2\Delta p^{(i)}(z)}{\mathrm{d}z^2} - \frac{\Delta p^{(i)}(z)}{\tau^{(i)}(z)} = -\rho(z),\ i = \overline{1,n}.$$

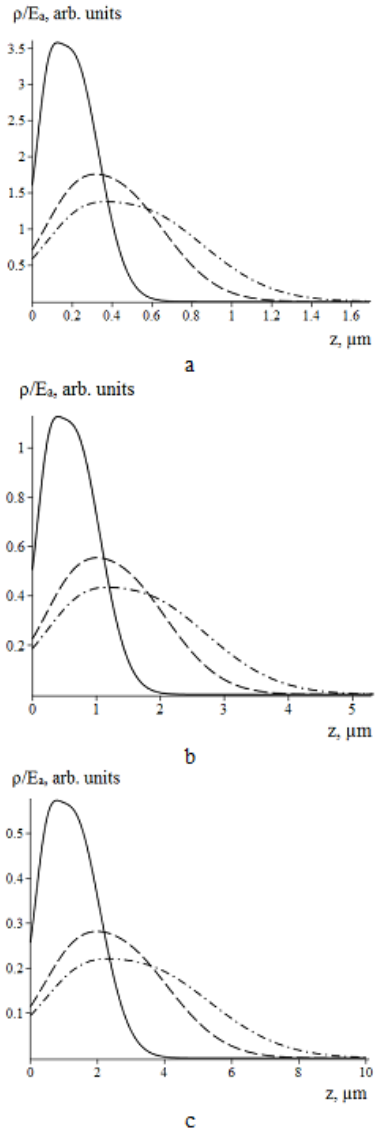

Fig. 1. Normalized to the power E_a, released in targets by an electron beam, energy losses by electrons in single-crystal gallium nitride (solid curves), silicon carbide (dashed lines) and silicon (dash-dotted lines). Energies of the beam electrons: 10 (a), 20 (b) and 30 (c) keV.

Рис. 1. Нормированные на мощность E_a, выделяемую в мишени электронным пучком, потери энергии электронами в монокристаллическом нитриде галлия (сплошные кривые), карбиде кремния (штриховые линии) и кремнии (штрихпунктирные линии). Энергии электронов пучка: 10 (a), 20 (b) и 30 (c) кэВ

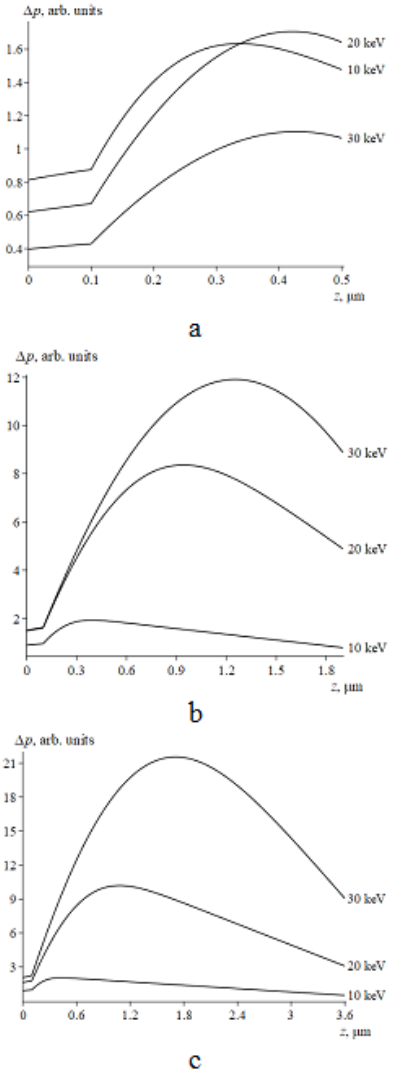

Fig. 2. Depth distributions of MCCs generated by an electron beam in a two-layer semiconductor structure of gallium nitride: a – 0.5 μm thick (0.1 μm GaN film and 0.4 μm GaN substrate); b – 1.9 μm thick (0.1 μm GaN film and 1.8 μm GaN substrate); c – 3.6 μm thick (0.1 μm GaN film and 3.5 μm GaN substrate). Electron energy of the beam: 10, 20, 30 keV.

Рис. 2. Распределение МСС по глубине, генерируемых электронным пучком в двухслойной полупроводниковой структуре из нитрида галлия: а — толщина 0,5 мкм (пленка GaN 0,1 мкм и подложка GaN 0,4 мкм); б — толщина 1,9 мкм (пленка GaN 0,1 мкм и подложка GaN 1,8 мкм); с — толщина 3,6 мкм (пленка GaN 0,1 мкм и подложка GaN 3,5 мкм). Энергия электронов пучка: 10, 20, 30 кэВ

5. Conclusions

The analysis of the considered models showed that the most acceptable is the matrix method, which allows one to obtain a solution to the problem in an analytical form. In this case, the best results are obtained when using as a substrate material one that has close parameters characterizing the energy dissipation in the film and substrate. In this case, the substrate parameters can be used on the right side of the differential equation.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research (RFBR), project no. 19-03-00271, and by the RFBR and the Government of Kaluga Region, project no. 18-41-400001.

References

1. Properties, processing and application of GaN and related semiconductors. J. H. Edgar, ed. London : INSPEC, 1999. 830 p.
2. Nitride (GaN) // Physics. Devices, and Technology. Farid Medjdoub and Krzystof Iniewski, eds. CRC Press, 2003. Chapter 3. P. 63–109.
3. Group III nitride semiconductor compounds. B. Gil, ed. Oxford : Oxford University Press, 1998. 492 p.
4. Scanning Microscopy for Nanotechnology. Techniques and Applications. W. Zhou and Z. L. Wang, eds. New York : Springer, 2007. 522 p.
5. SEM Microcharacterization of Semiconductors. D. B. Holt and D. C. Joy, eds. London : Academic Press, 1989. 452 p.
6. Wittry D. B., Kyser D. F. Measurements of diffusion lengths in direct-gap semiconductors by electron beam excitation // J. Appl. Phys. 1967. Vol. 38, no. 1. P. 375–382.
7. Everhart T. E., Hoff P. H. Determination of kilovolt electron energy dissipation versus penetration distance in solid materials // J. Appl. Phys. 1971. Vol. 42, no. 13. P. 5837–5846.
8. Mikheev N. N., Stepovich M. A. Distribution of energy losses in interaction of an electron probe with material // Industrial Laboratory. 1996. Vol. 62, no. 4. P. 221–226.
9. Stepovich M. A., Khokhlov A. G., Snopova M. G. Model of independent sources used for calculation of distribution of minority charge carriers generated in two-layer semiconductor by electron beam // Proc. SPIE. 2004. Vol. 5398. P. 159–165.
10. Burylova I. V., Petrov V. I., Snopova M. G., Stepovich M. A. Mathematical simulation of distribution of minority charge carriers, generated in multy-layer semiconducting structure by a wide electron beam // Semiconductors. 2007. Vol. 41, no. 4. P. 444–447.
11. Kalmanovich V. V., Seregina E. V., Stepovich M. A. Mathematical Modeling of Heat and Mass Transfer Phenomena Caused by Interaction between Electron Beams and Planar Semiconductor Multilayers // Bulletin of the Russian Academy of Sciences : Physics. 2020. Vol. 84, no. 7. P. 844–850.
12. Kalmanovich V. V., Seregina E. V., Stepovich M. A. Comparison of analytical and numerical modeling of distributions of nonequilibrium minority charge carriers generated by a wide beam of medium-energy electrons in a two-layer semiconductor structure // Journal of Physics : Conf. Series. Applied Mathematics, Computational Science and Mechanics : Current Problems. 2020. Vol. 1479, art. no. 012116.

Информация об авторах

Степович Михаил Адольфович, доктор физико-математических наук, профессор кафедры физики и математики Калужского государственного университета им. К. Э. Циолковского, Российская Федерация.

Калманович Вероника Валерьевна, старший преподаватель кафедры физики и математики Калужского государственного университета им. К. Э. Циолковского, Российская Федерация.

Филиппов Михаил Николаевич, доктор физико-математических наук, профессор, заведующий лабораторией Институт общей и неорганической химии им. Н. С. Курнакова РАН, Москва, Российская Федерация.

Information about the authors

Mikhail A. Stepovich, Doctor Sci., Professor of the Department of Physics and Mathematics, Kaluga State University n. a. K. E. Tsiolkovsky, Russian Federation.

Veronika V. Kalmanovich, Senior Lecturer of the Department of Physics and Mathematics, Kaluga State University n. a. K. E. Tsiolkovsky, Russian Federation.

Mikhail N. Filippov, Doctor Sci., Professor, Head of the Laboratory, Institute of General and Inorganic Chemistry n. a. N. S. Kurnakov of RAS, Moscow.