



UDC 621.382.323; 621.382.82

**ELECTRON TRANSPORT IN QUANTUM WELL HETEROTRANSISTORS**  
**ЕЛЕКТРОННИЙ ТРАНСПОРТ У ГЕТЕРОТРАНЗИСТОРАХ З КВАНТОВОЮ ЯМОЮ****Kulikov Kostyantyn,***postgraduate,*ORCID: <http://orcid.org/0000-0001-9743-0047>**Moskaliuk Vladimir,***Professor, PhD,*ORCID: <http://orcid.org/0000-0002-2753-0744>**Timofeyev Vladimir,***Professor, Doctor of Technical Sciences,*ORCID: <http://orcid.org/0000-0003-0515-1580>*Department of Electronic Engineering (<http://ee.kpi.ua>)**National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"**Kyiv, Ukraine*

**Abstract** The paper presents an analysis of electron transport processes in quantum wells of submicron heterostructural transistors. Techniques for modeling processes in nanoheterostructures have been developed, considering specific quantum effects and scattering mechanisms observable for ternary compounds. Based on the system of relaxation equations, modeling of submicron heterostructures with quantum wells is developed. The modeling takes into account the scattering of optical, acoustic, inter-valley, impurity mechanisms and scattering at the alloy deformation potential. The relaxation times for these scattering mechanisms are calculated and the influence on the initial characteristics of the submicron heterostructural transistor is prognosed.

**Keywords:** electron transport, scattering mechanisms; alloying potential; relaxation times; submicron heterostructural transistors; quantum wells.

**Introduction**

Heterostructure Field-Effect Transistors (HFETs) with high electron mobility demonstrate an internal field in the channel due to the bulk charge of the electrons pressed against the walls of the heterojunction, which in turn leads to electrical quantization of electron motion perpendicular to the heterojunction plane.

Prospects for the use of wide-band semiconductor materials, in particular GaN, to create HFETs with a gate length of 15-30 nm are shown in [1]. It is assumed that the cutoff frequencies of such transistors based on GaN above 500 GHz, and based on InP above 1 THz. Technological methods [2–4] are being improved to reduce surface effects both at the free boundaries of heterostructural transistors and interface phenomena at the quantum well boundary, which lead to additional electron scattering factors (alloy scattering, scattering at dislocations and charged centers, scattering on the roughness of the heterointerface). Ternary compounds transistors are also widely used for low-noise devices. For example, HFETs based on AlGaIn/GaN compounds shows [5] low noise at high values of the surface concentration of two-dimensional electron gas at the heterojunction boundary.

Methods of modeling HFETs on ternary compounds are being improved. The processes of electron energy quantization in a quantum well based on a one-dimensional model in the one-electron approximation (Schrödinger level) and distributed potential (Poisson level) were developed in [6].



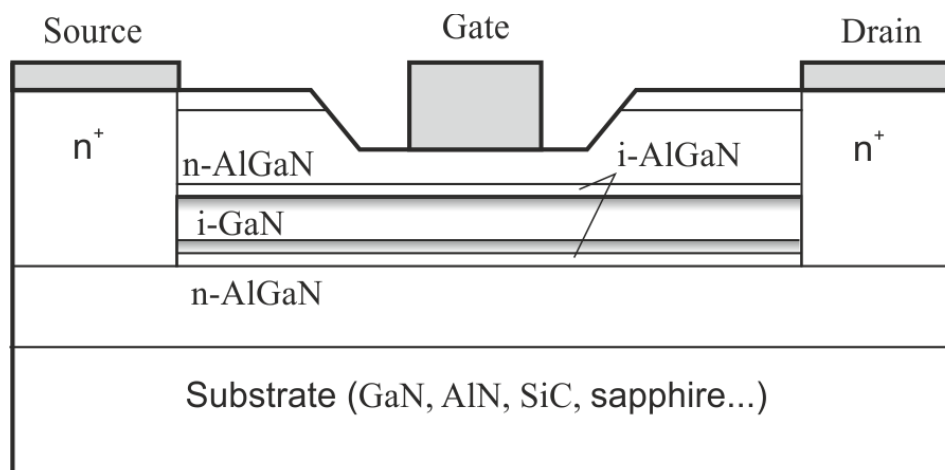
The main structural "element" in HFETs is the region of two-dimensional electron gas (2DEG). It is formed in the heterojunction zone between the wider-band AlGaN barrier layer and the undoped channel GaN with a narrower band gap.

The transition of electrons to a potential well is caused by the fact that due to different energies of electron affinity in the contact region a strong electric field is formed, which is usually modeled by breaking the bottom of the conduction band, which initiates the transition of free electrons to the potential well. Therefore, in the channel layer directly under the heterojunction, a thin layer of space charge with high density and mobility of free electrons is formed, which is called two-dimensional electron gas.

The aim of this study is to model and analyze the influence of scattering mechanisms characteristic of submicron structures based on a two-dimensional mathematical model in the approximation of relaxation times considering quantum effects for heterostructural transistors with a system of quantum wells. The main stages of the study are the formation of a system of two-dimensional differential equations in partial derivatives, which include the equations of conservation of energy and momentum, Poisson's and Schrödinger's equations to take into account quantum effects and a description of charge carrier scattering mechanisms. Integration of a system of equations for calculating the output current of a transistor and its output volt-ampere characteristics, in particular, to analyze the effect of charge carrier scattering on the alloying potential, which affects their motion even in the case of "quasi-ballistic" drift.

### Simulation of heterotransistor

Devices containing active regions with size in the direction of charges movement near of free path length and less are ballistic. The flight of electrons in the active region occurs due to the energy accumulated during injection. At the same time, the transfer of electrons in transistors with the size of the active region, commensurate with the wavelength of the electron, is quantum in nature. Figure 1 shows the structure of a two-junction transistor in which a channel is formed in a layer of undoped gallium nitride with a thickness of 30...50 nm between two layers of wider-band  $n^+$ -AlGaN. In an electron gas bounded by potential barriers on two sides, the quantum properties of 2DEG are even more pronounced than in a single-barrier structure.



**Figure 1. Typical structure of a heterostructural GaN/AlGaN transistor**



A simplified version of the transistor is used typically for simulation with fewer layers that form heterojunctions than in real structures. Layer thickness, longitudinal dimensions and energy characteristics of materials are parameters of the model. There are a number of approaches to modeling certain characteristics of submicron devices, including complete software products with built-in functions for solving the fundamental system of equations for semiconductors, taking into account the characteristics of structures. But, despite this diversity, the current problem is the description of physical processes in strong electric fields for submicron heterostructures with quantum well (QW) systems of various shapes. A combined approach to constructing a physic-topological model of a heterotransistor with a QW is possible, which includes relaxation equations and equations that describe processes in quantum systems and are solved in a self-consistent manner. Since large field gradients must be taken into account when modeling submicron structures, the convergence of one or another method strongly depends on the choice of the initial approximation and the grid step.

To describe stationary processes in semiconductors, we can use a system of relaxation equations derived from the Boltzmann equation [7]. The complete system of differential equations of the model of submicron structures includes in addition to the relaxation equations of momentum (1), electron temperature (2), the equation of charge conservation (3) and the Poisson equation (4) and current density (5) in the notation [7]:

$$d\vec{p} / dt - e\vec{E} = -\vec{p} / \tau_p, \quad (1)$$

$$\frac{dT_e}{dt} = -\frac{T_e - T}{\tau_E} + \frac{m^* \mu^2 \mathbf{E}^2}{3k_B \tau_E} (\gamma - 1), \quad (2)$$

$$dn / dt = 0, \quad (3)$$

$$\nabla^2 V = -\rho / \epsilon \epsilon_0, \quad (4)$$

$$\vec{j} = -en\vec{v}. \quad (5)$$

For a two-dimensional physical-topological model, it should be borne in mind that  $d / dt$  here is a complete derivative of the function of time and coordinates:

$$df(x, y, t) = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial t} dt \quad (6)$$

For computational solution of the system of equations it is necessary to carry out procedure of their sampling on the set grid. In this case, the sampling on the rectangular grid is chosen for static fields. The choice of the sampling step is due to the presence of inhomogeneities in the submicron structures at the interface and the size of the structure, and, as a consequence, the presence of large potential gradients. The iterative procedure involves adapting the integration step depending on the stability of the process and approaching the conditions of a given accuracy.

The potential distribution as a result of solving the Poisson equation (4) is taking into account the distribution of the concentration of mobile charge carriers in the right part of the equation in each outer cycle.

The conservation equations for the electron temperature (2) and for the velocity (1) are nonlinear strongly bound differential equations in first-order partial



derivatives. These include the electric field strength, which is related to the potential as  $\vec{E} = -\text{grad}V(x, y)$ . Together with the Poisson equation, they form a closed system of equations that can be solved by iterative methods using the initial approximation for velocity. In strong electric fields in structures with thin functional layers, the discretization of the energy spectrum and the Fermi character of filling the corresponding two-dimensional energy quantization subbands should also be taken into account. This is possible by self-consistent solution of the Poisson and Schrödinger equations.

### Quantum effects in heterostructural channels

In doped heterostructures with a high concentration of charge carriers there is a strong modification of the electrostatic potential near the quantum well. This causes a strong shift in the energy levels of quantization and redistribution of the concentration of charge carriers. For a two-dimensional electron gas, it is possible to approach the approximation of a rectangular quantum well by means of a self-consistent solution of the Poisson and Schrödinger equations:

$$-\frac{\hbar^2}{2m^*} \Delta \psi(x, y) + [V(x, y) - E_0] \psi(x, y) = 0. \quad (7)$$

An example of such a solution is given in Figure 2. For each level of energy quantization, wave functions are calculated, the "tails" of which extend beyond the quantum well. The distribution of the concentration of free carriers, taking into account the curvature of the zones can be found by a typical formula:

$$n(x, y) = N_c \frac{2}{\sqrt{\pi}} F_{1/2} \left( -\frac{E_c - E_\Phi - eV(x)}{k_B T} \right),$$

where  $N_c$  is the effective density of states in the conduction band;  $F_{1/2}$  - Fermi integral for three-dimensional electronic gas;  $E_c$  - the bottom of the conduction band;  $E_\Phi$  - Fermi energy.

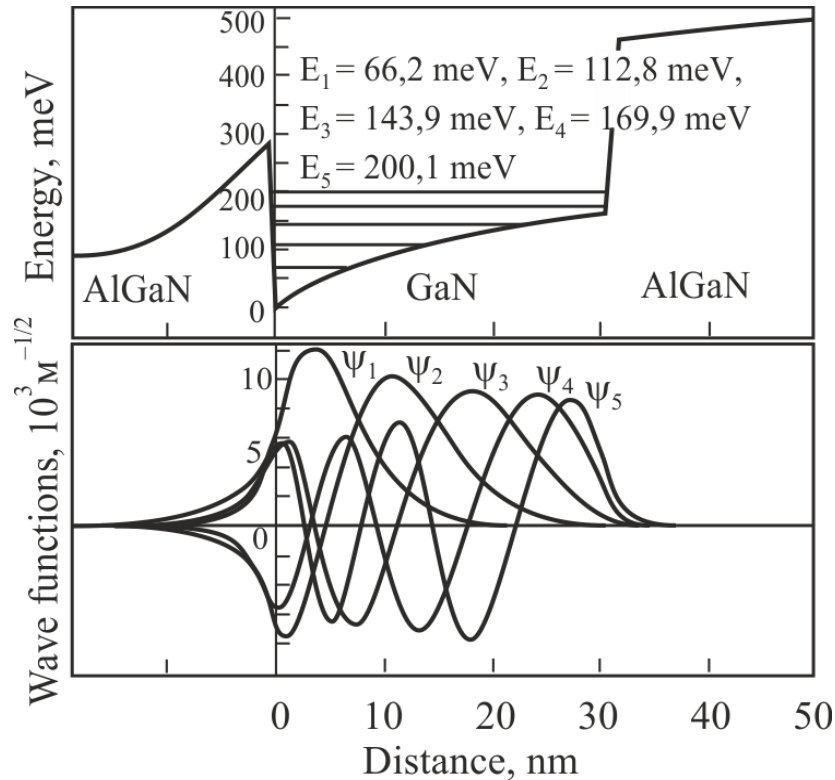
To calculate the concentration of charge carriers in the region of the quantum well for each level, it is necessary to take into account that in two directions the electrons move freely, forming transverse subbands of dimensional quantization. The concentration of "two-dimensional" charge carriers without taking into account the bending of the zones is the integration of the states of the subband, taking into account the Fermi-Dirac distribution [8]:

$$n(x, y) = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{E_\Phi - E_i}{k_B T} \right) \right] |\psi(x, y)|^2.$$

Bending of energy zones near the heterojunction due to the presence of Coulomb repulsion forms additional energy barriers and leads to the appearance of additional quasi-resonant states. Since a simple summation of two-dimensional and three-dimensional electrons will lead to a systematic error in the calculations and complications in the crosslinking of solutions, the authors [8] use the model of a "quantum box" with perfectly solid walls on which the wave function rotates to zero. In this model, the concentration of charge carriers is calculated "inside the quantum box" for the well region by solving the Schrödinger equation in the effective mass



approximation. Near the edges of the "box" and beyond, a quasi-classical approach is used to calculate the concentration of free carriers from the Fermi integral, taking into account the curvature of the zones [9]. The energy of dimensional quantization subbands in the approximation of a rectangular symmetric quantum well can be determined from [10].



**Figure 2. Potential relief shape and quantization levels and corresponding wave functions in the transistor channel between two heterobarriers**

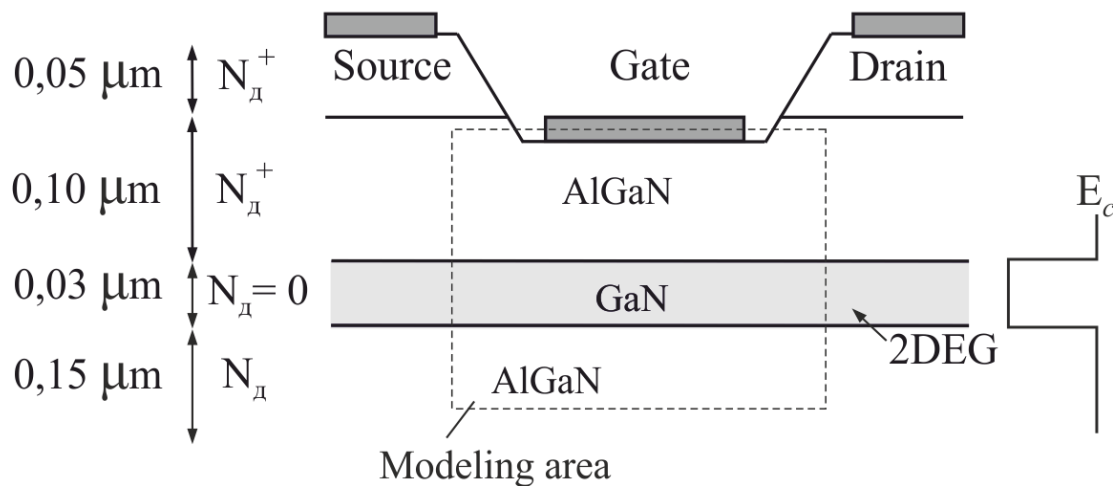
To achieve greater accuracy, you need to solve the Schrödinger equation by numerical methods. However, to estimate the position of the basic energy level, we can use the assumption of a "shallow" quantum well, for which  $U_0 \ll \hbar^2 / ma^2$  and the position of the basic level can be estimated by the formula  $E_0 \approx U_0 - \frac{ma^2}{2\hbar^2} U_0^2$ .

### Process simulation in a heterotransistor

The test structure of a heterotransistor with one channel and two heterojunctions for simulation is shown in Figure 3.

It is characterized by the following physical and topological parameters: gate length  $0.3 \mu\text{m}$ , interelectrode distances leakage gate  $0.4 \mu\text{m}$  and gate drain  $0.6 \mu\text{m}$ , a layer of wide-band doped AlGaIn under the gate with an effective thickness of  $0.1 \mu\text{m}$ , a layer of undoped AlGaIn  $50 \text{ \AA}$  (spacer), a layer of undoped GaN on a semi-insulated substrate several tens of micrometers thick, in the surface layer of which a potential well is formed as a result of the rupture of the zones. The x-axis is directed along the channel of the transistor, the y-axis is perpendicular to the channel from the gate surface. Since all electronic processes are associated with the surface layer and two-dimensional electron gas (2DEG) in the potential well, the simulation area can be limited to an effective thickness of a few micrometers.

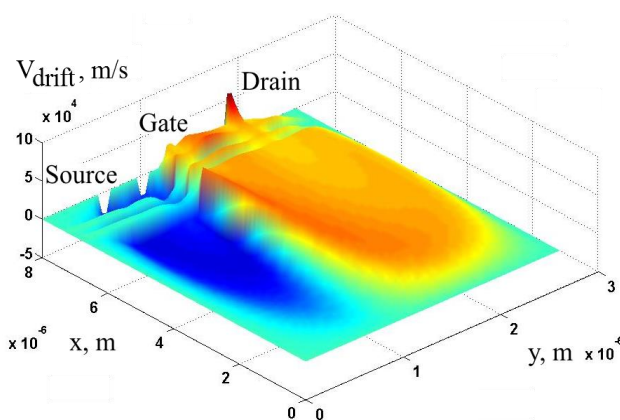




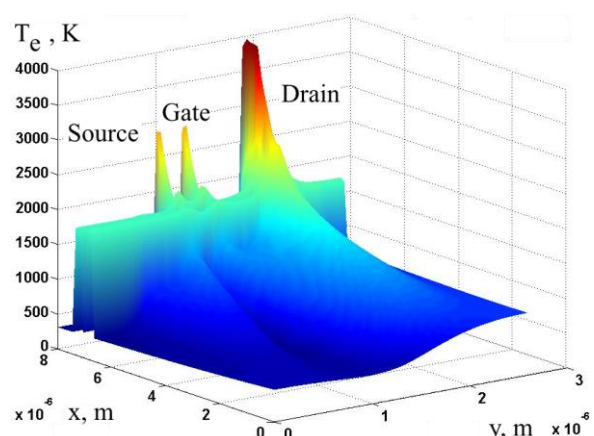
**Figure 3. Topological structure of a heterotransistor with 2DEG with one channel.**

As in traditional submicron heterotransistors, structures with several heterojunctions are dominated by strong field effects and submicron effects: quasi-ballistic transfer, heating under conditions of predominance of inter-valley and optical scattering of charge carriers, the effect of "overshoot" of electron drift velocity, and so on. The strong field region and nonstationary processes are related to the two-dimensional region under the shutter and the two-dimensional distributions of the characteristics of the electron gas – electron temperature (energy), momentum (velocity), effective mass, etc. A feature of the processes in such structures is the redistribution of carriers between potential wells, when the distance between them does not exceed the free path of electrons.

In Figures 4–7 show some results of two-dimensional modeling of physical characteristics in the submicron heterotransistor channel. These distributions are calculated according to the electrical displacements at the electrodes of the source, gate and drain – 0 V; – 0.8 V; 3.0 V. The discontinuity of the zones at the boundary of the heterojunction is given in the process of solving the Poisson equation as a built-in potential of about 0.8 V.



**Fig.4. Drift velocity distribution in a heterotransistor with a gate length of 0.3 μm**



**Fig. 5. Electron temperature distribution in a heterotransistor with a gate length of 0.3 μm**

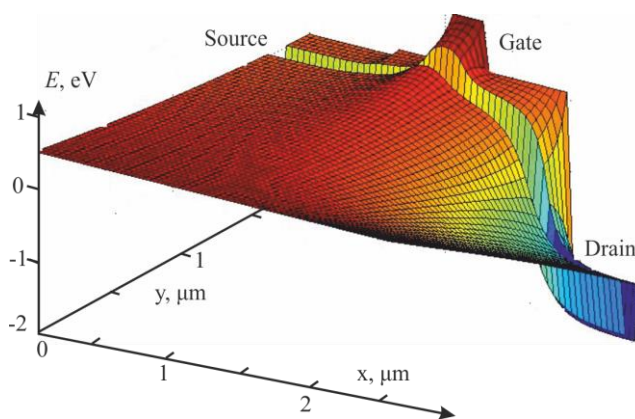


As the simulation results show, the heating of the electron gas and the increase in the temperature of the electrons are more related to the electrons drifting in the potential well at the boundary of the heterojunction. The effect of the "overshoot" of drift velocity is noticeable both for electrons of the heterojunction and for electrons drifting in the high-doped AlGa<sub>N</sub> layer. However, since the area under the gate is depleted of charge carriers, only a small number of them have high velocity values. Finding charge carriers in the quantum well is energetically advantageous, which explains the fact of redistribution of carriers in the channel between the quantum well and the substrate.

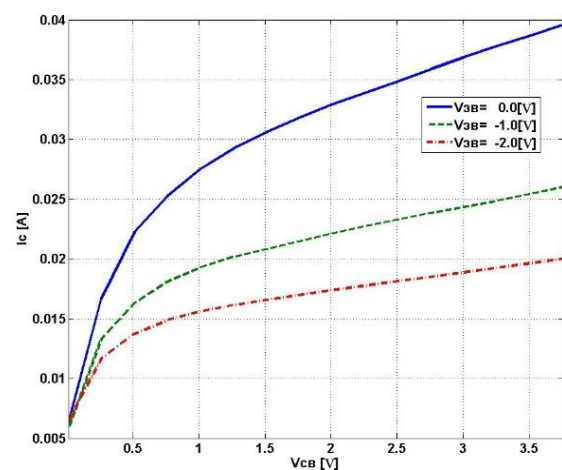
The output current of the transistor was calculated as the normal component of the current before the contact of the drain for known two-dimensional distributions of electron concentration, electric field strength and velocity based on the results of solving the initial system of equations in the case of grid nodes.

The average pulse relaxation times for different mechanisms were found by analytical relations [7] by averaging the known scattering rates over the electron distribution function. This takes into account the scattering mechanisms characteristic of submicron heterostructures.

*Impurity scattering* is almost elastic and effectively chaoticizes motion, making a significant contribution to the relaxation of the pulse. *Acoustic scattering* is characterized by a linear dependence of the scattering rate on the crystal lattice temperature, which is associated with a decrease in free path length with increasing number of phonons, and the carrier velocity proportional to energy as  $E^{1/2}$ , using a similar dependence on electron temperature.



**Fig. 6. Potential energy surface in a heterotransistor with a gate length of 0.3  $\mu\text{m}$**



**Fig. 7. Volt-ampere characteristics of the heterotransistor without taking into account the alloying potential**

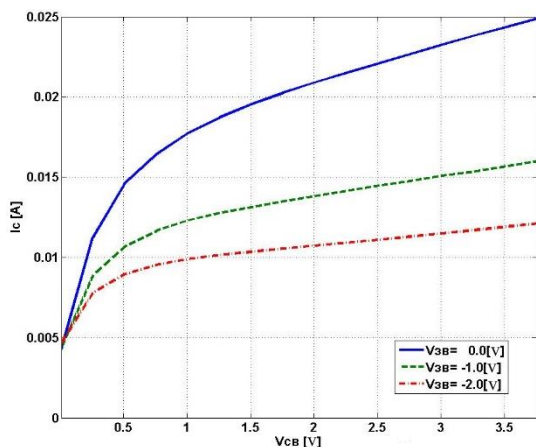
*Optical scattering* is inelastic. At each interaction of this kind, the energy of the electron changes in magnitude  $\pm\hbar\omega_0$ . Since this value of the optical phonon can be commensurate with the energy of the carriers, the scattering rates with the absorption of the phonon and its excitation differ markedly.

*Intervalley scattering* is also inelastic, because in each act of scattering an intervalley phonon with an energy  $\hbar\omega_{ij}$  close to the energy of optical phonons is

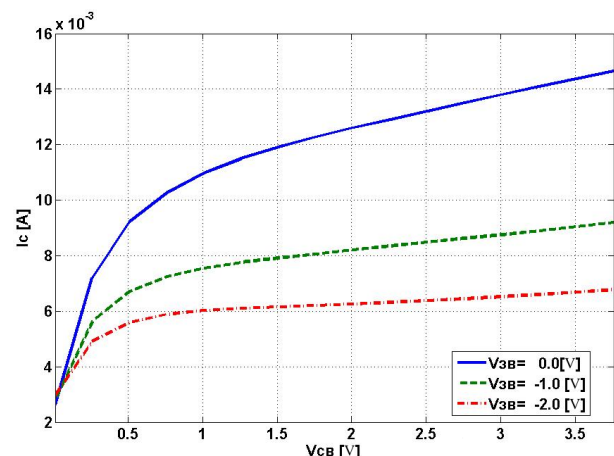


absorbed or released. When considering inter-valley scattering, in contrast to other mechanisms, the averaging of the kinetic equation is not carried out over the entire Brillouin zone, but over the characteristic states of individual valleys, so with a constant number of particles in the zone their concentration can be redistributed between valleys. The inertia of this process is determined by the concentration relaxation time  $\tau_n$  which is, as well as the relaxation time of the pulse  $\tau_p$  by averaging the inter-valley scattering rate. In [12], based on the analysis of the results of calculation of relaxation times, field-velocity and energy characteristics for the main scattering mechanisms in semiconductors of type  $A_3B_5$ , the predominant influence on the heating of polar optical and intervalley scattering electrons is shown. The influence of *scattering on the alloying potential* was investigated separately in these calculations. This type of scattering is related to the statistical nature of the distribution of the binary components GaN and AlN, when the molar composition  $x$  may change randomly. This is especially critical in the field of heterojunction. But for the model of "hard" walls, if the wave functions do not extend beyond the heterochannel into the AlGaIn layers, then for the channel this scattering can be neglected.

The analysis of the effect of alloy scattering was performed for the structure of a single-channel transistor and was integrally evaluated as the effect on the volt-ampere characteristics (Fig. 7–9). These dependences show that significant reductions in drain current are observed for values of alloy potential greater than 0.5 eV (Fig. 8) and range from 6 to 24 mA for both large and small levels of drain current depending on the gate voltage. The mechanisms of "cooling" of the electron gas in the strong electric field of submicron field-effect transistors are described in detail in [7]. The alloying potential affects not only the additional factor of electronic gas heating, but also to some extent "deforms" the configuration of energy valleys. The influence of this factor requires further study.



**Fig. 8. Volt-ampere characteristics of the heterotransistor for the value of the alloy potential  $\Delta U_a = 0,3$  eV**



**Fig. 9. Volt-ampere characteristics of the heterotransistor for the value of the alloy potential  $\Delta U_a = 1,0$  eV**

When modeling the relaxation time of the pulse, acoustic, impurity, optical, polar optical and intervalley scattering were taken into account. When calculating the





energy relaxation time, the same scattering mechanisms were taken into account, but without impurity scattering, which is considered to be elastic.

### Conclusion

Based on the developed model, it is possible to optimize the topology and electrophysical parameters of HFETs, in particular, the parameters of heterojunction materials, the location of quantum wells in the structure and the choice of optimal electrical regime for powerful and low-noise devices in the millimeter wavelength range.

Analysis of the scattering effect on the alloy potential allows us to conclude a more physically and quantitatively justified (including changes in the output current levels of the transistor) is a value of  $\Delta U_a$  close to 0.3 eV.

The increase in the average drift velocity in the structure with two quantum wells in comparison with the HFETs with one QW is up to 30%, which is largely due to the redistribution of electrons between potential wells with energy loss in overcoming barriers. The reduction of the effect of a strong electric field in a two-channel structure is associated with a decrease in the scattering probability both at polar optical phonons and due to injection processes to the lower heterojunction of electrons with high initial velocities and low energy values.

The developed models of taking into account the influence of quantum wells on the longitudinal transport of charge carriers in field-effect transistors with submicron gate length can be used to calculate not only transistor heterostructures but also other multilayer devices with quantum well systems under strong electric fields.

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**Реферат** У роботі наведено аналіз процесів електронного транспорту у квантових ямах субмікронних гетероструктурних транзисторів. Розроблено методики моделювання процесів у наногетероструктурах з урахуванням деяких квантових ефектів та специфічних для потрійних сполук механізмів розсіювання. На основі системи релаксаційних рівнянь проведено моделювання субмікронних гетероструктур з квантовими ямами. При моделюванні враховано розсіювання оптичне, акустичне, міждолинне, домішкове механізмів і розсіювання на сплавному деформаційному потенціалі. Розраховано часи релаксації для цих механізмів розсіювання і враховано вплив на вихідні характеристики субмікронного гетероструктурного транзистора.

У Вступі зроблено огляд наявного стану питання та сформульовано завдання моделювання і аналіз впливу механізмів розсіювання, характерних для субмікронних структур на основі двовимірної математичної моделі у наближенні часів релаксації з урахуванням квантових ефектів для гетероструктурних транзисторів з системою квантових ям. Розділ Чисельне моделювання гетеротранзистора складається з опису структури та математичної моделі ГСПТ. Третій розділ Квантові ефекти у гетероструктурних каналах наводить детальний опис фізичних процесів та дає розуміння можливих припущень та спрощень моделі. Результати використання моделі наведено у наступному розділі Моделювання процесів у гетеротранзисторі. Висновки окрім аналізу отриманих та описаних у статті результатів описують перспективи подальшого використання моделі і практичну користь.

**Ключові слова:** електронний транспорт, механізми розсіювання; сплавлений потенціал; часи релаксації; субмікронні гетероструктурні транзистори; квантові ями.

Article was sent: 10-Dec-2020.

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