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Monte Carlo simulation of hot electron effects in compensated GaN semiconductor at moderate electric fields

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Abstract. The electron distribution function and transport characteristics of hot electrons in GaN semiconductor are calculated by the Monte Carlo method. We studied the electron transport at temperatures of 10, 77, and 300 K under low and moderate electric fields. We found that, at low temperatures and low electric fields (a few hundreds of V/cm), the second "ohmic" region is to be observed on the *I-V* characteristic. In this case, the mean energy is very slowly dependent on the field. The streaming effect can occur in bulk GaN with low electron concentration ($<10^{16}$ cm^{-3}) at low temperatures and electric fields of a few kV/cm.

Keywords: Monte Carlo method, hot electrons, electron transport.

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1. Introduction

In recent years, a new class of semiconductors – the group-III nitrides – is actively investigated due to their possible usage in both power electronics and opto-electronics. Several materials such as InN, GaN, and AlN are included to this group of semiconductors. The investigation of kinetic properties of these materials and especially those of GaN is carried out in wide ranges of electric fields and temperatures. A number of works has been done to investigate kinetic properties of electrons in bulk GaN at high electric fields under room or higher temperatures. In most of these investigations, relatively high electron concentrations have usually considered. For example, in [1-4], electron kinetic properties have been studied at electric fields of 100-600 kV/cm and electron concentrations of 10^{16}–10^{18} cm^{-3}. It is noted that GaN has become of great interest for the use in many high-power semiconductor devices [5, 6].

The group-III nitride semiconductors, in particularly GaN, differ from other semiconductor $A^{III}B^{V}$ compounds well studied at the present moment. The nitrides have specific material characteristics: the large optical phonon energy ε_{LO}, the large energy splitting between the Γ-minimum and the lowest satellite valleys in the conduction band $\Delta\varepsilon$, and strong electron-polar-optical-phonon coupling (characterized by the Fröhlich constant α). For GaN, these quantities are equal to $\varepsilon_{LO} \approx 0.092$ eV, $\Delta\varepsilon \approx 1.4 - 1.8$ eV [3], and $\alpha = 0.41$, respectively. These material properties allow one to assume the existence of new electron phenomena at a moderate electric field which are hardly to be observable in other known polar semiconductors such as GaAs. The one of such effects is the streaming regime induced by optical phonon emission. In this regime, the electron motion is quasiperiodic in the energy space with alternating quasiballistic acceleration and emission of a polar optical phonon. The streaming regime can be realized at low lattice temperatures (10 – 77 K) and low electron concentrations (10^{14}–10^{15} cm^{-3}) [7, 8].

The main purpose of this work is to study characteristic properties of the electron transport in GaN at moderate electric fields by the Monte Carlo method. This numerical method is one of the most effective tools to study the electron transport in semiconductors. It allows one to take into account the band structure and all actual scattering mechanisms and is well described in the literature, in particular in [9-11].

2. Subject of investigation

We studied the transport characteristics of hot electrons in a bulk GaN of the cubic modification. Applied electric fields are assumed to be steady. The compensated GaN samples with low electron concentrations (10^{14}–10^{15} cm^{-3}) are considered. The ionized impurity concentration is of 10^{16} cm^{-3}. All material parameters used in the simulation are taken from [12].

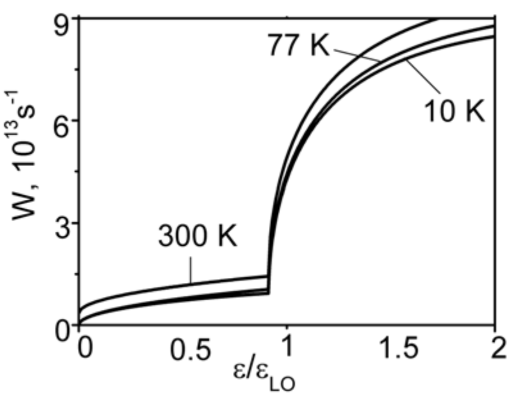

Fig. 1. Total scattering rate as a function of the electron energy in compensated GaN at 10, 77, and 300 K.

The following scattering mechanisms are taken into account: the scattering by acoustic phonon, polar optical phonon, and ionized impurities. The large intervalley separation in group-III-nitride semiconductors allows us to neglect the intervalley scattering in the considered range of electric fields. The electron band is assumed parabolic for the simulation of the electron transport. Importantly, the electron concentration is chosen low to neglect the electron-electron scattering.

Under these assumptions, the obtained dependences of the scattering rate on the electron energy at different lattice temperatures are shown in Fig. 1. In the "passive" energy region ($\varepsilon < \varepsilon_{\rm LO} = \hbar\omega_{\rm LO}$), the ionized impurity scattering dominates at 10 and 77 K. In the "active" energy region ($\varepsilon > \varepsilon_{\rm LO}$), the polar optical-phonon emission is always the dominant scattering mechanism. For 300 K, two scattering mechanisms, i.e. the ionized impurity scattering and the polar optical-phonon absorption, are essential in the "passive" energy region.

3. Electron distribution function

In this section, we demonstrate an analytical method of solving the Boltzmann equation in case of weak electric fields and compare the analytical solution with a numerical one obtained by the Monte Carlo method.

3.1. Analytical model

The momentum electron distribution function $f(\vec{p})$ contains the full information about electron properties and is traditionally the main subject of the research. The distribution function is used to calculate the mean kinetic characteristics. Moreover, the knowledge of $f(\vec{p})$ allows us to give the full qualitative picture of kinetic phenomena taking place in the semiconductor.

The electron distribution function $f(\vec{p})$ in a homogeneous steady electric field $\vec{E}$ can be determined from the Boltzmann transport equation

$$e\vec{E}\frac{df(\vec{p})}{d\vec{p}} = \left(\frac{\partial f}{\partial t}\right)_{\rm col}. \qquad (1)$$

Here $\left(\frac{\partial f}{\partial t}\right)_{\rm col}$ is the collision integral. Under certain conditions, the integro-differential equation (1) can be reduced to a chain of differential equations by using the Legendre polynomial expansion of the distribution function [13]. In other words, the distribution function is expanded as

$$f(\vec{p}) = \sum_k f_k(\varepsilon) P_k(\cos\theta), \qquad (2)$$

where $f_k(\varepsilon)$ are coefficients of expansion of the distribution function, $P_k(\cos\theta)$ are the Legendre polynomials, and θ is the angle between the electron momentum $\vec{p}$ and the electric field $\vec{E}$.

Coefficients of the expansion of the electron distribution $f_k(\varepsilon)$ can be used to determine different mean kinetic characteristics. For example, in order to calculate the mean energy $\langle\varepsilon\rangle$ and the drift velocity $v_{\rm dr}$, we must find two first coefficients $f_0(\varepsilon)$ and $f_1(\varepsilon)$:

$$\langle\varepsilon\rangle = \int \varepsilon\, f(\vec{p})\, d^3\vec{p} = 4\pi\int \varepsilon\, f_0(\varepsilon)\, p^2 dp\,, \qquad (3)$$

$$v_{\rm dr} = \int v_x\, f(\vec{p}) d^3\vec{p} = \frac{4\pi}{3}\int v\, f_1(\varepsilon) p^2 dp\,. \qquad (4)$$

The determination of the coefficients $f_0(\varepsilon)$ and $f_1(\varepsilon)$ is the main task of the analytical theory.

3.2. Case of weak fields

At small electric fields and low lattice temperatures, the electron distribution is formed by the elastic and quasielastic scattering mechanisms. The electron distribution function calculated by the Monte Carlo method in the momentum space is shown in Fig. 2, *a*. Here, p_x and p_y are the components of the momentum, and p_x is parallel to the electric field. On the contour plot (Fig. 2, *b*), we show the contour lines representing the lines of constant values of the distribution function from 0.1 to 0.9 with a step of 0.1. Two first coefficients of the Legendre polynomial expansion of the distribution function are shown on Fig. 2, *c*. It is clearly seen that the coefficient $f_0(\varepsilon)$ is essentially larger than $f_1(\varepsilon)$ anywhere in the energy region. This means that the electron distribution function is quasiisotropic at this electric field.

Thus, at weak fields, we can use the diffusion approximation which assumes that $|f_1(\varepsilon)| << |f_0(\varepsilon)|$ and $f_2 = \ldots = f_k = 0$. In the diffusion approximation, Eq. (1) can be written as

$$\frac{eE}{3p^2}\frac{d(p^2 f_1)}{dp} = (L_{\rm ac} + L_{\rm op}) f_0, \quad eE\frac{df_0}{dp} = -\frac{f_1}{\tau(p)}. \qquad (5)$$

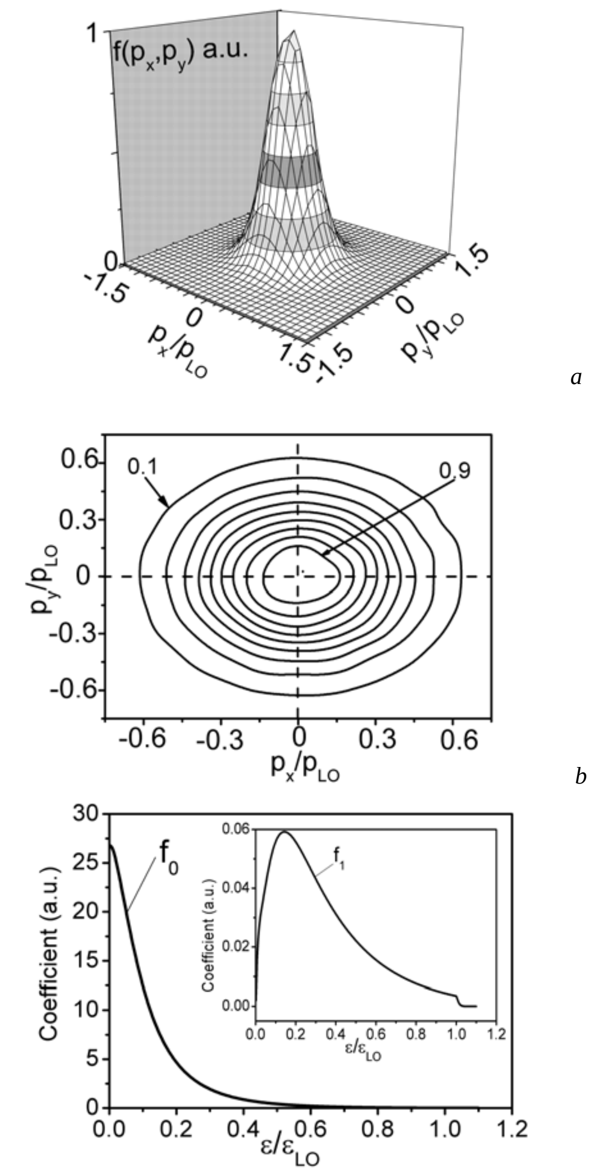

Fig. 2. Electron distribution function (*a*), contour plot (*b*), and coefficients of expansion (2) of the distribution function (*c*) for GaN at 10 K and E = 100 V/cm, $p_{\mathrm{LO}} = \sqrt{2m\varepsilon_{\mathrm{LO}}}$.

In (5), L_{ac} and L_{op} are the collision operators for acoustic phonons (quasielastic interaction) and polar optical phonons (inelastic interaction); L_{ac} is a differential second-order operator, the effect of L_{op} is reduced to an algebraic expression in finite differences [13]; and $1/\tau(p) = 1/\tau_{\mathrm{ac}}(p) + 1/\tau_{\mathrm{imp}}(p)$, where $\tau_{\mathrm{ac}}(p)$, $\tau_{\mathrm{imp}}(p)$ are the momentum relaxation times on acoustic phonons and ionized impurities, respectively. Solving (5), we can find the analytical expression for $f_0(\varepsilon)$, $f_1(\varepsilon)$ and then will calculate the mean kinetic characteristics.

3.3. Comparison of numerical and analytical results

It is appropriate now to compare the mean kinetic characteristics obtained analytically with those calculated by the Monte Carlo method. The results of calculations are shown in Fig. 3, where the mean electron energy (Fig. 3, *a*), the electron drift velocity (Fig. 3, *b*), and the longitudinal $D_{\parallel}$ and transverse $D_{\perp}$ diffusion coefficients (Fig. 3, *c*) are presented as functions of the electric field. The calculations are carried out by assuming a compensated GaN at 10 K. It is clear that the analytical solution coincides with the numerical one in a range of low electric fields. With increase in the applied field, the distribution function takes a more anisotropic form. The diffusion approximation is disturbed, and one can see a weak divergence between curves 1 and 2 in Fig. 3.

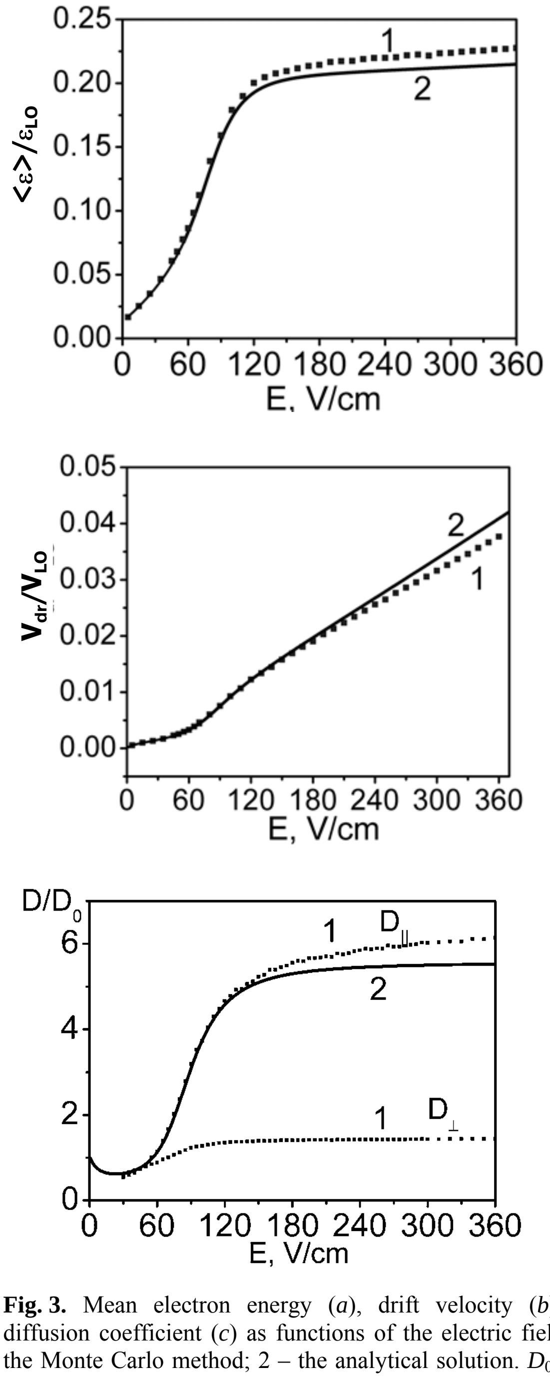

Fig. 3. Mean electron energy (*a*), drift velocity (*b*), and diffusion coefficient (*c*) as functions of the electric field: 1 – the Monte Carlo method; 2 – the analytical solution. D_0 is the diffusion coefficient in the equilibrium state.

3.4. Case of strong fields

A strongly anisotropic electron distribution is formed in the strong applied field. The formation of the anisotropic electron distribution is characteristic of the streaming phenomenon. This anisotropic electron distribution function calculated by the Monte Carlo method at an electric field of 4 kV/cm is shown in Fig. 4, *a*. Here, the *x*-component of the momentum, p_x, is parallel to the electric field. Contour lines on the plot shown in Fig. 4, *b* are not spherical as those in Fig. 2, *b*, but they are elongated along the applied field. Three first coefficients of expansion (2) of the electron distribution function are shown in Fig. 4, *c*. In the streaming regime, these moments are quantities of the same order. This is strongly different from the case of low electric fields when the spherically symmetric part f_0 entirely dominates (Fig. 2, *c*).

4. Mean kinetic characteristics of electrons

In this section, we describe some specific properties of the mean kinetic characteristics. At first, we consider a case of weak electric fields. Then we will discuss a peculiarity of the electron motion in the streaming regime and analyze the kinetic properties of electrons under strong electric fields.

4.1. Case of weak fields

At low temperatures (from 10 to 77 K) and fields less than 50 V/cm, the mean energy grows rapidly with increase in the field (see Fig. 5, *a*). In this range of temperatures and fields, electrons interact mainly with acoustic phonons and ionized impurities. So the energy and momentum relaxations occur on acoustic phonons and ionized impurities, respectively. These scattering mechanisms cannot restrict the growth of the mean energy as an

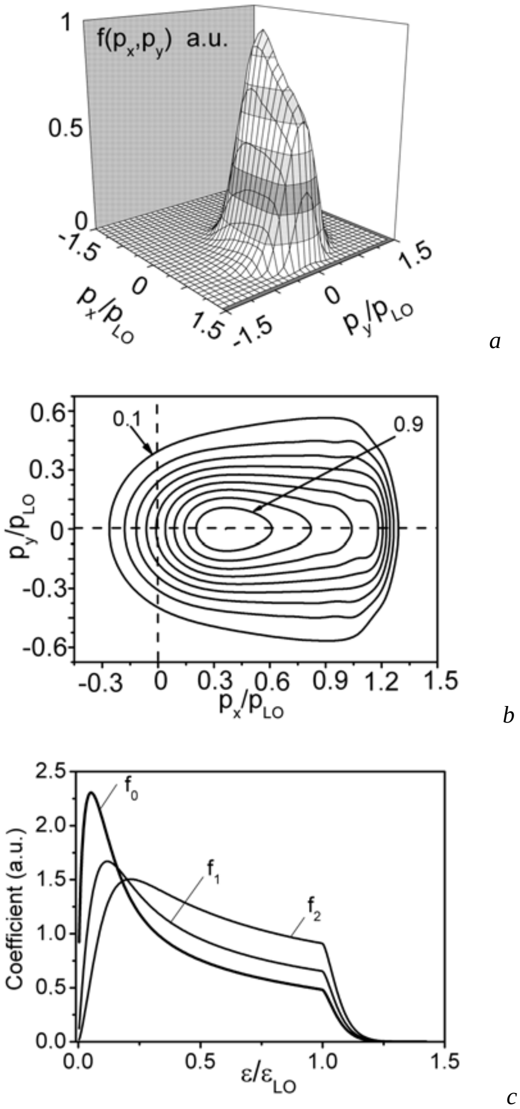

Fig. 4. Electron distribution function (*a*), contour plot (*b*), and coefficients of expansion (2) of the distribution function (*c*) for GaN at 10 K and E = 4 kV/cm.

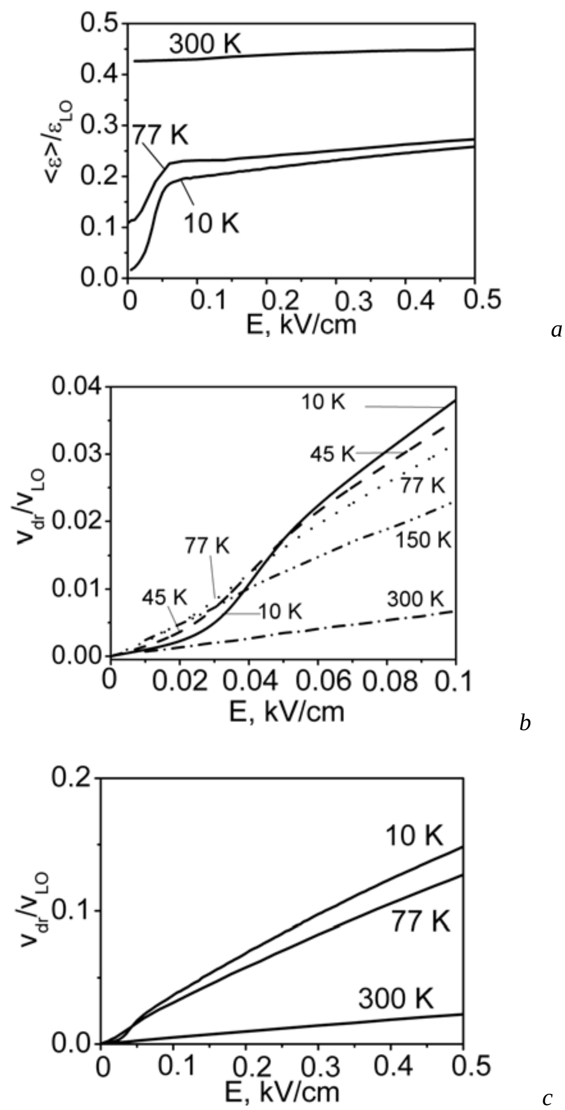

Fig. 5. Mean electron energy (*a*) and drift velocity (*b*) and (*c*) as functions of the electric field for GaN ($N_i = 10^{16}$ cm^{-3}, $N_e = 10^{14}$ cm^{-3}).

applied field increases. In larger electric fields, the role of the electron interaction with polar optical phonons (emission phonons) becomes more important. This scattering mechanism suppresses a growth of the mean energy. As a result, the saturation of the mean electron energy is observed at a field of 100 V/cm and more.

At fields less than 50 V/cm, the dependence of the drift velocity on the electric field has two unusual properties. At heating fields and temperatures from 10 to 77 K, we observe the anomalous growth of mobility with temperature (see Fig. 5, *b*). This mobility growth is due to a decrease of the role of the ionized impurity scattering with increase in the lattice temperature in the Brooks-Herring model. For temperatures from 77 K and higher, the role of electron-phonon scattering mechanisms (acoustic and polar optic phonons) becomes more important, and the electron mobility decreases with increase in the temperature.

At electric fields of 100 V/cm and higher (Fig. 5, *c*) where the quasisaturation of the mean energy takes place, we observe the so-called second "ohmic" region for the drift velocity [14, 15]. In case of the second "ohmic" region, the main mechanism of electron energy relaxation is the emission of polar optical phonons. The electron momentum relaxation comes from ionized impurities. Electron mobility is estimated as $1.5\cdot10^4\ \mathrm{cm^2/(V\cdot s)}$ for 10 K and $1.1\cdot10^4\ \mathrm{cm^2/(V\cdot s)}$ for 77 K on this part of the *I-V* characteristic. For comparison, for the electron mobility on the first "ohmic" region, we have the following estimations: $4\cdot10^3\ \mathrm{cm^2/(V\cdot s)}$ for 10 K and $8.5\cdot10^3\ \mathrm{cm^2/(V\cdot s)}$ for 77 K.

For the lattice temperature equal to 300 K, drastically another situation occurs. At 300 K, the inelastic scattering mechanism – the polar optical-phonon absorption – is essential in the "passive" energy region in addition to the elastic scattering mechanism (the ionized impurity scattering). As a result, the mean energy depends weakly on the applied field and the *I-V* characteristic is quasiohmic in the wide range of electric fields with the mobility estimated to be $1.8\cdot10^3\ \mathrm{cm^2/(V\cdot s)}$.

4.2. Case of strong fields

In higher electric fields (a few kV/cm), we can observe another hot electron effect. The low lattice temperature, a low electron concentration, and the domination of the polar optical-phonon emission over other scattering mechanisms provide conditions for the appearance of the streaming effect at some range of steady electric fields.

In the streaming regime, the electron motion becomes almost periodic [7, 15]. During one period *T*, an electron accelerates quasiballistically until it reaches the critical velocity $v_{\mathrm{LO}} = \sqrt{2\varepsilon_{\mathrm{LO}}/m}$. The electron then loses its energy by emitting an optical phonon and starts the next period of acceleration. The scheme of this motion is shown in Fig. 6.

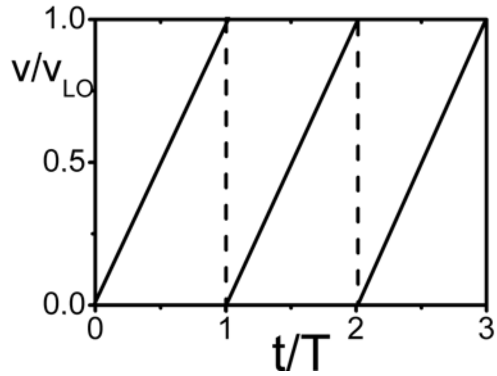

Fig. 6. Sketch of changing the electron velocity with time in the streaming regime.

The streaming regime is characterized by the saturation of both the mean energy and the drift velocity. These quantities as functions of the electric field are shown in Fig. 7. At fields of 2–10 kV/cm, it can see the region of the saturation of the mean energy and the drift velocity. At this region of the *I-V* characteristic, the drift velocity is equal to $\sim 0.5v_{\mathrm{LO}}$. At the lattice temperature equal to 300 K, the streaming is not possible in the considered range of electric fields. This is clearly seen from the last figure.

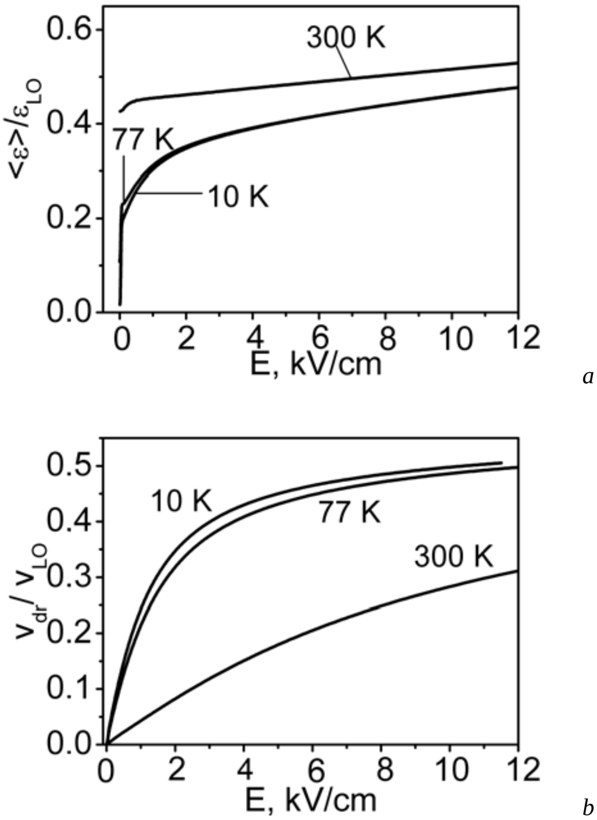

Fig. 7. Mean electron energy (*a*) and drift velocity (*b*) as functions of the electric field for GaN.

5. Conclusions

We have studied the distribution function and properties of the electron transport in group-III nitride semiconductors at moderate electric fields. In bulk GaN, at low temperatures in the wide range of heating electric fields, the electron distribution function is quasiisotropic, and the second "ohmic" region on the *I-V* characteristic is observed. Simultaneously, the saturation of the mean electron energy is observed. As the electric field increases, the electron distribution takes on the spindle shape, and the electrons demonstrate the streaming regime. In compensated GaN, particularly, the streaming effect occurs at 10 K and 77 K at fields of 2–10 kV/cm.

The novel transport effects studied in this paper can find applications to the construction of devices. The existence of an extended quasisaturation region for the mean electron energy on a growth of the drift velocity corresponds to the steady noise level of hot electrons and the increase of the signal/noise ratio. This can be used in the development of new semiconductor devices, in particular, of sensitive photodetectors. The peculiar features of the electron transport in the streaming regime can be used in the design of tunable sources of tera-Hertz radiation [16].

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