Mathematical Modelling and Analysis
Volume 12 Number 3, 2007, pages 379–388
 ISSN 1392-6292 print, ISSN 1648-3510 online

NUMERICAL SIMULATION OF THE CONDUCTIVITY RELAXATION IN THE HIGH RESISTIVITY SEMICONDUCTOR

A. PINCEVIČIUS[1], M. MEILŪNAS[2] and N. TUMANOVA[2]

[1] *Military Academy of Lithuania*
[2] *Vilnius Gediminas Technical University*

E-mail: pincev@takas.lt;MecislavasMeilunas@fm.vtu.lt
E-mail: tumnat@gmail.com

Received March 7, 2007; revised March 17, 2007; published online September 15, 2007

Abstract. A theoretical model describing the relaxation of charge carriers in semiconductors of high resistance under the influence of the laser pulses is presented. It is demonstrated that parameters of the trapping states relevant to the processes of the conductivity relaxation can be defined by fitting the experimental data. Time evolution of the conductivity of the $GaAs$ bulk semiconductor under the influence of nanosecond and picosecond laser pulses is considered. Effect of two laser pulses, when the first one results in population of the trapping state and the second one induces its depopulation, is also considered.
Key words: simulation, relaxation photoconductivity, parameters of the trapping states, parameters identification

1. Introduction

High resistance semiconductors (e.g. $GaAs$) are widely used by manufacturing the basic elements of microelectronics such as transistors, Schottky diodes, etc. [4]. As a rule they are used for fabrication of the isolated substrate, on which the relevant device is designed by means of the molecular beam epitaxy. Properties of those devices depend very much on the quality of any separate layer due to compensation of residual impurities by intrinsic defects. Impurities and structural defects cause a presence of electron/hole trapping states in the band gap characterized by activation energies E_i and the trapping coefficients γ_i. It is noteworthy that those defect states predetermine the photoelectric properties of the system since they are responsible for electron-hole recombination processes. Light-induced conductivity (i.e. photoconductivity) relaxation is mainly defined by the band – band transitions or by transitions into the impurity/defect states. Thus the relaxation kinetics contains

the information about characteristics of those states, such as the trapping cross-sections of electrons/holes, positioning of the states in the band gap and the amount of those states (concentration). The scheme convenient for the practical use to study the relaxation kinetics and its application by analyzing the experimental data will be presented here. This scheme is a simplified version of a more complex scheme, when the diffusion and drift of the charge carriers are taken into account, when better understanding of such phenomena is needed, for instance, by studying the heterostructures.

2. Formulation of the Problem

The scheme of electronic transitions related to a single deep trapping state in the forbidden energy band gap is presented in Fig. 1 [6]. E_C determines the conduction band and E_V is the valence band, thus, E_g qualifies the band gap, E_1 defines the activation energy of electrons from the trapping state. Arrows 1, 2, 3, 4 indicate the possible electronic transitions to the trapping state and to the valence or to the conduction band, $g(t)$, $g_1(t)$ are electron generation paths by the laser pulses generated from the valence band or from the trapping state. Usually, the set of multiple trapping states appears in the forbidden energy band gap of the binary or multi-component semiconductors, thus, a few of principle states have to be taken into account for modelling the relaxation processes.

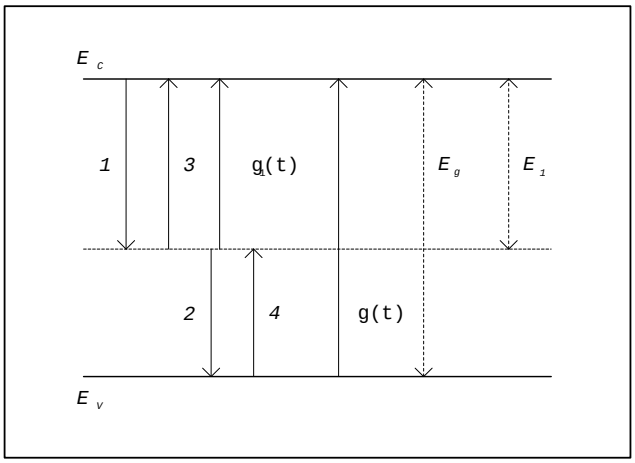

Figure 1. A simplified relaxation scheme in the doped semiconductor.

Electrons transitions, as shown by arrows in Fig. 1, are usually defined as follows [6]:

$$1 - \gamma_n N_{CM}(m_0 + m), \qquad 2 - \gamma_n (M - m_0 - m)(n_0 + n),$$
$$3 - \gamma_p P_{VM}(M - m_0 - m), \quad 4 - \gamma_p (m_0 + m)(p_0 + p),$$

where M is the concentration of the trapping states under consideration, m_0 is the population of those states by electrons under thermal equilibrium conditions, m is the non equilibrium concentration of electron population of the same states (i.e., the difference of those populations, Δm, is defined), electron trapping rates: γ_n - electron trapping by the trapping state from the conduction band or γ_p - hole trapping from the valence band, respectively, N_{CM}, P_{VM} are statistical factors determined by the depth of the trapping states E_i and temperature T, n_0, n and p_0, p are concentrations of electrons and holes under conditions of thermal equilibrium and caused by laser irradiation, respectively.

The electron-hole recombination in such a system irradiated by the laser beam and the corresponding initial conditions are defined by the following set of nonlinear differential equations [2, 3, 7]:

$$\begin{cases} \dfrac{dn}{dt} = \sum_{i=1}^{4}[\gamma_n^i(n_0 + N_{CM}^i)m_i - \gamma_n^i(M_i - m_{0i} - m_i)n] + g(t), \\ \dfrac{dm_i}{dt} = -m_i[\gamma_p^i(p_0 + P_{VM}^i) + \gamma_n^i(n_0 + n + N_{CM}^i)] \\ \qquad\qquad + \gamma_n^i(M_i - m_{0i})n - \gamma_p^i(m_{0i} + m_i), \\ p = n + \sum_{i=1}^{4} m_i, \end{cases} \tag{2.1}$$

$$n(0) = 0, \quad p(0) = 0, \quad m_i(0) = 0. \tag{2.2}$$

In the case of electron generation from the deep trapping state (say, from the second level, $i = 2$), the first and third expressions of equation (2.1) are given by:

$$\begin{cases} \dfrac{dn}{dt} = \sum_{i=1}^{4}[\gamma_n^i(n_0 + N_{CM}^i)m_i - \gamma_n^i(M_i - m_{0i} - m_i)n] + g(t) \\ \dfrac{dm_2}{dt} = -m_2[\gamma_p^2(p_0 + P_{VM}^2) + \gamma_n^2(n_0 + n + N_{CM}^2)] + \gamma_n^2(M_2 - m_{0i})n \\ \qquad - \gamma_p^2(m_{02} + m_2)p, \end{cases}$$

i.e., the electron from this particular state is also taken into account.

The laser pulse is usually assumed to be of the Gaussian shape:

$$g(t) = \alpha\beta I_0 \exp\Big(-\frac{(t - t_0)^2}{2\sigma_t^2}\Big), \tag{2.3}$$

where α is the absorption coefficient, β is the quantum yield, I_0 is the maximum fluence of a laser pulse, t_0 is the time moment, when the pulse of the laser achieves its maximum value, σ_t is the shape of a laser pulse.

In the case, when the energy of the pulse laser E_0 is known, equation (2.3) can be rewritten as:

$$g(t) = \frac{\alpha\beta E_0}{h\nu\sqrt{2\pi}\sigma_t} \exp\Big(-\frac{(t - t_0)^2}{2\sigma_t^2}\Big),$$

where $h\nu$ is the energy of light quantum.

In any particular case the amount of trapping states and their positioning in forbidden energy region have to be chosen to fulfil calculations by means of the differential equations defined above. If the conductivity of the non-irradiated semiconductor at several temperatures is known, the initial selection of parameters can be "tuned". Under conditions of thermal equilibrium for each electronic level the detailed balance relationship has also to be fulfilled for every electronic state, thus, giving:

$$p_{0i} + \frac{M_{d1}N_{CM}^{1i}}{n_{0i} + N_{CM}^{1i}} + \frac{M_{d2}N_{CM}^{2i}}{n_{0i} + N_{CM}^{2i}} = n_{0i} + \frac{M_{a1}P_{VM}^{1i}}{p_{0i} + P_{VM}^{1i}} + \frac{M_{a2}P_{VM}^{2i}}{p_{0i} + P_{VM}^{2i}}. \quad (2.4)$$

In the following the parameters of four levels will be taken into account: two donor levels M_{di} and two acceptor levels M_{ai}. By solving the system of four nonlinear algebraic equations (n_{0i}, p_{0i} are known at four temperatures and for chosen state positioning), the populations of those states will be defined.

The final goal is to identify parameters of the trapping states, which cannot be defined directly. Having experimentally observed data of the conductivity relaxation in the semiconductor volume at different temperatures and at different levels of laser irradiation, parameters of the trapping states and their amount can be defined from fitting those experimental data by means of the solution of equations (2.1). The set of equations (2.4) is sensitive to variation of parameters, thus, the solution has to be fulfilled with enhanced precision. Optimization goal function is defined as follows:

$$\Delta\sigma = \min\left(\sum_i \left|\frac{\sigma_{Exp}(t_i) - \sigma_{Cal}(t_i)}{\sigma_{Exp}(t_i)}\right|\right), \quad (2.5)$$

where $\sigma_{Exp}(t_i)$ is experimental conductivity value at time t_i, $\sigma_{Cal}(t_i)$ is the conductivity value calculated at the same time point. So, the inverse problem is under consideration, and the goal is to minimize the relative error. Model adequacy can be evaluated by bringing weights into optimization goal function – at the end of the conductivity relaxation period the weight should be smaller as the influence of other factors on charge carriers increases. Finally, it is supposed that each trapping state parameter belongs to the interval $[10^{-11}; 10^{-6}]$.

3. Solution of Direct Problem

For studies of the conductivity for the model with 4 trapping states the set of nonlinear differential equations (2.1) under the initial conditions (2.2) has to be solved for a selected values of eight parameters γ_{ni} and γ_{pi}, $i = 1,\ 2,\ 3,\ 4$. Eigenvalues of the model system (2.1) are scattered, therefore, methods of solutions developed for stiff systems have to be applied. Since the problem has to be considered on a wide time scale (10^{-9} – 10^{-4} s) or (10^{-13} – 10^{-8} s), when the electron/hole concentration varies with different rate and at different

times, the Gear method [5] with variable steps was applied. The reliability of the obtained results is improved if the fitting is carried out for different temperatures and for different excitation fluences. To assure the adequacy of the model for the experimental conditions, further more extended modelling as well as more costly experiments can be carried out.

The conductivity (Si/cm) of the volume of a semiconductor is defined as follows:

$$\sigma = e(n_0 + n)\mu_n + e(p_0 + p)\mu_p, \tag{3.1}$$

where e is the charge of the electron, μ_n, μ_p are the mobilities of the electrons and holes, respectively.

4. Parameters Identification

A goal function of the given stiff system generally defines a very ravined surface. Most of optimization methods reach the bottom of the ravine very quickly, however, the optimization process stops far from the real minimum point. The results of the optimization procedure also depend on initial parameters set. To avoid these problems genetic algorithm [1] was applied.

Discrete optimization problem was solved – all parameters were optimized with rank precision. It is assumed that each parameter can obtain a value from the interval $\{10^{-11}, 10^{-10}, 10^{-9}, 10^{-8}, 10^{-7}, 10^{-6}\}$. Elitist algorithm modification was applied with random mutation possibility and population evolution of 30 generations.

5. Calculation Results and Discussions

Typical temporal evolution of the conductivity (experimental results [7] as well as those from the theoretical fitting) under the action of the nanosecond laser pulse is shown in Fig. 2. It is evident that the calculations give a qualitative fit of the experimental results, however, there are still some deviations. Results at different excitation fluences are shown in Fig. 3 and at different temperatures in Fig. 4. The fitted results are obtained for parameters as indicated in Tab. 1. The parameters of trapping states given in Tab. 1 were indicated on the grounds of physical experience by testing several probable sets.

Table 1. The fitting results.

$M_i(cm^{-3})$	$E_i(eV)$	$\gamma_{ni}(cm^3s^{-1})$	$\gamma_{pi}(cm^3s^{-1})$
$2,52 \cdot 10^{16}$	$0,2$	$1 \cdot 10^{-6}$	$1 \cdot 10^{-7}$
$1,00 \cdot 10^{14}$	$0,4$	$1 \cdot 10^{-11}$	$1 \cdot 10^{-9}$
$5,30 \cdot 10^{16}$	$0,78$	$1 \cdot 10^{-9}$	$1 \cdot 10^{-11}$
$2,52 \cdot 10^{16}$	$1,2$	$1 \cdot 10^{-7}$	$1 \cdot 10^{-6}$

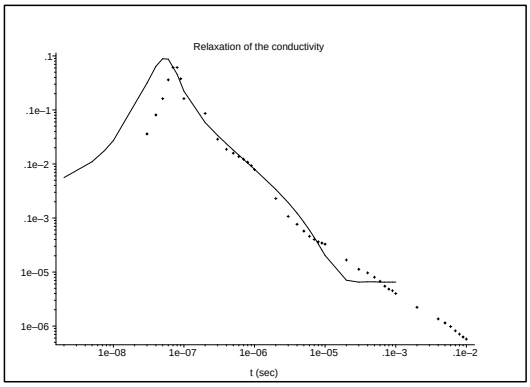

Figure 2. Conductivity relaxation under the influence of the nanosecond laser pulse. Experimental results are indicated by dots and the fitting data by the solid line.

Other situations corresponding to different temperatures and excitation conditions are shown in Fig. 3 – Fig. 7. Parameters of trapping states values

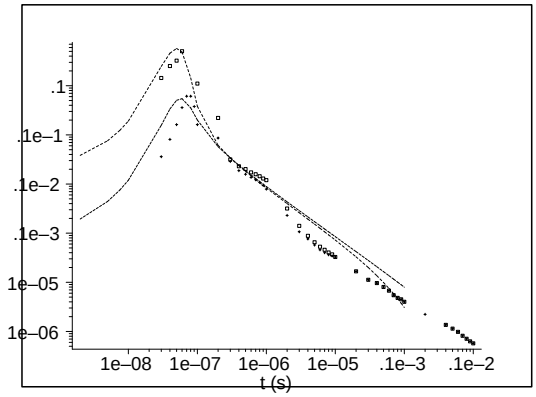

Figure 3. Conductivity relaxation under the influence of the nanosecond laser pulse at different fluences. The upper data corresponds to $4\ 10^{23}\ photons/cm^2$ and the lower data - to $4\ 10^{24}\ photons/cm^2$.

were also identified using genetic algorithm. The results of 20 calculation sets are presented in Tab. 2.

The results of the optimization procedure for three experimental data sets with different temperatures and excitation conditions are presented in Tab. 3. Since optimization procedure results depend on experimental data accuracy, calculation based on few data sets is obviously more reliable than the one based on single experiment data.

The best result of the set 1 disagrees with the best result of the set 2 only by single parameter value.

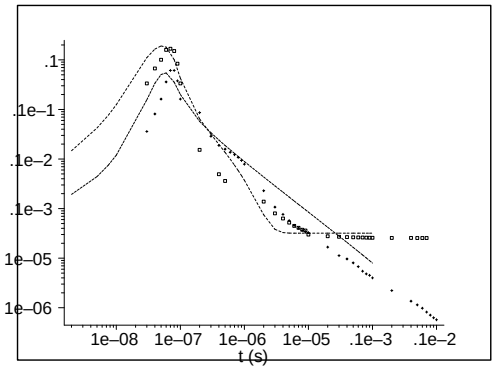

Figure 4. Conductivity relaxation under the influence of the nanosecond laser pulse at different temperatures. Dashed line corresponds to $T = 400\ K$, crosses – to $T = 300\ K$.

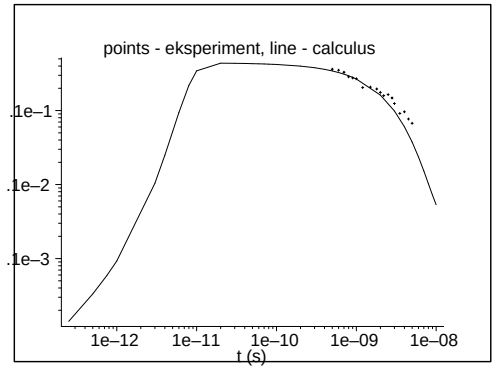

Figure 5. Conductivity relaxation under the influence of the picosecond laser pulse. The solid line corresponds to calculations, the dots – to the experiment.

Table 2. Parameters of trapping states values identified using a genetic algorithm.

	$\gamma_{ni}(cm^3s^{-1})$	$\gamma_{pi}(cm^3s^{-1})$	$\Delta\sigma$	Fall density
1	$\{10^{-6}, 10^{-6}, 10^{-11}, 10^{-11}\}$	$\{10^{-7}, 10^{-6}, 10^{-11}, 10^{-6}\}$	8.71	0.35
2	$\{10^{-6}, 10^{-6}, 10^{-11}, 10^{-10}\}$	$\{10^{-7}, 10^{-6}, 10^{-11}, 10^{-6}\}$	8.72	0.20
3	$\{10^{-6}, 10^{-6}, 10^{-7}, 10^{-11}\}$	$\{10^{-7}, 10^{-11}, 10^{-10}, 10^{-6}\}$	8.94	0.20
4	$\{10^{-6}, 10^{-11}, 10^{-6}, 10^{-11}\}$	$\{10^{-7}, 10^{-6}, 10^{-10}, 10^{-6}\}$	9.11	0.05
5	$\{10^{-6}, 10^{-7}, 10^{-11}, 10^{-11}\}$	$\{10^{-7}, 10^{-7}, 10^{-11}, 10^{-6}\}$	9.12	0.05
6	$\{10^{-6}, 10^{-6}, 10^{-6}, 10^{-11}\}$	$\{10^{-6}, 10^{-8}, 10^{-11}, 10^{-6}\}$	15.03	0.05
7	$\{10^{-6}, 10^{-6}, 10^{-6}, 10^{-7}\}$	$\{10^{-6}, 10^{-6}, 10^{-9}, 10^{-6}\}$	15.83	0.10

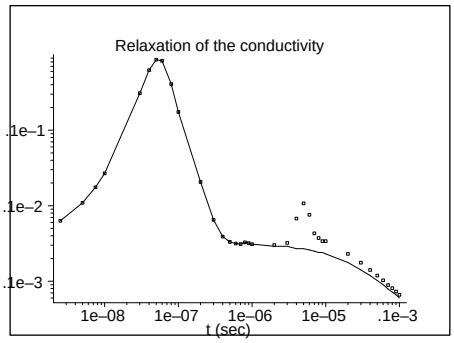

Figure 6. Conductivity relaxation under the influence of one and two nanosecond laser pulses. The first laser pulse induces the band – band transition while the second pulse generates electrons from trapping state ($E = 0,4\ eV$, $t_0 = 5\ 10^{-6}\ sec$). The solid curve corresponds to a single pulse, the dots demonstrate results corresponding to the case of two pulses.

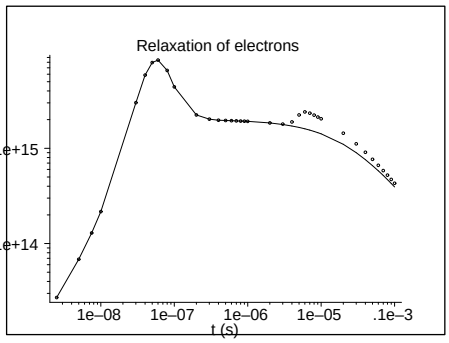

Figure 7. Relaxations of the electron concentration in the trapping state ($E = 0,4\ eV$) in the case of excitation by one and two nanosecond laser pulses. The solid curve corresponds to the case of one pulse, dots - to two pulses.

Table 3. The results of the optimization procedure for different temperatures.

	$\gamma_{ni}(cm^3s^{-1})$	$\gamma_{pi}(cm^3s^{-1})$	$\Delta\sigma$	Fall density
1	$\{10^{-6},10^{-6},10^{-7},10^{-11}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-6}\}$	29.95	0.25
2	$\{10^{-6},10^{-6},10^{-7},10^{-8}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-6}\}$	29.96	0.20
3	$\{10^{-6},10^{-6},10^{-7},10^{-11}\}$	$\{10^{-7},10^{-7},10^{-11},10^{-6}\}$	30.09	0.05
4	$\{10^{-6},10^{-6},10^{-7},10^{-11}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-7}\}$	30.16	0.05
5	$\{10^{-6},10^{-6},10^{-8},10^{-11}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-6}\}$	30.28	0.05
6	$\{10^{-6},10^{-6},10^{-6},10^{-11}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-6}\}$	30.52	0.10
7	$\{10^{-6},10^{-7},10^{-6},10^{-11}\}$	$\{10^{-7},10^{-6},10^{-11},10^{-6}\}$	31.04	0.10
8	$\{10^{-6},10^{-11},10^{-6},10^{-11}\}$	$\{10^{-7},10^{-9},10^{-11},10^{-6}\}$	31.55	0.25

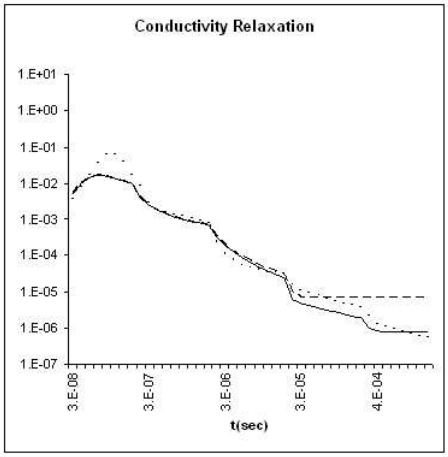

Figure 8. Conductivity relaxation under the influence of the nanosecond laser pulse. The dashed line corresponds to the parameters indicated in Tab. 1 and the solid line – to the first set in Tab. 2.

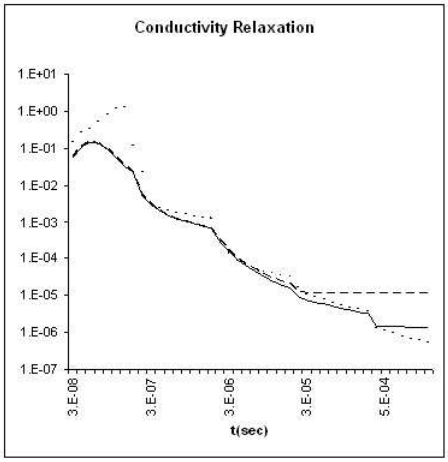

Figure 9. Conductivity relaxation under the influence of the nanosecond laser pulse at fluence $4\ 10^{23}\ photons/cm^3$. The dashed line corresponds to the parameters indicated in Tab. 1, and the solid line – to the first set in Tab. 3.

6. Conclusions

As demonstrated by fitting the experimental data, the parameters of the trapping states, such as the energy depth, the concentration of the trapping states, trapping efficiencies for electrons and holes, can be well determined using optimization algorithms, though specific optimization methods should be applied. To increase optimization reliability experimental data errors should be evaluated. As soon as those values are defined, more complex experimental conditions can be considered. For instance, the diffusion and drift of charge carriers can be taken into account. Conditions with two excitation pulses provide the possibilities to estimate the "inertness" of the system under consideration and its dependence on the excitation level as well as the competition of the population/depopulation between each of the trapping states. The latter is sensitive to the wavelength of the excitation pulses. And finally, this fitting procedure is valid for any semiconducting system providing better understanding of the processes under consideration.

Acknowledgment

This work was supported by the Lithuanian State Science and Studies Foundation within the project on B-03/2007 "Global optimization of complex systems using high performance computing and GRID technologies" and by the Eureka Project EUREKA E!3691 OPTCABLES.

References

[1] D. Batishev and S. Isaev. Optimization of multiextremum functions using genetic algorithms. (in Russian)

[2] A. Pincevičius, R.J. Rakauskas and S. Vošterienė. The numerical models of the estimation of the electrooptical parameters of $GaAs$. *Lithuanian Journal of Physics*, **42**, 340–344, 1992. (in Russian)

[3] A. Pincevičius and J. Storasta. Determination of the parameters of the deep levels of photosensitive semiconductors. *Theses of the IX World Lithuanian Symposium of Science and Arts*, 86–87, 1995. (in Lithuanian)

[4] J.V. DiLorenzo and D.D. Khandelwal. *GaAs FET principles and technology.* Radio and Communication, 1988. (in Russian)

[5] C.W. Gear. *Numerical initial value problem in ordinary differential equations.* Prentice Hall, Englewood Cliffs, New York, 1971.

[6] S.M. Rivkin. *Photoelectric phenomena in semiconductors.* Fizmatgiz, 1963. (in Russian)

[7] J. Vaitkus, J. Storasta, A. Pincevičius, M. Petrauskas and V. Kažukauskas. Determination of the parameters of the deep levels in semi-insulating $GaAs$ by relaxation of the photoconductivity at pulse laser excitation. *Lithuanian Journal of Physics*, **28**(6), 744–751, 1988. (in Russian)