On some problems of mathematical modeling of diffusion of non-equilibrium minority charge carriers generated by kilovolt electrons in semiconductors

M A Stepovich¹, E V Seregina², V V Kalmanovich¹ and M N Filippov³

¹ Tsionkovskiy Kaluga State University, 26 Stepan Razin Street, Kaluga, 248023 Russia
² Bauman Moscow State Technical University (National Research University), Kaluga Branch, 2 Bazhenov Street, Kaluga, 248000 Russia
³ Kurnakov Institute of General and Inorganic Chemistry RAS, 31 Leninsky prospect Street, Moscow, 119991 Russia

E-mail: m.stepovich@rambler.ru

Abstract. Some problems of mathematical modeling of the diffusion of non-equilibrium minority charge carriers generated by kilovolt electrons in semiconductor targets are considered. The calculations were carried out by the matrix method, which makes it possible to solve the equations of heat and mass transfer in multilayer planar structures with an arbitrary number of layers. Estimates of the distributions of minority charge carriers in two-layer semiconductor structures of the “film-substrate” type are obtained.

1. Introduction

One of the few methods that allow for the implementation of non-contact nondestructive diagnostics of solids are electron probe methods based on the use of beams of kilovolt electrons of low (up to about 8-10 keV) or medium (from 8-10 to 50 keV) energies. 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 [1].

In semiconductor materials science, when researching materials using electron beams, most often, as an informative signal, a signal associated with the generation and diffusion of non-equilibrium minority charge carriers (MCC) in a semiconductor target is recorded and/or signals are recorded whose characteristics significantly depend on the distribution of the MCC, for example cathodoluminescent radiation arising from radiative recombination of MCCs [2].

The usage of sharply focused electron beams (electron probes) makes it possible to study the local properties of materials. However, in this case, substantial heating of the targets is possible [3, 4], which can affect, sometimes irreversibly, the characteristics of the material. When simulating and experimentally studying the processes associated with the interaction of an electron probe with a semiconductor target, heating of a semiconductor may not be considered - see, for example, [5], although calculations indicate a significant increase in temperature under an electron probe in heavy semiconductors [6, 7]. It is possible to exclude the effect of heating on the material under study by using wide electron beams to excite an informative signal. This approach was used earlier to identify the electrophysical parameters of the near-surface layer of a homogeneous semiconductor [8, 9], and...
an analytical solution of the differential equation was obtained. We also investigated some of the possibilities of using numerical methods for modeling: 1) a one-dimensional process of heat and mass transfer caused by a wide electron beam [10-13] or electromagnetic radiation [14] in homogeneous semiconductor targets and 2) a one-dimensional diffusion process of MCCs in a two-layer semiconductor structure [15]. Simulation of MCC diffusion for a sharply focused electron probe was also carried out [16, 17]. In general, numerical methods made it possible to solve the considered problems of heat and mass transfer with an accuracy sufficient for practical use, but this approach turned out to be rather laborious. Therefore, when modeling the processes of heat and mass transfer in multilayer planar semiconductor structures, the approach described in [8, 9] was used. Initially, to solve this problem, standard methods of mathematical analysis were used [18, 19]. However, we failed to generalize this method to an arbitrary number of layers of a multilayer semiconductor structure. An analytical solution to this problem was obtained using the matrix method [20-22]. Preliminary results obtained in the simulation of a specific informative signal, cathodoluminescence [23], have shown that this approach is promising. At the same time, some problems of mathematical modeling of diffusion of non-equilibrium MCC generated by kilovolt electrons in multilayer semiconductors emerged. In this work, we continue to study the possibilities of using the matrix method for mathematical modeling of informative signals in specific multilayer semiconducting structures.

2. Statement of the problem

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 \( z \in [0, l] \), the depth distribution of the MCC is found as a solution to the differential equation

\[
\frac{d}{dz} \left( D^{(i)}(z) \frac{d\Delta p^{(i)}(z)}{dz} \right) - \frac{\Delta p^{(i)}(z)}{\tau^{(i)}(z)} = -\rho^{(i)}(z), \quad i = 1, n,
\]

with boundary conditions

\[
D^{(i)} \frac{d\Delta p^{(i)}(z)}{dz} \bigg|_{z=0} = v_{s}^{(i)} \Delta p^{(i)}(0), \quad D^{(n)} \frac{d\Delta p^{(n)}(z)}{dz} \bigg|_{z=l} = -v_{s}^{(n)} \Delta p^{(n)}(l).
\]

The superscript in parentheses indicates the layer number. For a multilayer semiconductor structure, we denote: \( z_{1} = 0, \ z_{n+1} = l \) - the outer boundaries of the semiconductor, \( z_{2}, z_{3}, \ldots, z_{n} \) - the coordinates of the interfaces of the layers; \( D^{(i)} \), \( L^{(i)} \), \( \tau^{(i)} \) are electrophysical parameters: diffusion coefficient, diffusion length and lifetime of the MCC in the i-th layer, respectively, while \( L^{(i)} = \sqrt{D^{(i)} \tau^{(i)}} \). At the boundaries of the semiconductor (at \( z = 0 \) and at \( z = l \)) the reduced rates of surface recombination \( S^{(i)} = L^{(i)} v_{s}^{(i)}/D^{(i)}, \ S^{(n)} = L^{(n)} v_{s}^{(n)}/D^{(n)} \), where \( v_{s}^{(1)} \) and \( v_{s}^{(n)} \) 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.

In connection with the above, the main goal of this work is to assess the possibilities of using the proposed method for carrying out calculations in planar semiconductor structures with different values of the electrophysical parameters: for two-layer structures made of two different materials and for two layers of one material, but with different electrophysical parameters of each of the layers. In this case, the main attention is paid to the possibility of using one expression in the right-hand side of differential equation (1) for each layer of a two-layer target.
3. Results of mathematical modeling

In carrying out the calculations, the matrix method was used, which was described in sufficient detail by us earlier [20-22]. The calculations were carried out for two-layer structures of semiconductor micro-, nanoelectronics and microwave technology. Below are the results of calculations for structures based on gallium nitride used in optoelectronics and microwave technology and solid solutions of cadmium telluride used in infrared technology. The following are considered as substrate materials: silicon carbide and silicon for gallium nitride, and cadmium telluride for solid solutions of cadmium telluride. In the calculations for $\rho^{(i)}(z)$, we used the parameters characteristic of the substrate material – see figure 1 and figure 2.

![Figure 1](image1.png)

**Figure 1.** Normalized to the power $E_p$, 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) for various energies of the beam electrons: 10 (a), 20 (b) and 30 (c) keV.

![Figure 2](image2.png)

**Figure 2.** Normalized to the power $E_p$ released in targets by an electron beam, energy losses by electrons in single-crystal cadmium telluride (solid curves), its solid solutions Cd$_{0.6}$Hg$_{0.4}$Te (dotted lines), Cd$_{0.2}$Hg$_{0.8}$Te (dashed lines) and mercury telluride (dash-dotted lines) for various energies of the beam electrons: 10 (a), 20 (b), and 30 (c) keV.

An analysis of the distributions of energy losses in the film and substrate materials showed that in the case when the parameters of these materials differ significantly, the solution of equation (1) with boundary conditions (2) for the fixed right-hand side of equation (1) (the same $\rho^{(i)}(z)$ for both the film and the substrate) gives distributions $\Delta \rho^{(i)}(z)$ that can only be regarded as estimates.

Figure 3 shows the distributions of the MCC generated by the electron beam in the semiconductor structure Cd$_{0.2}$Hg$_{0.8}$Te/CdTe for various beam electron energies: 5 (curve 1), 10 (2), 15 (3), 20 (4), 25 (5), and 30 keV (6). The following parameter values were used: $L_1 = 35$ nm, $\tau_1 = 10^{-6}$ s, $S_1 = 0.0857$ for Cd$_{0.2}$Hg$_{0.8}$Te and $L_2 = 30$ nm, $\tau_2 = 10^{-5}$ s, $S_2 = 10$ for CdTe.
Figure 3. a – depth distributions of MCCs generated by an electron beam in a two-layer semiconductor structure Cd$_{0.2}$Hg$_{0.8}$Te/CdTe 7 mkm thick (0.5 mkm Cd$_{0.2}$Hg$_{0.8}$Te and 6.5 mkm CdTe); b – distributions of MCCs generated by an electron beam in a two-layer semiconductor structure Cd$_{0.2}$Hg$_{0.8}$Te/CdTe with a thickness of 0.4 mkm (0.1 mkm Cd$_{0.2}$Hg$_{0.8}$Te and 0.3 mkm CdTe). Electron energy of the beam: 5 (curves 1), 10 (2), 15 (3), 20 (4), 25 (5), 30 (6) keV.

From the analysis of the dependences of energy losses by kilovolt electrons, it can be concluded that the solution by the matrix method of the considered diffusion equation of non-equilibrium MCCs in the above semiconductor materials with the right-hand side corresponding to the electrophysical parameters of the film (in our case, gallium nitride, including when performing calculations in substrate material) gives only estimates of the distributions of non-equilibrium MCCs. In this case, to obtain acceptable results, there are restrictions on the thickness of the considered two-layer structure – for example, for $E_0 = 20$ keV, the structure thickness is estimated to be no more than about 2 mkm. The results of some model calculations of the depth distribution of MCCs generated by an electron beam in a two-layer semiconductor structure based on gallium nitride with a thickness of 0.4 mkm (0.1 mkm for a GaN film and 0.3 mkm for a GaN substrate) for various electron beam energies: 10 (solid line), 20 (dashed line) and 30 keV (dash-dotted line) are shown in figure 4.

Figure 4. Depth distributions of MCCs generated by an electron beam in a two-layer semiconductor structure of gallium nitride with a thickness of 0.4 mkm (0.1 mkm – GaN film and 0.3 mkm – GaN substrate) with different electrophysical parameters on the layers: for a GaN film $\tau = 10^{-6}$ s, $S = 30$, $L = 35$ mkm, $v_s = 105 \cdot 10^7$ mkm/s, $D = 122 \cdot 10^7$ mkm$^2$/s; similar values for a GaN substrate $\tau = 10^{-5}$ s, $S = 30$, $L = 30$ mkm, $v_s = 9 \cdot 10^7$ mkm/s and $D = 9 \cdot 10^7$ mkm$^2$/s. Electron energy of the beam: 10 (solid line), 20 (dashed line) and 30 keV (dash-dotted line).

The curves shown in figure 4 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 0.4 mkm thick target – see figure 2a. An increase in
the beam energy for a film of this thickness leads to a decrease in the energy lost in the target (figure 2b and figure 2c) and, as a consequence, to a decrease in the generated MCCs – see figure 4.

On the whole, taking into account the relatively small thickness of the film in real structures, it seems reasonable when performing calculations for two-layer structures on the right-hand side of expression (1) to use \( \rho^{01}(z) \) the electrophysical parameters characteristic of the substrate for calculations. This approach gives good results if the parameters of the layers differ insignificantly, as, for example, for the structure \( \text{Cd}_{0.6}\text{Hg}_{0.4}\text{Te}/\text{CdTe} \) – this also follows from the analysis of the data in figure 2, from which it can be seen that the distributions of energy losses for these two materials are very close. For the structure \( \text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}/\text{CdTe} \), the difference in energy losses for these two materials is larger, but calculations in this case give quite acceptable results as well. A somewhat different situation is realized for gallium nitride structures when silicon, silicon carbide, and gallium arsenide are used as substrates.

4. Conclusions

The use of the matrix method in the mathematical modeling of heat and mass transfer processes in a multilayer planar medium makes it possible to obtain an analytical solution to the problem. However, the features of the interaction of a primary monoenergetic beam of kilovolt electrons with a multilayer target, first of all, the loss of monoenergeticity of electrons, can only give estimates of the distributions of non-equilibrium MCCs in the structure. For a two-layer structure of the “film-substrate” type, the best estimates for films up to 1–2 mkm thick can be obtained if the parameters characteristic of the substrate material are used to describe the electron energy losses in these structure.

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