Mathematical simulation of distribution of minority charge carriers, generated in multy-layer semiconducting structure by a wide electron beam[1]

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The method of calculation of distributions of minority charge carriers generated in the two-layer semiconductor by a wide electron beam with energies 5–30 keV based on use of model of independent sources is described.

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1. Introduction

Usually for the quantitative description of diffusion of minority charge carriers (MCC) in semiconductors the following two approaches can be used: 1) model of collective movement of the generated carriers in which on diffusion of MCC from each microvolume of the semiconductor also with the carriers generated in other areas of a target are influenced [1–3]. Mathematically it is expressed that as function of generation MCC the differential equation of diffusion includes the function describing of electron beam energy losses density in all volume of a target. Such model can be used for the quantitative description of processes in homogeneous semiconductors; 2) model of independent sources in which all over again it is considered diffusive process of the carriers generated in each separate microvolume of the semiconductor, and resulting distribution of MCC can be obtained by integrating of the received distributions from each of microvolumes [4]. It can be made by using of Green's function [5] and for stationary case — by using method, suggested in [6] — in this work we used this method. Mathematically it is expressed that the diffusion equation for each of dot sources of MCC then by means of integration on the volume occupied MCC, there is their distribution in the semiconductor as a result of diffusion [5] all over again is solved. This model can be applied for the quantitative description of processes in non-uniform and multilayered structures and consequently is perspective at studying planar structures of semiconductor electronics [6,7].

At studying micro- and nanoelectronic structures the informative signal is excited simultaneously in several layers of multilayered structure and consequently the problem of diagnostics of each separate layer at use a strongly focused electronic probe powerfully becomes complicated. Partially to solve this problem we can use ideas of works [1,2,6,7] in which parameters of a homogeneous target are offered to be defined from dependences intensity monochromatic cathodoluminescence (CL) from energy of a wide electron beam; some opportunities of application of this method are considered in [8]. At the same time for studying multilayered structures, development of the approach is necessary, allowing to describe the basic physical phenomena and the processes occurring at interaction of electron beam with such targets and on the basis of this to define informative opportunities of a considered method. One of the main moments in the decision of this problem is the description of MCC distributions generated by an electron beam after their diffusion in nonuniform planar structure. The knowledge of distributions allows to create adequate models of CL of such structures.

In the present work, the idea of work [9] based on a model of independent planar sources MCC is used for the decision of a problem of MCC distribution in the multilayered structure.

The purpose of the present work is studying opportunities of usage of an independent sources model for calculation of distributions MCC generated in the two- and three-layer semiconductor by a wide electron beam.

2. Statement of a problem

Statement of a problem is considered on an example of two-layer structure [10]. The structure such as „epitaxial film–substrate", created is considered on the basis of the same semiconductor material or at use of two various materials, but having close density, charge numbers and atomic weights. In this case the process of interaction of electron beam with the target can be described as for a homogeneous one then to consider diffusion generated MCC separately in the first material (film) and the second material (substrate). Really such model can be applied, for example, to structure „epitaxial film–monocrystal substrate"

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with a different level by doping an impurity that provides various values of electrophysical parameters (diffusion length L, diffusion constant D, factor of absorption α, etc.) in each of materials. For one-dimensional diffusion in half-infinite semiconductor distribution of nonequilibrium MCC on depth z is given by expression [7]:

$$\Delta p(z) = \int_0^\infty \Delta p(z, z_0) dz_0. \tag{1}$$

Here function $\Delta p(z, z_0)$ describes distribution of MCC, generated by the plane indefinitely thin source which is taking place on depth z_0, $z_0 \in [0, \infty)$; and z — the coordinate counted from a plane surface deep into of the semiconductor. Distribution $\Delta p(z, z_0)$ can be obtained as the decision of the differential equation:

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

with boundary conditions

$$D\frac{d\Delta p(z, z_0)}{dz}\bigg|_{z=0} = v_s \Delta p(0, z_0), \quad \Delta p(\infty, z_0) = 0.$$

For two-layer structure we shall designate: z_1 — coordinate of border of the unit of two layers D_1, D_2, L_1, L_2 and τ_1, τ_2 — factors of diffusion, diffusion lengths and life-times of MCC in the first and the second materials, S_1 — the resulted reduced surface recombination rate MCC (in the first layer), S_2 — the same parameter on the border of film-surface, $\rho(z)$ — distribution of energy-loss density in the target. Thus $L_1 = \sqrt{D_1\tau_1}$ and $L_2 = \sqrt{D_2\tau_2}$, $S_1 = v_{s1}L_1/D_1$ and $S_2 = v_{s2}L_2/D_2$; here v_{s1} — surface rate of nonequilibrium MCC in a surface of film, v_{s2} — the same parameter on the border of film-surface. Then for the first material (film) we have:

$$D_1\frac{d\Delta p_{11}(z, z_0)}{dz}\bigg|_{z=0} = v_{s1}\Delta p_{11}(0, z_0), \tag{3}$$

for the second material (substrate)

$$\Delta p_{22}(\infty, z_0) = 0, \tag{4}$$

and on the border film–substrate

$$\lim_{z \to z_1 - 0} \Delta p_1(z, z_0) = \lim_{z \to z_1 + 0} \Delta p_2(z, z_0). \tag{5}$$

Here

$$\Delta p(z, z_0 \le z_1) = \begin{cases} \Delta p_{11}(z, z_0), & \forall z \in [0, z_0], \\ \Delta p_{12}(z, z_0), & \forall z \in [z_0, z_1], \\ \Delta p_{22}(z, z_0), & \forall z \in [z_1, \infty), \end{cases}$$

$$\Delta p(z, z_0 \ge z_1) = \begin{cases} \Delta p_{11}(z, z_0), & \forall z \in [0, z_1], \\ \Delta p_{12}(z, z_0), & \forall z \in [z_1, z_0], \\ \Delta p_{22}(z, z_0), & \forall z \in [z_0, \infty). \end{cases}$$

The sense of boundary conditions (3) and (4) is obvious, and the condition (5) provides a continuity of function $\Delta p(z, z_0)$ on border of two materials (at $z = z_1$).

3. Results and discussion

Distribution of MCC as a result of their diffusion in two-layer structure was as follows: 1) all over again was solved the diffusion equation (2) for the first material, thus one of two constants of differentiation was determined from a boundary condition (3); 2) the diffusion equation (2) for the second material was solved, and one of the constants was determined from a condition (4); 3) decisions in the first and second materials were „sewed" on their borders with using of a condition (5). It allowed determining the staying constants.

In result for each of the chances schematically represented of Fig. 1, required decisions $\Delta p(z, z_0)$ are received:
1) for $z_0 \le z_1$

$$\Delta p(z, z_0) = \begin{cases} \Delta p_{11}(z, z_0) = \frac{\rho(z_0)\tau_1}{2L_1}\exp\left(-\frac{z_0}{L_1}\right) \\ \quad\times\left[\exp\left(\frac{z}{L_1}\right) - \frac{S_1-1}{S_1+1}\exp\left(-\frac{z}{L_1}\right)\right], \quad \forall z \in [0, z_0], \\ \Delta p_{12}(z, z_0) = \frac{\rho(z_0)\tau_1}{2L_1}\exp\left(-\frac{z}{L_1}\right) \\ \quad\times\left[\exp\left(\frac{z_0}{L_1}\right) - \frac{S_1-1}{S_1+1}\exp\left(-\frac{z_0}{L_1}\right)\right], \quad \forall z \in [z_0, z_1], \\ \Delta p_{22}(z, z_0) = \frac{\rho(z_0)\tau_1}{2L_1}\exp\left(\frac{z_1-z}{L_2} - \frac{z_1}{L_1}\right) \\ \quad\times\left[\exp\left(\frac{z_0}{L_1}\right) - \frac{S_1-1}{S_1+1}\exp\left(-\frac{z_0}{L_1}\right)\right], \quad \forall z \in [z_1, \infty); \end{cases}$$

2) for $z_0 \ge z_1$

$$\Delta p(z, z_0) = \begin{cases} \Delta p_{11}(z, z_0) = \tilde{N}_1(z_0)\exp\left(\frac{z}{L_1}\right) \\ \quad + C_2(z_0)\exp\left(-\frac{z}{L_1}\right), \quad \forall z \in [0, z_1], \\ \Delta p_{21}(z, z_0) = \frac{\rho(z_0)\tau_2}{2L_2}\exp\left(-\frac{z_0}{L_2}\right) \\ \quad\times\left[\exp\left(\frac{z}{L_2}\right) - \frac{S_2-1}{S_2+1}\exp\left(-\frac{z}{L_2}\right)\right], \quad \forall z \in [z_1, z_0], \\ \Delta p_{22}(z, z_0) = \frac{\rho(z_0)\tau_2}{2L_2}\exp\left(-\frac{z}{L_2}\right) \\ \quad\times\left[\exp\left(\frac{z_0}{L_2}\right) - \frac{S_2-1}{S_2+1}\exp\left(-\frac{z_0}{L_2}\right)\right], \quad \forall z \in [z_0, \infty), \end{cases}$$

where

$$\tilde{N}_1(z_0) = \frac{\rho(z_0)\tau_2}{2L_2}\exp\left(-\frac{z_0}{L_2}\right)\left[\exp\left(\frac{z_1}{L_2}\right) - \frac{S_2-1}{S_2+1}\right.$$
$$\left.\times\exp\left(-\frac{z_1}{L_2}\right)\right]\left[\exp\left(\frac{z_1}{L_1}\right) - \frac{S_1-1}{S_1+1}\exp\left(-\frac{z_1}{L_1}\right)\right]^{-1},$$

$$\tilde{N}_2(z_0) = \frac{\rho(z_0)\tau_2}{2L_2}\left[\exp\left(\frac{z_1 - z_0}{L_2}\right) - \frac{S_2-1}{S_2+1}\right.$$
$$\left.\times\exp\left(-\frac{z_1+z_0}{L_2}\right)\right]\left[\exp\left(-\frac{z_1}{L_1}\right) - \frac{S_1+1}{S_1-1}\exp\left(\frac{z_1}{L_1}\right)\right]^{-1}.$$

Using the received partities, distributions MCC on depth $\Delta p(z)$ it is calculated under the formula (1).

For three-layer structure target of type the „film-film-substrate", created on the basis of the same semiconductor materials are considered or at use of three various, but having close density, serial numbers and nuclear weights of materials.

For three-layer structure we shall designate: z_1 — coordinate of border of section of the first and second layer, z_2 — coordinate of border of section of the second and third layer. The system of the equations for the three-layer semiconductor is made to similarly boundary conditions for the two-layer semiconductor. In a result the expression is received more unwieldy, but similar written for the two-layer semiconductor. Below the received equation is written only for a case $z_0 < z_1$; thus:

$$\Delta p(z, z_0 < z_1) = \begin{cases} \Delta p_{11}(z, z_0) = C_1(z_0)\exp\left(\frac{z}{L_1}\right) \\ \qquad + C_2(z_0)\exp\left(\frac{-z}{L_1}\right), \quad \forall z \in [0, z_0], \\ \Delta p_{12}(z, z_0) = C_3(z_0)\exp\left(\frac{z}{L_1}\right) \\ \qquad + C_4(z_0)\exp\left(\frac{-z}{L_1}\right), \quad \forall z \in [z_0, z_1], \\ \Delta p_{22}(z, z_0) = C_5(z_0)\exp\left(\frac{z}{L_2}\right) \\ \qquad + C_6(z_0)\exp\left(\frac{-z}{L_2}\right), \quad \forall z \in [z_1, z_2], \\ \Delta p_{33}(z, z_0) = C_7(z_0)\exp\left(\frac{z}{L_3}\right) \\ \qquad + C_8(z_0)\exp\left(\frac{-z}{L_3}\right), \quad \forall z \in [z_2, \infty). \end{cases}$$

Analytical expressions for constants $\tilde{N}_i = \tilde{N}_i(z_0, \boldsymbol{\Theta})$, where $\boldsymbol{\Theta}$ — the vector of parameters of the given semiconductor layer $i = \overline{1, 8}$ are received.

For example

$$\tilde{N}_1(z_0, \boldsymbol{\Theta}) = \frac{\rho(z_0)\left[\exp\left(\frac{2z_0}{L_2}\right) + \frac{1-S_2}{1+S_2}\right]}{\left[\exp\left(\frac{2z_0}{L_2}\right)\left(\frac{D_3}{L_3} + \frac{D_2}{L_2}\right) + \frac{1-S_2}{1+S_2}\left(\frac{D_3}{L_3} - \frac{D_2}{L_2}\right)\right] \times \times \left[\exp\frac{z_0}{L_1} + \frac{1-S_1}{1+S_1}\exp\left(-\frac{z_0}{L_1}\right)\right]}.$$

Here $\boldsymbol{\Theta} = \{L_1, L_2, L_3, D_2, D_3, S_1, S_2\}$.

Similar results are received for cases when source of MCC is in the second and third materials of structure.

The checking of the received results is lead numerically by using of expressions for distributions $\Delta p(z, z_0)$, and the formula (1). As reference the similar expressions received for two-layer structure are used; we shall note, that validity of expressions for two-layer structure has been confirmed earlier [10]: in limiting cases of infinitely thin or infinitely thick first layer the expressions resulted in [9] for homogeneous semiconductor have been received.

4. Results of calculations

Calculations are carried out for parameters, characteristic for semiconductor structure „epitaxial film GaAs — monocrystal substrate GaAs" (and for three-layer structure with a thick second layer). The following values of parameters are used: $L_1 = 0.69\,\mu$m, $\tau_1 = 9.5 \cdot 10^{-10}$ s, $S_1 = 50$ — for the first material (film) and $L_2 = 0.4\,\mu$m, $\tau_2 = 3.2 \cdot 10^{-10}$ s, $S_2 = 50$ — for the second material (substrate); value z_1 was necessary to equal $z_1 = 1.5\,\mu$m. The distributions of energy-loss density $\rho(z)$ was used in accordance with [7].

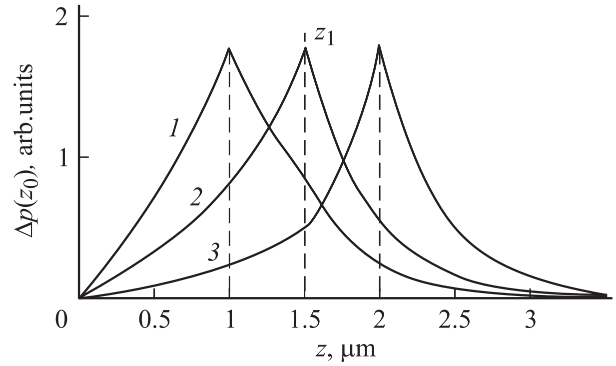

Figure 1. Distribution of MCC after diffusion from the thin planar source situated at the depth z_0 under a surface of the two-layer semiconductor. Calculations are carried out for parameters, the typical for semiconductor structure „epitaxial film GaAs–monocrystal substrate GaAs".

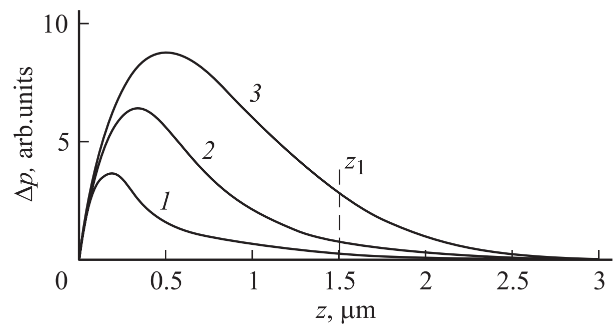

Figure 2. Distribution of MCC, generated by an electron beam in two-layer semiconducting structure „epitaxial film GaAs–monocrystalling substrate GaAs".

Results of calculations of dependences $\Delta p(z, z_0)$ for considered structure are submitted of Fig. 1. Distributions of MCC which is turning out as a result of diffusion from indefinitely thin planar sources, are shown: on depth $z_0 = 1\,\mu$m (i.e. in the first material — curve *1*), $z_0 = 1.5\,\mu$m (i.e. on border of materials — curve *2*), $z_0 = 2\,\mu$m (i.e. in the second material — curve *3*). For each curve it is carried out normalization on the maximal value of the density MCC, and the maximum of all three curves $\Delta p(z, z_0)$ answers the same value. Energy of an electron beam $E_0 = 20$ keV.

Results of calculations of dependences $\Delta p(z)$ for considered structure are submitted of Fig. 2. Distributions of MCC, generated by an electron beam with energy of electrons $E_0 = 10$ (curve *1*), 15 (*2*) and 20 (*3*) keV, — after their diffusion are shown; value $z_1 = 1.5\,\mu$m.

5. Conclusion

Some opportunities of using of the model of independent sources for calculation of distributions of MCC are considered as a result of their diffusion in multilayer semiconductor planar structure. For materials with close values of density (charge numbers and atomic weights) are received the analytical expressions, allowing to carry out calculations of distributions of MCC generated by plane indefinitely thin planar sources by using of any function of generation of electron-hole pairs. The modeling calculations which have been carried out for structure such as „film GaAs–substrate GaAs“ in a range of energy of electrons from 5 up to 30 keV, have shown an opportunity of using of the received expressions for calculation of distributions of MCC in considered semiconductor target.

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