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# NUMERICAL MODELLING OF SEMICONDUCTOR STRUCTURES INCLUDING ELECTRON-HOLE SCATTERING AND RECOMBINATION RADIATION RECYCLING EFFECT

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## Abstract

A charge carrier transport model is developed which allows in a phenomenologically more constant way to take into account the effects of electron-hole scattering on the mobilities of the charge carriers in a semiconductor. Also a mathematical model of charge carrier generation due to the photon reabsorption process in a direct gap semiconductor is given and some photon transport aspects are discussed.

*Keywords:* electron-hole scattering, charge carrier mobility, direct gap semiconductor, recombination.

## Introduction

The influence of electron-hole scattering on the electrical characteristics of a diode structure was first considered by FLETCHER (1957). He suggested to apply Mathiessen's rule also in the case of electron-hole scattering. Since then this way is commonly used for the total mobility calculations. The role of recombination radiation recycling process in GaAs diodes and thyristors was first discussed by ALFEROV et al (1977, 1978, 1979). It was shown that the recombination radiation emitted mostly from the $n$-base and $p^+$-emitter had a considerable strong effect on the electrical parameters of devices. More general treatment of the photon recycling effects was given by ALFEROV et al (1976) and VELMRE and FREIDIN (1979), by using numerical methods to solve corresponding boundary value problems.

The aim of this paper is to summarize some results in numerical modelling of semiconductor bipolar devices obtained at Tallinn Polytechnic Institute.

## Semiconductor Equations and Recombination-Generation Laws

The initial set of semiconductor equations contains the Poissons' equation and the continuity equations for electrons and holes which in one-dimensional approximation read as follows:

$$\frac{\partial^2 \varphi}{\partial x^2} = -\frac{q}{\varepsilon\varepsilon_0}(p - n + N), \qquad N = N_D^+ - N_A^- \tag{1}$$

$$\frac{\partial j_p}{\partial x} = -q(R - G + \frac{\partial p}{\partial t}), \tag{2}$$

$$\frac{\partial j_n}{\partial x} = q(R - G + \frac{\partial n}{\partial t}). \tag{3}$$

The total recombination rate $R$ is a sum of Shockley-Read-Hall, Auger and radiative recombination rates

$$R = R_{\mathrm{SRH}} + R_{\mathrm{A}} + R_{\mathrm{R}},$$

where

$$\begin{aligned} R_{\mathrm{SRH}} &= (pn - n_i^2) / [\tau_{p0}(n + n_1) + \tau_{n0}(p + p_1)], \\ R_{\mathrm{A}} &= (pn - n_i^2)(\gamma_p p + \gamma_n n), \\ R_{\mathrm{R}} &= B(pn - n_i^2). \end{aligned}$$

Apart from the generation caused by an external excitation into the total generation rate $G$ may be included the generation rate due to the impact ionization of carriers

$$G_{\mathrm{I}} = \frac{1}{q}(|j_p| \cdot \alpha_p + |j_n| \cdot \alpha_n),$$

and the generation rate due to the photon recycling process. In (VELMRE et al (1981)) it was shown that in case of self-absorption in the base region with the thickness $w$ the generation rate can be determined as follows:

$$G_{\mathrm{R}} = \int_0^x R_{\mathrm{R}}(x')F(u)\,du + \int_0^{w-x} R_{\mathrm{R}}(x')F(u)\,du, \tag{4}$$

$$F(u) = -\frac{1}{2}\int_0^\infty \beta(\varepsilon)\varrho(\varepsilon)\alpha(\varepsilon)\mathrm{Ei}(-\alpha(\varepsilon)u)\,d\varepsilon,$$

where

$u = |x - x'|$ and $\beta(\varepsilon)$ is the internal photoeffect coefficient,

$\varrho(\varepsilon)$ is the normalised spontaneous emission spectrum in the base region,

$\alpha(\varepsilon)$ is the photon absorption coefficient,

$\varepsilon = h\nu$ is the photon energy and

$\mathrm{Ei}(-z)$ is the exponential integral function.

A more detailed consideration of the effect of photon recycling on the carrier transport will be given later.

## Transport Models in Case of Electron-Hole Scattering

The carrier transport in semiconductors is usually described by two current equations in the form as follows:

$$j_p = q\left(\mu_p p E - D_p \frac{\partial p}{\partial x}\right) \tag{5}$$

$$j_n = q\left(\mu_n n E + D_n \frac{\partial n}{\partial x}\right) \tag{6}$$

The conventional way to take into account the electron-hole scattering is to modify the carrier mobilities in Eqs. (5–6) using the formula introduced by FLETCHER (1957):

$$\mu_{n,p}^{-1} = \mu_{n0,p0}^{-1} + \mu_{np}^{-1} \tag{7}$$

where $\mu_{np}$ is the mobility related to the electron-hole scattering and the subscript 0 denotes the mobility components independent of electron-hole scattering. In a number of papers (e.g. DYKMAN and TOMCHUK (1964); GRIBNIKOV and MEL'NIKOV (1968)) it has been pointed out that in the case of electron-hole scattering Einstein's relation between the mobility and diffusion coefficient will be injured. So the insertion of Eq. (7) into Einstein's relation will result in a dependence of ambipolar diffusion coefficient on carrier density, which contradicts to many theoretical and experimental results for not extremely high carrier densities.

Another way to take into account the influence of electron-hole scattering on the carrier transport was proposed by AVAK'IANTS et al (1963). From their carrier motion equations one can derive the current equations as follows:

$$j_p = q\left(\mu_{p1} p E - \varphi_T \mu_{p2} \frac{\partial p}{\partial x} - \varphi_T \mu_{p3} \frac{\partial n}{\partial x}\right), \tag{8}$$

$$j_n = q\left(\mu_{n1} n E + \varphi_T \mu_{n2} \frac{\partial n}{\partial x} + \varphi_T \mu_{n3} \frac{\partial p}{\partial x}\right), \tag{9}$$

where

$$\mu_{p1} = \mu_{p2} - \frac{n}{p}\mu_{p3},$$
$$\mu_{n1} = \mu_{n2} - \frac{p}{n}\mu_{n3}.$$

These equations are derived from a phenomenological plasma-like model for electrons and holes. However, the same equations can be obtained starting from the Boltzmann equation variation principle solution (MEYER (1980)).

It is easy to convert the equations Eq. (8) and Eq. (9) into a form more convenient for numerical calculations:

$$j_p = \beta_{pp} j_{p0} - \beta_{pn} j_{n0}, \tag{10}$$
$$j_n = \beta_{nn} j_{n0} - \beta_{np} j_{p0}, \tag{11}$$

where

$$\beta_{pp} = \frac{\mu_{p2}}{\mu_{p0}}, \qquad \beta_{pn} = \frac{\mu_{p3}}{\mu_{n0}},$$
$$\beta_{nn} = \frac{\mu_{n2}}{\mu_{n0}}, \qquad \beta_{np} = \frac{\mu_{n3}}{\mu_{p0}},$$

and

$$j_{p0} = q\left(\mu_{p0} p E - D_{p0}\frac{\partial p}{\partial x}\right),$$
$$j_{n0} = q\left(\mu_{n0} n E + D_{n0}\frac{\partial n}{\partial x}\right)$$

For practical calculations it is necessary to determine the coefficients $\beta_{ij}$ in Eq. (10) and Eq. (11). The theoretical evaluation of coefficients is cumbersome and the results scarcely give the needed accuracy. Therefore, a search for an appropriate experimental method could be more reasonable.

Below we discuss a way utilizing the zero-order approximation to the solution of Boltzmann equation. Referring to MEYER (1980) we can obtain:

$$\beta_{pp}^{(0)} = (1 + p\mu_{n0}^{(0)} I^{ch}) / M,$$
$$\beta_{pn}^{(0)} = p\mu_{p0}^{(0)} I^{ch} / M,$$
$$\beta_{nn}^{(0)} = (1 + n\mu_{p0}^{(0)} I^{ch}) / M,$$
$$\beta_{np}^{(0)} = n\mu_{n0}^{(0)} I^{ch} / M$$
$$M = 1 + (p\mu_{n0}^{(0)} + n\mu_{p0}^{(0)}) I^{ch}.$$

Now the further specification of the electron-hole scattering function $I^{ch}$ is needed. One can use for evaluating $I^{ch}$ the conductivity measurements on a lightly doped semiconductor under high excitation condition, so that

$$n \cong p = \overline{n} \gg N_A + N_D.$$

In this case

$$\sigma_{\text{exp}} = q\overline{n}\,(\,\mu_n + \mu_p\,)_{\text{exp}}$$

On the other hand, the theoretical conductivity may be written as

$$\sigma_{\text{theor}} = q\overline{n}\,(\,\mu_{n1} + \mu_{p1}\,)$$

Now, assuming that $\sigma_{\text{exp}} \cong \sigma^{(0)}_{\text{theor}}$ we obtain

$$\begin{aligned} I^{ch}(\overline{n}) &= \frac{1}{\overline{n}\,(\,\mu^{(0)}_{n0} + \mu^{(0)}_{p0}\,)}\left[\frac{\mu_{n0} + \mu_{p0}}{(\,\mu_n + \mu_p\,)_{\text{exp}}} - 1\right] = \\ &= \frac{1}{n}\left[\frac{1}{(\,\mu_n + \mu_p\,)_{\text{exp}}} - \frac{1}{(\,\mu_{n0} + \mu_{p0}\,)}\right]. \end{aligned}$$

*Fig. 1* shows $I^{ch}$ against $\overline{n}$, obtained from different conductivity measurements on lightly doped silicon at $T = 290$K. In numerical calculations for silicon in the case of $T = 300$K we have used the approximative formula

$$I^{ch}(\overline{n}) = 9.88 \times 10^{-21}\,\frac{1 + 7.91 \times 10^{-19}\overline{n}}{1 + 8.51 \times 10^{-18}\overline{n}}, \tag{12}$$

where $\overline{n}$ is given in $\text{cm}^{-3}$.

The temperature dependence $I^{ch} \sim T^{-3/2}$ is predicted theoretically. In case $n \neq p$ (emitter regions of a diode structure, for instance) we have used $\overline{n} = (p+n)/2$ in Eq. (12) but now the formula could be treated only as a qualitatively accurate one. For estimation of the function $I^{ch}$ for highly doped silicon an additional experimental and theoretical research is needed.

The discretization scheme of the set of equations Eqs. (1–3), Eq. (8), Eq. (9) and the numerical algorithm have been described in detail previously VELMRE et al (1985). This algorithm was realized in the computer program DYNAMIT-1 developed at the Electronics Department of Tallinn Polytechnic Institute for 1D modelling of multijunction bipolar structures on isothermal steady state and transient conditions.

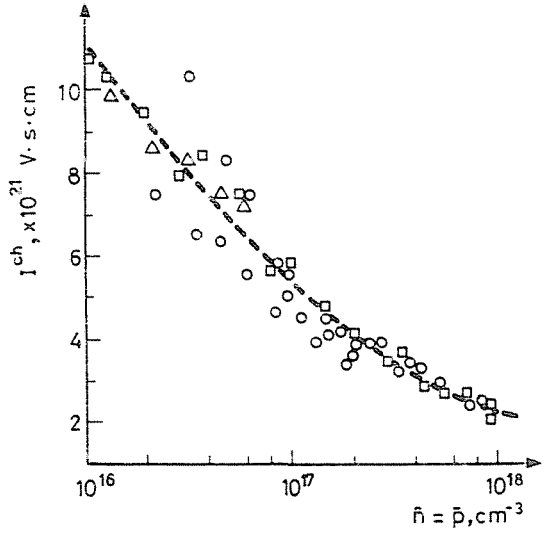


*Fig. 1.* Function $I^{ch}$ characterizing the electron-hole scattering versus carrier density in silicon at $T = 290$K.
o KRAUSSE, 1972;
△ DANNHÄUSER, 1972;
□ GRIVITSKAS, WILLANDER and VAITKUS, 1984.

## Photon Recycling and Relevant Effects in Direct-Gap Semiconductors

As it was mentioned above the reabsorption of the band-to-band recombination radiation may strongly affect the device parameters at high excitation levels, so that this physical phenomenon has to be included in mathematical models of device structures based on direct-gap semiconductors. The generation rate in the integral form Eq. (4) was used in numerical models and computer programs, which work at Tallinn Polytechnic Institute. There are different computer programs for isothermal and nonisothermal analysis of direct-gap material structures in 1D approximation. Details of numerical modelling and calculation results can be found in references (VELMRE and FREIDIN (1979), VELMRE et al (1981), VELMRE and FREIDIN (1983A), VELMRE and FREIDIN (1983B)).

In more transparent explanation of the influence of photon recycling on the carrier transport let us consider analytically the diffusion equation under the assumption that no electron-hole scattering and impact ionization

generation take place. In one-dimensional case

$$D\frac{\partial^2 p}{\partial x^2} = R_{\mathrm{SRH}} + R_{\mathrm{A}} + R_{\mathrm{R}} - G_{\mathrm{R}}, \tag{13}$$

where $D = D_p$ for low injection level and $D = D_a$ (the ambipolar diffusion coefficient) for high injection level. If we suppose now that $G_{\mathrm{R}}$ in Eq. (13) is given by expression Eq. (4), then the diffusion equation Eq. (13) turns into an integro-differential equation. As an approximation from the above-mentioned integro-differential equation a non-linear differential equation of second order can be derived as utilizing the Taylor series expansion for the radiative recombination rate:

$$G_{\mathrm{R}} = \Phi_0(x,w) + \Phi_1(x,w)\frac{dR_{\mathrm{R}}}{dx} + \frac{1}{2}\Phi_2(x,w)\frac{d^2R_{\mathrm{R}}}{dx^2} + \cdots . \tag{14}$$

Then, keeping just the first three terms of the Taylor expansion and inserting Eq. (14) into Eq. (13) we obtain:

$$\frac{d}{dx}\left\{\left[D + \tfrac{1}{2}\Phi_2(x,w)B(2p+N)\right]\frac{dp}{dx}\right\} + \left[\Phi_1(x,w) - \tfrac{1}{2}\frac{d\Phi_2(x,w)}{dx}\right] B(2p+N)\frac{dp}{dx} = R_{\mathrm{SRH}} + R_{\mathrm{A}} + [1-\Phi_0(x,w)]R_{\mathrm{R}}. \tag{15}$$

The term added to the diffusion coefficient $D$ in Eq. (15) can be interpreted as a photon diffusion coefficient

$$D_{\mathrm{ph}} = \frac{1}{2}\Phi_2(x,w)B(2p+N).$$

The second term on the left-hand side of Eq. (15) contains a factor which can be considered as an equivalent drift velocity of carriers caused by the photon transport mechanism:

$$\begin{aligned} v_{\mathrm{ph}} &= \left[\Phi_1(x,w) - \frac{1}{2}\frac{d\Phi_2(x,w)}{dx}\right] B(2p+N) \cong \\ &\cong \Phi_1(x,w)B(2p+N). \end{aligned}$$

The right-hand side of Eq. (15) is a sum of non-radiative recombination rates $R_{\mathrm{SRH}}$ and $R_{\mathrm{A}}$ and a term $[1-\Phi_0(x,w)]R_R$ which can be treated as a virtual non-radiative recombination channel related to the fly-out losses of photons. Taking some simplifying assumptions the functions $\Phi$ can be derived analytically.

To illustrate the role of different photon transport mechanisms the hole density distribution in a lightly-doped $n$-type GaAs layer with thickness

$w = 10\ \mu$m and $w/\sqrt{D_a\,\tau_{SRH}} = 2$ was calculated. The boundary conditions $p = p_0$ at $x = 0$ and $p = 0$ at $x = w$ were chosen, so that the internal quantum efficiency at $x = 0$ was

$$\eta_i(0) = R_R(0) / [R_R(0) + R_{SHR}(0) + R_A(0)] = 0.99$$

We can see in *Fig. 2* that taking into account only the fly-out losses and neglecting the photon transport at all ($\Phi_1,\ \Phi_2 = 0$) we get the lowest carrier density distribution curve 1 which corresponds to the shortest effective diffusion length of carriers and the worst carrier transmission rate through the layer. In case of $\Phi_1,\ \Phi_2,\ \Phi_3, \neq 0$ (curve 2) the photon transport significantly improves the carrier transmission. Nevertheless, at the

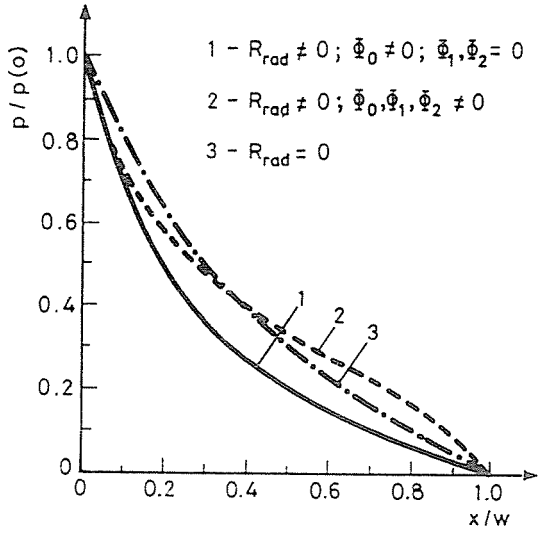


*Fig. 2.* Hole density distributions in a lightly doped $n$-$GaAs$ layer with $w = 10\mu$m

left boundary, where the recombination radiation is the strongest, there is still dominating the fly-out mechanism diminishing the effective diffusion length of carriers. Curve 3 in *Fig. 2* displays the carrier distribution in case $R_R = 0$. This is a well-known distribution of carriers in the base of non-drift bipolar transistor.

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