

**Influence of high energy radiation on transport characteristics
of electrons in semiconductor structures.
Simulation by Monte Carlo method**

N.V.Demarina*, S.V.Obolensky, V.K.Kiselev**

*Nizhni Novgorod State University
Gagarin avenue 23, Nizhni Novgorod, 603950, Russia*

Influence of radiation-induced defects (charged point defects and disordered regions) on electron transport characteristics in *n-GaAs* is studied with the help of Monte Carlo method.

Introduction

The experimental researches of generation of defects in solids began in nineteenth century. However processes of high-energy radiation interaction with semiconductors were begun to study systematically soon to the end of the Second World War. It was because the creation of the nuclear weapons and also development of atomic engineering and space development followed after them. These events caused appearance of a radiation resistance problem [1].

However don't forget, that semiconductors are very sensitive to presence even of small quantity of defects. It caused that more than forty years ago radiation defects have been specially formed in semiconductor materials for modification of their properties [2]. Since the problem of interaction of high-energy particles with materials has left the frameworks of radiation resistance tasks and has got universal character.

Nowadays together with traditional methods (for example ion implantation) the new radiation methods are developed. They are isolation of a material by ion irradiation, various variants of gettering and others [2]. Now extensive experimental material on researches of the electrophysical characteristics of the basic semiconductors (*Si*, *Ge*, *GaAs*) for a case of irradiation by ions, neutrons, electrons has been accumulated. In the conditions of irradiation of the semiconductor by high-energy particles we frequently face damages considerably differing by their complexity, nature and character of display in modification of initial material properties. Therefore in some cases there are not only quantitative and even qualitative explanations of the experimentally observed phenomena.

Development of the authentic models describing transport of charge carriers in semiconductor structures allows to overcome difficulties concerned with prediction of the material and devices characteristics modification under radiation influence successfully. Such models were developed as required.

In the seventies the frequency of serial devices was about 10GHz. In this range of frequencies the sizes of active areas of devices exceeded 1 μm . In that time method of the equivalent circuit was used as usual method of the theoretical analysis of low-frequency devices [3]. It means that semiconductor device was replaced with a set of resistors, ca-

* Phone: +7-8312-656032; Fax: +7-8312-656416; E-mail: demarina@rf.unn.runnet.ru

** Phone: +7-8312-656032; Fax: +7-8312-656416; E-mail: obolensk@rf.unn.runnet.ru

capacitors and inductors. The characteristics of the semiconductor device were calculated by the solution of the equations based on the Kirhgoff laws. Since the computer speed was low the elements parameters of the equivalent circuit were determined approximately. Usually result was obtained with the use of one-dimensional local-field approach, which included the following equations [3]:

$$\begin{aligned} \Delta V &= \frac{q}{\varepsilon_s} (n + N_+ - N_-), \\ \frac{\partial n}{\partial t} &= \frac{1}{q} \nabla \mathbf{j} + G - R, \quad \mathbf{j}_n = -qn \mathbf{v}_n + q \nabla (D_n n), \\ \mathbf{j} &= \mathbf{j}_n + \frac{\partial \mathbf{E}}{\partial t}, \quad \mathbf{E} = -\nabla V, \end{aligned} \quad (1)$$

where V is the electrostatic potential, n is electron concentration, N_+ , N_- are the concentrations of positive and negative charged ions (donor and acceptor impurities, radiation-induced defects), \mathbf{j}_n , \mathbf{j} are the electron and full currents densities, D_n is the coefficient of electron diffusion, \mathbf{v}_n is the drift velocity of electrons, E is the electric field, G is the generation rate, R is recombination rate, ε_s is the permittivity, q is the electron charge.

It was supposed that the charge carrier velocity was proportional to an electrical field in the each point and the previous history of electron motion wasn't considered. Main effects, which taken into account in such model of radiation influence were increase of carriers concentration due to material ionization and decrease of mobility, concentration and lifetime of charge carriers as a result of defect generation.

The significant change of a situation has occurred in the late eighties and in the early nineties, when the maximum frequency of transistors have amounted to about 100-200 GHz and the sizes of active areas were reduced up to tenth micron. In the case of such sizes of active areas the effects concerned with nonlocal properties and non-uniformity of electron-hole plasma are significant. In such case it is necessary to use two or three-dimensional model and to take into account a lot of new effects. These effects deal with electron gas heating and charge carriers scattering on radiation-induced defects. Use of numerical methods has become inevitable. In the early nineties the approach based on quasi-hydrodynamic system of the equations was offered [3]:

$$\begin{aligned} \Delta V &= \frac{q}{\varepsilon_s} (n - N_+ + N_-), \quad \frac{\partial n}{\partial t} = \frac{1}{q} (\nabla, \mathbf{j}_n) + G - R, \\ \frac{d(m(W_n) \mathbf{v}_n)}{dt} &= q \mathbf{E} - \frac{m(W_n)}{\tau_p} \mathbf{v}_n, \end{aligned} \quad (2)$$

$$\frac{\partial(W_n n)}{\partial t} = (\nabla, \mathbf{j}_{W_n}) + (\mathbf{j}_n, \mathbf{E}) - \frac{n(W_n - W_0)}{\tau_W} + G W_i,$$

$$\mathbf{j}_n = -qn v_n + q \nabla(D_n n), \quad \mathbf{j}_{W_n} = -n W_n v_n + \nabla(D_n n W_n),$$

$$\mathbf{j} = \mathbf{j}_n + \frac{\partial \mathbf{E}}{\partial t}, \quad \mathbf{E} = -\nabla V,$$

where V is the electrostatic potential, n is electron concentration, N_+ , N_- are the concentrations of positive and negative charged ions (donor and acceptor impurities, radiation-induced defects), \mathbf{j}_n , \mathbf{j} are the electron and full currents densities, \mathbf{j}_{W_n} is the electron energy flux density, W_n , W_0 are the non-equilibrium and equilibrium energies of electrons, respectively; τ_W is the time of energy relaxation, τ_p is the time of pulse relaxation, m is conduction band effective mass, D_n is the coefficient of electron diffusion, v_n is the drift velocity of electrons, \mathbf{E} is the electric field, G is the generation rate, R is recombination rate, ϵ_s is the permittivity, q is the electron charge. This system is for macroscopic physical magnitudes and includes the large number of kinetic characteristics

New problem has appeared as a result. It deals with necessity of determination of electron-hole gas transport characteristics in semiconductors during and after radiation influence for electrical field value up to 100kV/cm. They are drift velocity, mobility, energy and pulse relaxation times and others.

The analysis of the charge carrier transport phenomena traditionally is based on a solution of transport Boltzmann equation. The Monte Carlo method is extremely attractive for the solution of this equation [4]. It allows inserting in the model additional scattering mechanisms, to vary semiconductor band structure. Thus it is very visual and gives an opportunity to investigate influence of various processes on the material characteristics in detail. But despite of all advantages, it has one sufficient disadvantage. It deals with enormous expenses of machine time and therefore difficulty in its realization. Nevertheless, in contrary to all difficulties, the purpose of this work was the study of electron transport in *GaAs* structures under defect-induced and ionizing radiation influence by numerical simulation with use of the Monte Carlo method.

In the paper it is written briefly about the features of high energy particles interaction with semiconductors firstly, the methods of calculation of the electron gas characteristics in *GaAs* under radiation influence are described and opportunities of these methods by some of the obtained results are shown.

1. Monte Carlo method

The principle of the Monte Carlo method as applied to the determination of distribution function is to simulate the motion of one electron in momentum space. This motion consists alternately of a drift with constant velocity in the electric field followed by scattering by phonons. The equation of electron motion in the electrical field of intensity \mathbf{E} between the scattering events is following [4,5]

$$\frac{d\mathbf{k}}{dt} = -\frac{q}{\hbar} \mathbf{E}, \quad (3)$$

where \mathbf{k} is wave vector of electron, t is time, q is electron charge, \hbar is Planck's constant.

The time which electron drifts in the electric field, the type of scattering processes and the final state are random quantities with probability distributions which can be expressed in terms of the transition rates due to the various processes and the strength of the electric field. Computer in accordance with special techniques generates these random values. For example the time of free flights of electron t_s is determined by expression

$$t_s = -\frac{1}{\Gamma} \ln(r), \quad (4)$$

where r is random number generated with equal probability between 0 and 1 and Γ is following

$$\Gamma = \sum_{q=1}^n \lambda_q(\mathbf{k}), \quad (5)$$

where total λ_q is total transition rate from the state \mathbf{k} due to the q 'th process. Having determined the time of free flight with the help of the next random number the scattering process responsible for terminating the flight is determined. Further random numbers are required to determine the final state after the scattering.

In order to determine energy distribution function histogram is set up energy space. Time that the electron spends in a particular cell is proportional to the distribution function at this point in energy space. The physical quantities such as the drift velocity, mean energy and so on can be obtained by numerical integration of distribution function. But it is more convenient to calculate them directly from the initial and final k -components of each free flight.

In the paper the transport characteristics of electrons in n-type *GaAs* were calculated by the Monte Carlo method. The three-valley Γ -L-X model of conduction band was used [6]. Polar optical, deformation potential acoustic, ionizing impurity and relevant intervalley scattering processes were considered together with the non-parabolicity in each type of valleys.

The results obtained with the Monte Carlo technique for n-type *GaAs* without radiation induced defects were in a good agreement with experimental data represented in literature [6].

2. Main features of interaction of high-energy radiation with semiconductor

The influence of high-energy radiation on the semiconductors is accompanied firstly by producing of a various kinds of structural damages of a crystal lattice and secondly generation of non-equilibrium charge carriers due to energy radiation. The first process causes the irreversible modification of material parameters, in the second case the initial properties of the semiconductor are restored after determination of irradiation. Therefore work consisted of two parts devoted to investigation of electron transport after firstly de-

fect-induced and secondly, ionizing radiation influences. It will be paid attention only to the first part in the paper.

Mention should be made that term radiation-induced defect means more or less steady structure damage of crystal lattice appearing as a result of high energy particles action [1].

During motion through a material a particle with the high energy transfers a part of energy to atoms of the substance. Depending on a kind of a particle this process occurs differently. To describe this process in detail is not purpose of this paper but it is necessary to stress, that it is supposed, that the atom is always displaced from the steady position in a crystal lattice, if the energy, obtained by it is more than some threshold energy of displacement. Threshold energy of displacement is minimal energy which is necessary for displacement of atom from a crystal lattice point to interstice. If energy obtained by atom as a result of interaction with a high energy particle is about threshold energy of displacement the atom is just displaced from the steady crystal lattice point with creation of the elementary point defect - empty lattice point (vacancy) and interstitial atom. This defect is called Frenkel' pair. If the energy obtained by atom considerably exceeds threshold energy of displacement the atom during the motion in a material comes into consecutive collisions with other atoms, knocks out them from their crystal lattice points, transmitting to them superfluous energy. Knocked out atoms, in their turn, create the following generation of knocked out atoms and so on. The collision cascade is developing. It decays when the energy transmitted by primary atom (ancestor of the cascade) at the next collision is less or about threshold one [7].

The developing cascade of collisions causes producing of cluster of prime (initial) radiation-induced defects. Relaxation of prime defects cluster results in under due conditions appearance of thermodynamically steady cluster, which is called disordered region. It should be note that the irradiation by electrons and protons usually is accompanied by appearance of point defects. While an irradiation by neutrons causes disordered regions and point defects.

Therefore the paper devoted to study of electron transport in structures with radiation induced defects includes two parts. In one part the point defects influence on charge carrier kinetic characteristics was investigated and in another – disordered regions were considered.

3. Influence of the charged point defects on n-GaAs electrophysical characteristics

The point defects influence on the electrophysical characteristics of *GaAs* was considered for case of defects created in a material by protons with energy of about tens keV.

At the first I shall stop on the model of point defect. It is known that the producing in the semiconductor of simple defects such as Frenkel' pairs is accompanied by creation in the semiconductor gap of the whole system of energy levels [8]. It was supposed that the energy level could be occupied by one electron or is empty. Therefore the lattice defect could be in two charging states. Born approach for screened Coulomb potential was used to calculate the total transition rate from the state with energy W for scattering by charged point radiation-induced defect. The expression for transition rate is following

$$\lambda_{pdj}(W) = \frac{2\sqrt{2}\pi N_{pd} q^4 \sqrt{m^*}}{\epsilon^2 \hbar^2 \beta^2} \frac{1 + 2\alpha_j W}{\sqrt{W(1 + \alpha_j W)}}, \quad (6)$$

$$\beta^2 = 4\pi \frac{nq^2}{\epsilon k_B T},$$

where W is the electron energy counted from the appropriate valley bottom, N_{pd} is the defects concentration, n is the electron concentration, m^* is the effective electron mass, α_j is the non-parabolicity constant j 'th valley, ϵ_s is the permittivity, \hbar is Planck's constant, k_B is Boltzmann's constant.

Some results obtained with the help of described model are represented below.

Drift velocity, mobility, energy and pulse relaxation times and some other electron transport characteristics in n-type GaAs with concentration of doping impurity $6 \cdot 10^{17} \text{ cm}^{-3}$, before and after an irradiation by protons with average energy 20 keV by a dose 0.1 and 0.2 μCi were calculated.

The dependencies of electron drift velocity and mobility on the electric field, pulse and energy relaxation time of electrons as a function of average electron energy for different defect concentration are presented in Fig. 1 and 2.

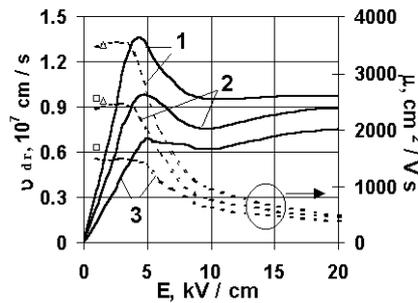


Fig. 1

Electric field strength E dependence of the electron drift velocity v_{dr} (—) and mobility μ (- -) before 1 and after irradiation of n-GaAs by protons with the energy 20 keV with dose 2 $-D_p=0.1 \mu\text{Ci}$, 3 $-D_p=0.2 \mu\text{Ci}$; \square – analytical approach, Δ – experimental data. Concentration of doping impurity is $6 \cdot 10^{17} \text{ cm}^{-3}$

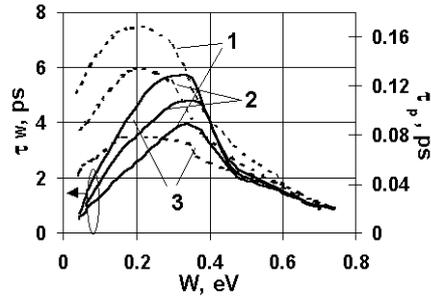


Fig. 2

Energy τ_w (—) and pulse τ_p (- -) relaxation times as a function of the electron average energy W before 1 and after irradiation of n-GaAs by protons with the energy 20 keV with dose 2 $-D_p=0.1 \mu\text{Ci}$, 3 $-D_p=0.2 \mu\text{Ci}$; \square – analytical approach, Δ – experimental data. Concentration of doping impurity is $6 \cdot 10^{17} \text{ cm}^{-3}$

It is clear that due to presence in material of the charged radiation-induced defects total scattering transition rate increases considerably. It causes that the pulse relaxation time decreases twice at concentration of defects compared with concentration of doping impurity. Length of free flight also decreases, therefore electron during free flight picks up smaller energy. As a result radiation-induced charged defect scattering, despite of its small-angle character results in significant reduction of mobility and average drift velocity. But the scattering by defects is elastic (electron doesn't loss energy, but only changes the direction of its motion). It results in increase of energy relaxation time. In low electric fields the results of numerical calculation are in a good agreement with the data obtained with the help of analytical formula [7]. In Fig. 1 the badges mark experimental data. It is seen that they are close to theoretical values.

4. Influence of the charged point defects and disordered regions on *n-GaAs* electrophysical characteristics

The influence of both charged point defects and disordered regions on the electrophysical characteristics *n-GaAs* was investigated for case of defects formed in the material by fast neutrons with energy of about MeV.

For description of disordered region it was used model developed by Gossik [7,9] who proposed that there is electrically neutral kernel in center enriched with vacancies (Fig. 3). It is surrounded with the charged shell consisting of complexes of vacancies with impurity atoms and defects. Approximately disordered region is regarded as a sphere. The energy levels of defects inside disordered region assign certain state of the Fermi level in the gap, which is not the same as in bulk. Establishing of thermodynamic equilibrium between a semiconductor lattice and cluster is accompanied by Fermi levels equalization in both parts of a crystal. Around of disordered region the layer of spatial charge is formed. Therefore the disordered region looks like ordinary p-n-junction. The distribution of electric field and potential at the disordered region is represented in Fig. 4.

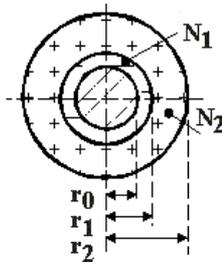


Fig. 3
Cross-section of disordered region (Gossik's model).

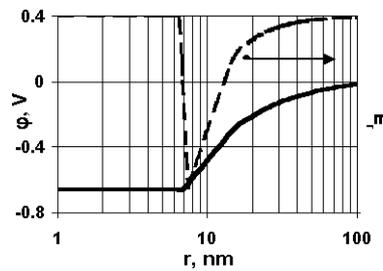


Fig. 4
Coordinate r dependence of the electrostatic potential φ and radial component of the electric field E_r in disordered region. Concentration of doping impurity is 10^{15} cm^{-3} .

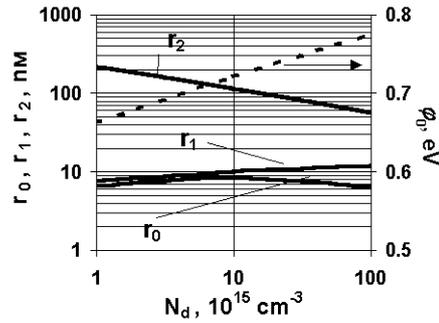


Fig. 5
Radiuses of damaged region r_1 , central kernel r_0 , lay of space charge r_2 and electrostatic potential ϕ_0 in the center of the disordered region as a function of doping impurity concentration N_d .

for the first time. The calculated dependencies r_0 , r_2 and ϕ_0 as function of doping impurity concentration are represented in the Fig. 5.

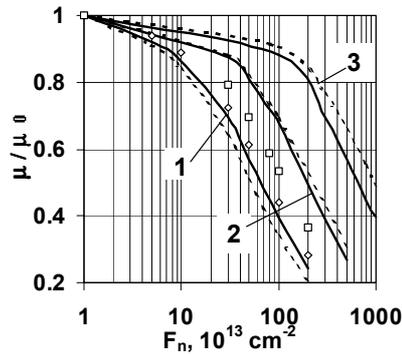


Fig. 6
Electron mobility in *n-GaAs* after irradiated by fast neutrons with average energy 1 MeV as a function of neutron fluence. Concentration of doping impurity: 1 - $N_d = 10^{15} \text{ cm}^{-3}$, 2 - $N_d = 10^{16} \text{ cm}^{-3}$, 3 - $N_d = 10^{17} \text{ cm}^{-3}$;
— method Monte Carlo, - - - empirical relation [10], analytical estimation - \diamond - $N_d = 10^{15} \text{ cm}^{-3}$, \square - $N_d = 10^{16} \text{ cm}^{-3}$

It was necessary to solve a task of determination of disordered region parameters to calculate transition rate of charge carriers by such heterogeneity (disordered region). This task was solved with the help of new experimental data represented in the literature [6] in approach of Gossik model. These data includes the sizes of the damaged area (r_1), concentration and energy levels of radiation induced defects. Radiuses of the kernel (r_0), spatial charge lay (r_2) and concentration of charges in the kernel shell of region were determined

Due to classical character of particles motion in relation to a large-scale picture charge which takes place close to disordered region the disordered region was considered as insuperable barrier for particles. The scattering transition rate was determined with the help of cross-section of disordered region, which depended on charge carrier energy. The derived expression transition rate is following

$$\lambda_j(W) = v_j \Sigma_{dr} N_{dr},$$

$$\Sigma_{dr} = 2\pi \times r_{ef}^2, \quad (7)$$

where r_{ef} is the effective radius of disordered region, N_{dr} is the disordered region concentration, v_j is the electron velocity in j 'th valley.

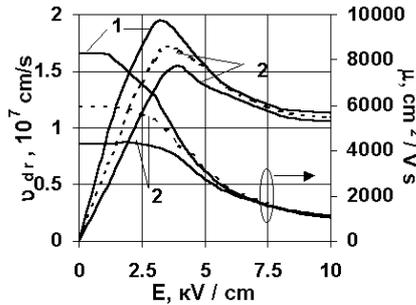


Fig. 7

Drift velocity v_{dr} and mobility μ as a function of electric field strength E in n -GaAs: 1 – without irradiation; 2 – after irradiation by neutron flux of $5 \cdot 10^{14} \text{ cm}^{-2}$: point defects and disordered regions (—); disordered regions (- - -). Concentration of doping impurities $N_d = 10^{15} \text{ cm}^{-3}$

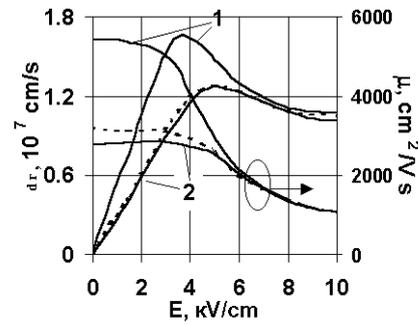


Fig. 8

Drift velocity v_{dr} and mobility μ as a function of electric field strength E in n -GaAs: 1 – without irradiation; 2 – after irradiation by neutron flux of $5 \cdot 10^{15} \text{ cm}^{-2}$: point defects and disordered regions (—); disordered regions (- - -). Concentration of doping impurities $N_d = 10^{17} \text{ cm}^{-3}$

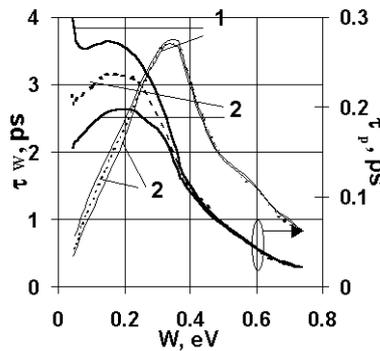


Fig. 9

Energy τ_W and pulse τ_p electron relaxation times as function of average electron energy in n -GaAs:

1 – without irradiation; 2 – after irradiation by neutron flux of $5 \cdot 10^{14} \text{ cm}^{-2}$: point defects and disordered regions (—); disordered regions (- - -). Concentration of doping impurities $N_d = 10^{15} \text{ cm}^{-3}$

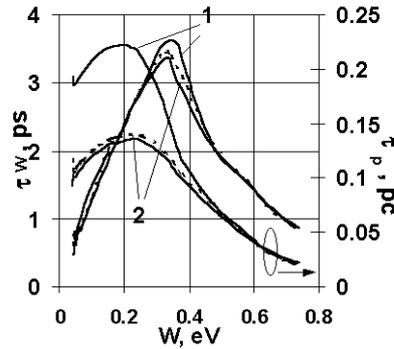


Fig. 10

Energy τ_W and pulse τ_p electron relaxation times as function of average electron energy in n -GaAs:

1 – without irradiation; 2 – after irradiation by neutron flux of $5 \cdot 10^{15} \text{ cm}^{-2}$: point defects and disordered regions (—); disordered regions (- - -). Concentration of doping impurities $N_d = 10^{17} \text{ cm}^{-3}$

At discussion of the results of this paper part it would be desirable to stop on two moments. Firstly kinetic characteristics of electrons were calculated for case of n-type *GaAs*, irradiated by fast neutrons for concentration of doping impurity 10^{15} , 10^{16} and 10^{17} cm^{-3} . The calculated mobility as function of neutron fluence is represented in the Fig. 6. Good agreement between theoretical and experimental data known earlier takes place. Drift velocity, energy and pulse relaxation times as a function of electric field strength for different neutron fluence were calculated (Figs. 7, 8, 9, 10).

Secondly, the influence of point defects and disordered regions on the electrophysical characteristics of *n-GaAs* was compared. For this purpose the calculations were carried out on the one hand for a material with radiation-induced defects of both types and one the other - with disordered region only. The result is represented in Figs. 7–10.

It is seen that in the case of small concentration of doping impurity (10^{15} cm^{-3} , Fig. 7 and 9) disordered regions give the contribution to change of the characteristics like point defects only when they occupy more than 10% of material volume. In the case of the high doping impurity concentration (10^{17} cm^{-3} , Fig. 8 and 10) their influence is dominant in compare with point defects. It is the important result, which has practical importance. It allows to state that forming in low doping material disordered regions with a combination of the point defects elimination is method to create a new material with high mobility and incredible small lifetime of non-equilibrium charge carriers.

5. Influence of radiation-induced defects on electron transport in nanometer structures

Monte Carlo method allows simulating electron transport in nanometer structures. In the paper the influence of radiation-induced defects on feature of ballistic electron transport in “short” structures was investigated.

It is known that stationary drift velocity in *GaAs* can not exceed value about $2 \cdot 10^7$ cm/s . However in a dynamic (non-stationary) conditions, for example, when the electrical field varies sharply from 0 up to some value electron can move without any scattering. The time of the free path is about pulse relaxation time. It means, that if electrons fly through active area of semiconductor structure during time, compared with pulse relaxation time, their average velocity in this area should exceed it's stationary value.

In Fig. 11 the average drift velocity is represented as function of electric field strength for semiconductor structure with length 100 nm. It is seen, that the velocity (solid line *l* in Fig. 11) is significant more in compare with stationary value in a bulk crystal.

Maximum average drift velocity of electron in the structure as a function of structure length is represented in Fig. 12 for different charged point defect concentration. It is obtained that the scattering by the charged point defects defect decreases free flight time, therefore peak value of drift velocity decreases. So, if concentration of the charged point defects is compared with concentration of doping impurity, the effect of velocity overshoot does not affect on electron motion in structures with lengths exceeding 250 nm.

The result of electron transport simulation in short structures with both disordered regions and point defects is represented in Fig. 12. It is supposed that length of structures is 100 nm and concentrations of doping impurity are 10^{15} and 10^{17} cm^{-3} . Obtained results allow to state that the influence of point defects on electron transport is dominant in low

doped structures. In highly doped material their effect can be neglected since the disordered region influence is dominant.

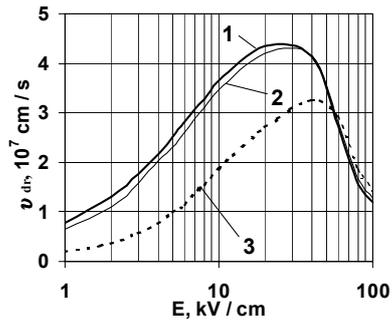


Fig. 11

Average electron drift velocity v_{dr} as a function of electric field strength E in n -GaAs without radiation-induced defects (1), with disordered regions (2), with disordered regions and point defects (3). Neutron fluence: $2.3 - 3 \cdot 10^{14} \text{ cm}^{-2}$. Structure length is 100 nm, concentration of doping impurity is 10^{15} cm^{-3} .

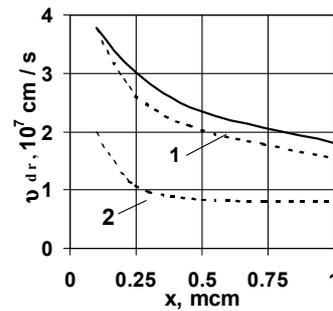


Fig. 12

Semiconductor structure length x dependence of drift velocity v_{dr} in n -GaAs before (—) and after (- - -) irradiation by protons (average energy is 20 keV) by dose: 1 – 0.1 μCl ; 2 – 0.2 μCl . Concentration of doping impurity is $6 \cdot 10^{17} \text{ cm}^{-3}$.

6. Experimental verification

For experimental approbation of model the $n^+ - n - n^-$ structures with various concentration of doping impurity in the n -layer were used. Schottky-gate field-effect transistors with gate length from 30 nm up to 1.5 μm were made. The photo of studied structure with gate length 0.25 μm is represented in Fig. 13. The structures were irradiated in one case with protons with average energy 20 keV, in the other - neutrons with average energy 1 MeV. The degradation of the material electrophysical characteristics after irradiation results in degradation of the device characteristics - reduction of the drain current and power gain coefficient. In Fig. 14 experimental data are represented for the transistor with 0.25 μm gate length irradiated by fast neutron with average energy about 1 MeV.

Kinetic characteristics of electron gas in GaAs with radiation induced defects calculated with the help of Monte Carlo method were approximated. As a result analytic formulas were derived for electron drift velocity, pulse and energy relaxation times and others. These expressions were used for calculation of current-voltage and high-frequency characteristics of Schottky-gate field-effect transistor with the help of quasi-hydrodynamic system of the equation (2). As seen on Fig. 14 a good agreement between experimentally and theoretically received characteristics takes place.

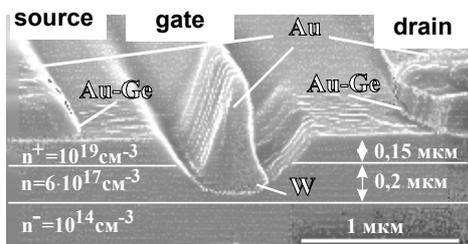


Fig. 13
Photomicrograph of field-effect transistor cross-section (gate length is 0.25 μm)

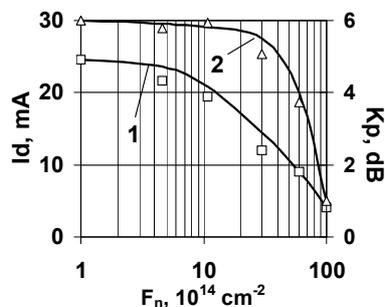


Fig. 14
Drain current (1) and power gain (2) of field-effect transistor as function of the neutron flux (gate length is 0.25 μm);
— theoretical results,
□, Δ – experimental data

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