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MONTE CARLO SIMULATION OF ELECTRON HEATING IN A ONE-DIMENSIONAL GaAs-QUANTUM CONDUCTOR

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The process of transport of one-dimensional electrons in a GaAs quantum conductor is investigated by the Monte Carlo method. It is shown that in addition to scattering by polar optical phonons, the heating of charge carriers is also appreciably affected, in the case of electric field intensities higher than $5\cdot 10^5$ V/m, by ionized-impurity scattering and the transverse dimensions of the conductor.

Many works devoted to electron transport in semiconductive quantum conductors have been published, primarily due to the possibility of using the unique properties of such structures in devices. Therefore, it is very important to investigate electron transport in semiconductor quantum conductors in the high-intensity electric fields typical of the operating conditions of actual micro- and nanoelectronic devices, since under these conditions electronic gas heating can exert a pronounced influence on the electrical characteristics of the devices.

It is known that one of the most promising approaches that allow sufficiently effective investigations of the specific features of electron transport in strong electric fields in three- and quasi-two-dimensional semiconductor devices is the Monte Carlo method (see, e.g., [1-3]). At the same time, a very limited number of works are known in which this method is employed to calculate the kinetic parameters of transport in quasi-one-dimensional GaAs quantum conductors [4-6], and the case of a rigorously one-dimensional quantum structure with an electrical quantum limit has been considered, as far as we know, only in [7]. In that work, the Monte Carlo method was used to calculate the drift electron velocity v_{dr} as a function of the electric field intensity E in a one-dimensional GaAs structure at the maximum electric intensity $E_{max} = 3\cdot 10^5$ V/m. It is pertinent to note that the model allowed for only one mechanism of electron scattering, namely, scattering by polar optical phonons.

Below we report the results of Monte Carlo simulation of the process of electron transport in one-dimensional GaAs quantum conductors of different cross-sections at temperatures $T = 30$ and $T = 77$ K in a uniform electric field with maximum intensity $E_{max} = 2\cdot 10^6$ V/m. In addition to scattering by polar optical phonons, the suggested model also allowed for remote ionized-impurity scattering. The algorithm used for Monte Carlo simulation is identical to that described in [7].

The total electron energy E in a quantum conductor in an approximation of a deep rectangular potential well can be represented in the form [7, 8]

$$E = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 \pi^2}{2m^*}\left(\frac{1}{L_y^2} + \frac{1}{L_z^2}\right), \tag{1}$$

where the first term on the right-hand side of (1) represents the kinetic energy of an electron with the wave vector k_x along the direction of motion x, while the second term is the bottom energy of the "zeroth" subband.

The intensities of scattering by polar optical phonons with their emission and absorption were calculated, respectively, by the formulas [8]

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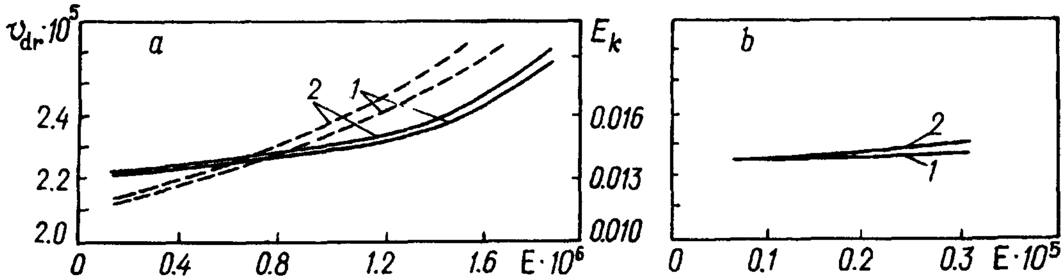

Fig. 1. Drift velocity and kinetic energy of electron motion along the x-coordinate as functions of the electric-field intensity in the case of scattering by polar optical phonons (v_{dr}, solid curves; E_k, dashed curves): 1, 2) (a), respectively, T = 30 and 77 K; 1, 2) (b) our results and the results of [7]. v_{dr}, m/sec; E_k, eV; E, V/m.

$$W^{em}(k_x) = \frac{\alpha\omega}{2\pi}(N_q + 1)\frac{I^{em}[q_+^{em}(k_x)] + I^{em}[q_-^{em}(k_x)]}{\sqrt{\left(\frac{\hbar k_x^2}{2m^*\omega} - 1\right)}}, \tag{2}$$

$$W^{a}(k_x) = \frac{\alpha\omega}{2\pi}N_q\frac{I^{a}[q_+^{a}(k_x)] + I^{a}[q_-^{a}(k_x)]}{\sqrt{\left(\frac{\hbar k_x^2}{2m^*\omega} + 1\right)}}, \tag{3}$$

where $q_\pm^{em} = k_x \pm \sqrt{k_x^2 - (2m^*\omega/\hbar)}$ and $q_\pm^{a} = -k_x \pm \sqrt{k_x^2 + (2m^*\omega/\hbar)}$. Expressions for the integrals I^{em} and I^{a} are given in [8]. They are rather bulky and therefore are not given here.

The intensity of remote-charged-impurity scattering was calculated by the formula [9]

$$W(k_x) = \frac{N_i m^* e^4}{\pi^2\hbar^3\varepsilon^2 k_x}K^2\left(2dk_x\sin\frac{\theta}{2}\right). \tag{4}$$

The final state of an electron after scattering by the given mechanism was determined with allowance for the fact that in the one-dimensional case an electron can move only forward or backward. We took into consideration only backscattering, since the scattering angle θ between the initial k_x and final k_x' wave vectors was equal to 180°. To simplify calculations, we used a stepwise approximation of the function $K(2dk_x)$ at $dk_x \leq 1$ and the approximate equality $K(2dk_x) \approx 1/2(\pi/dk_x)^{1/2}\exp(-2dk_x)$ at $dk_x > 1$.

Using the results of simulation of electron motion in the space of the wave vectors at different electric-field intensities E, we calculated the mean drift velocity v_{dr} and kinetic energy of charge carriers $E_k = \hbar^2 k_x^2/2m^*$. Figure 1a shows the results of calculation of v_{dr} and E_k as functions of ε without allowance for ionized-impurity scattering for two temperatures provided that $L_y = L_z = L_0 = \sqrt{\hbar/2m^*\omega}$ for fields with E < $2\cdot 10^6$ V/m. It is easy to see that for fields with $E > 3\cdot 10^5$ V/m, which were not considered in [7], electron heating begins to be observed and is manifested in a pronounced increase in electron drift velocity and energy [10]. This is attributed to the fact that as in the three-dimensional case [11], in the fields with a sufficiently high intensity, due to reduction of the intensity of electron scattering with emission of a polar optical phonon, a charge carrier can acquire an energy along the free path that is higher than its energy lost in scattering with phonon emission.

For comparison's sake, Fig. 1b shows the dependences v_{dr} (E) calculated for T = 30 K, $L_y = L_z = L_0$ and for the field range E < $4\cdot 10^5$ V/m. The practical coincidence of curves 1 and 2 indicates that calculations made for these conditions in [7] and in the present work are adequate.

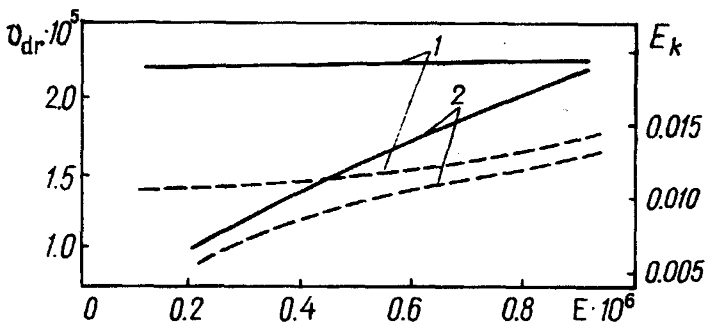

Fig. 2. Drift velocity and kinetic energy of electron motion along the x-coordinate as functions of the electric-field intensity with allowance for impurity scattering (ν_{dr}, solid curves, E_k, dashed curves): 1, 2) without and with allowance for impurity scattering. $L_y = L_z = L_0$, $d = 100$ Å; $T = 30$ K.

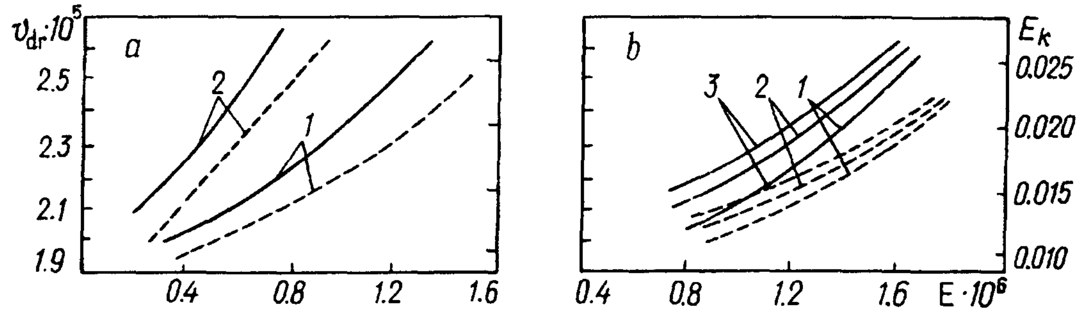

Fig. 3. Influence of transverse dimensions of quantum conductor (a) and distance from its center to charged impurity (b) on electron heating (ν_{dr}, solid curves, E_k, dashed curves): 1, 2) (a), respectively, $L_y = L_z = L_0$ and $L_y = L_z = 3L_0$, $d = 100$ Å, $T = 30$ K; 1, 2, 3 (b), respectively, $d = 100$, 150 and 200 Å, $L_y = L_z = L_0$, $T = 30$ K.

An example of the influence of impurity-scattering, which is elastic, on the drift velocity and the kinetic energy of an electron is represented in Fig. 2. As judged from the curves, this influence is more pronounced in the region of lower-intensity fields. This is attributable to the fact that according to formula (4) the intensity of impurity scattering decreases with an increase in electric-field intensity.

Figure 3 shows the influences, respectively, of the transverse dimensions of the quantum conductor L_y and L_z and the distance from its center to an impurity d on electron heating. In particular, it follows from Fig. 3a that with an increase in L_y and L_z, the curves $\nu_{dr}(E)$ and $E_k(E)$ become steeper. This is associated with a decrease in the intensity of scattering with phonon emission with increasing transverse dimensions of the conductor [8]. As is seen in Fig. 3b, ν_{dr} and E_k also increase with the parameter d, which is attributable to a decrease in the intensity of impurity scattering.

Thus, the results obtained allow us to conclude that with allowance only for scattering by polar optical phonons in the electrical quantum limit as well as for this mode of scattering and impurity scattering for fields with electric intensities higher than $E > 5\cdot 10^5$ V/m such a quantum structure shows the effect of electron heating. In the investigated range of parameters, the process of heating markedly depends on impurity scattering and the transverse dimensions of the conductor in addition to the electric-field intensity.

NOTATION

ν_{dr}, drift velocity of electrons; E, E_{max}, electric-field intensity and its maximum value; T, temperature of the crystal lattice, K; k_x, wave vector of an electron along the x-coordinate; L_y and L_z, transverse dimensions of quantum well along y and z; m^*, effective electron mass; $\hbar$, reduced Planck's constant; α, coupling constant of electron-phonon interaction; ω, frequency of polar optical phonon; N_q, number of thermodynamically equilibrium phonons; N_i, impurity concentration per unit length of conductor; e, electron charge; ε, dielectric permittivity of GaAs; $K(2dK_x)$, modified second-kind Bessel function; d, distance between charged impurity and coordinate origin located at the center of the square cross-section of conductor; θ, angle of scattering; E_k, kinetic energy of electron corresponding to the wave vector k_x.

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