NUMERICAL SIMULATION OF NONEQUILIBRIUM PROCESSES IN AN ELECTRON–HOLE PLASMA OF BINARY HETEROSTRUCTURES.

1. CALCULATION ALGORITHMS

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The algorithms of numerical solution of the system of quasihydrodynamic equations, simulating a dense electron–hole plasma in binary heterostructures, are considered and treated.

The nonequilibrium due to injection of hot electrons and holes can be substantial in semiconducting injection lasers, light diodes, bipolar transistors, and other devices based on heterostructures of an electron–hole plasma (EHP). In EHP with high charge carrier concentrations, such as EHP of semiconducting lasers, the pair collision frequencies are relatively high, so that Fermi or Maxwell electron and hole energy distributions are established. The effective electron and hole temperature, however, can substantially differ in this case from the lattice temperature. This deviation is most substantial when energy transfer from the EHP lattice is slowed shown, such as at low temperatures, for example [1, 2]. In a number of cases the "separation" of effective carrier temperatures from the lattice temperature in EHPs of lasers and light diodes can also occur at sufficiently high values of the lattice temperature, such as room temperature [3]. EHP heating in heterostructures can substantially affect the characteristics of semiconducting devices. For sufficiently strong EHP heating its stratification is possible [4], leading, in particular, to inhomogeneities of EHP optical properties.

The theoretical study of heating effects in an EHP is the subject of many studies, such as [4, 8], in which was analyzed the stability of a uniform state of a "hot" EHP, as well as studies of the effect of a heated EHP of the characteristics of devices of the type of lasers and light diodes [9, 10]. The complexity of physical processes in an EHP of semiconducting devices, related to its nonequilibrium and inhomogeneity, leads to the necessity of using mathematical simulation methods to study these processes. The quasiballistic model is used for a relatively dilute EHP. In this case the methodology based on simultaneous application of macroparticle and Monte Carlo methods is quite effective for numerical solutions of the corresponding problems [11]. This approach is not valid for a dense EHP with frequent pair collisions. In the situation under consideration the charge carrier distribution functions are similar to the Fermi (Maxwell) functions, and one can transform from the kinetic equations to the quasihydrodynamic EHP model [1].

Computer numerical simulation of processes on the basis of using quasihydrodynamic equations was carried out, for example, in [12, 13]. In these studies, however, was assumed constancy of the coefficients of diffusion, heat conduction, etc., i.e., constancy of the coefficients in terms with second spatial derivatives. For a real EHP this restriction can be substantial, because a strong nonlinearity is possible of the gradient terms, substantially complicating the mathematical treatment of the problem.

The present study is devoted to developing algorithms of numerical solution of the system of quasihydrodynamic equations for a dense "hot" EHP with account of nonlinearity of diffusion and heat conduction.

For definiteness we consider a binary p–i–n heterostructure with wideband p- and n-region junctions and a narrow-band i-region (Fig. 1). We confine ourselves to treating a quite dense, but nondegenerate EHP with equal electron and hole effective masses, for which the characteristic time of pair collisions τ satisfies the condition

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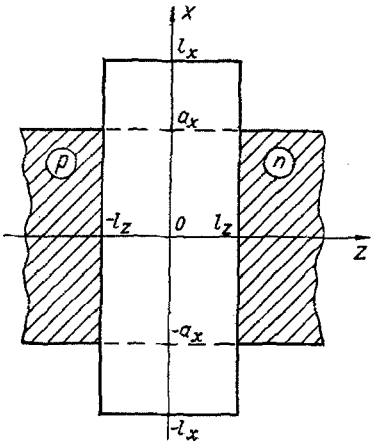

Fig. 1. Schematic representation of the geometry of the structure under consideration.

$$\tau_p \ll \tau \ll \tau_e, \tag{1}$$

where τ_p and τ_e are the relaxation times of momentum and energy due to interactions with impurities and phonons. Besides, it is assumed that the EHP in the active i-region is quasineutral, which imposes the following condition:

$$l_s \ll l_x, l_z. \tag{2}$$

For heterostructures based on $Pb_xSn_{1-x}Te$ at charge carrier energies corresponding to temperature ~ 100 K it can be assumed that the conditions adopted are satisfied if the concentrations are $N \sim 10^{14}$-10^{16} cm^{-3} and l_x, $l_z \geq 10^{-5}$-10^{-4} cm.

In the situation considered the EHP is characterized by a charge carrier concentration N and their effective temperature Θ, for which the following system of equations, derived, for example, in [4, 5], is valid in the two-dimensional geometry:

$$\frac{\partial N}{\partial \tau} = \frac{\partial^2}{\partial X^2}[D(N, \Theta)N] + \frac{\partial^2}{\partial Z^2}[D(N, \Theta)N] + R(N, \Theta), \tag{3}$$

$$\frac{\partial E(N, \Theta)}{\partial \tau} = \frac{\partial}{\partial X}\left\{\varkappa(N, \Theta)\frac{\partial \Theta}{\partial X} + \Pi(N, \Theta)\frac{\partial}{\partial X}[D(N, \Theta)N]\right\} +$$

$$+ \frac{\partial}{\partial Z}\left\{\varkappa(N, \Theta)\frac{\partial \Theta}{\partial Z} + \Pi(N, \Theta)\frac{\partial}{\partial Z}[D(N, \Theta)N]\right\} + P(N, \Theta). \tag{4}$$

When electron–hole scattering weakly affects the momentum relaxation, the following relation is valid $D(\Theta) = D_l(\Theta/\Theta_l)^{1+\alpha}$, $\varkappa(N, \Theta) = (5/2 + \alpha)ND(\Theta)$, where α is a numerical coefficient, determined by the energy dependence of the momentum relaxation time, $E(N, \Theta) = 3/2N\Theta$ is the EHP energy density (the nondegenerate case), and $\Pi(\Theta) = (5/2 + \alpha)\Theta$ is the energy transported by a single electtron (hole) into the flow. The shape of the terms $R(N, \Theta)$ and $P(N, \Theta)$ is determined by the dominant mechanisms of electron and hole recombination and their energy relaxation. We further put:

$$R(N, \Theta) = \frac{N_l - N}{\tau_r(\Theta)}, \tag{5}$$

$$P(N, \Theta) = \frac{N(\Theta_l - \Theta)}{\tau_\varepsilon(\Theta)}. \tag{6}$$

Here $\tau_r(\Theta) = \tau_r(\Theta/\Theta_l)^r$, $\tau_\varepsilon(\Theta) = \tau_\varepsilon(\Theta/\Theta_l)^\varepsilon$, where r and ε are numbers whose values are determined by the corresponding mechanisms.

Taking the active region to be rectangular (Fig. 1), the boundary conditions to Eqs. (3), (4) are assigned in the form

$$-\frac{\partial}{\partial Z}[D(N, \Theta)N]\Big|_{Z=\mp l_z} = \pm J, \tag{7}$$

$$-\left\{\varkappa(N,\ \Theta)\frac{\partial\Theta}{\partial Z}+\Pi(N,\ \Theta)\frac{\partial}{\partial Z}[D(N,\ \Theta)N]\right\}\Big|_{Z=\mp l_z}=\pm\Delta\cdot J, \tag{8}$$

$$\frac{\partial}{\partial X}[D(N,\ \Theta)N]\Big|_{X=\mp l_x}=0, \tag{9}$$

$$\left\{\varkappa(N,\ \Theta)\frac{\partial\Theta}{\partial X}+\Pi(N,\ \Theta)\frac{\partial}{\partial X}[D(N,\ \Theta)N]\right\}\Big|_{X=\mp l_x}=0. \tag{10}$$

Conditions (7)-(10) correspond to injection of "hot" carriers of junctions of size $2a_X$, located at the planes $Z = \mp l_Z$; here $J = J(\tau, X) = J(\tau)X(a^2_X - X^2)$ is the current density injected through electron and hole heterojunctions, where Δ is the energy of injected carriers, determined, in particular, by the jump values of the bottom of the conduction band and the top of the valence and in the heterojunction.

As initial conditions we take

$$N(X,\ Z)|_{\tau=0}=N_0=\text{const},\quad \Theta(X,\ Z)|_{\tau=0}=\Theta_0=\text{const}. \tag{11}$$

We introduce the following dimensionless quantities:

$$\frac{N}{N_l}=n,\quad \frac{\Theta}{\Theta_l}=T,\quad \frac{X}{l_z}=x,\quad \frac{Z}{l_z}=z,\quad \frac{l_x}{l_z}=l,\quad \frac{a_x}{l_z}=a,$$

$$\frac{\tau D_l}{l_z^2}=t,\quad \frac{\tau_r D_l}{l_z^2}=\tau_R,\quad \frac{\tau_\varepsilon D_l}{l_z^2}=\tau_E,\quad \frac{J(\tau,\ X)l_z}{N_l D_l}=I(t,\ x),\quad \frac{\Delta}{\Theta_l}=\delta. \tag{12}$$

In these variables the system (3)-(10), with account of the specific representation of the coefficients appearing in it, is

$$\frac{\partial n}{\partial t}-\frac{\partial^2}{\partial x^2}[nT^{1+\alpha}]-\frac{\partial^2}{\partial z^2}[nT^{1+\alpha}]=\frac{1-n}{\tau_r(T)}, \tag{13}$$

$$\frac{3}{2}\frac{\partial(nT)}{\partial t}-\left(\frac{5}{2}+\alpha\right)\left\{\frac{\partial^2}{\partial x^2}[nT^{2+\alpha}]+\frac{\partial^2}{\partial z^2}[nT^{2+\alpha}]\right\}=\frac{n(1-T)}{\tau_\varepsilon(T)}, \tag{14}$$

$$-\frac{\partial}{\partial z}[nT^{1+\alpha}]\Big|_{z=\mp 1}=\pm I(t,\ x), \tag{15}$$

$$-\left(\frac{5}{2}+\alpha\right)\frac{\partial}{\partial z}[nT^{2+\alpha}]\Big|_{z=\mp 1}=\pm\delta I(t,\ x), \tag{16}$$

$$\frac{\partial}{\partial x}[nT^{1+\alpha}]\Big|_{x=\mp l}=0, \tag{17}$$

$$\left(\frac{5}{2}+\alpha\right)\frac{\partial}{\partial x}[nT^{2+\alpha}]\Big|_{x=\mp l}=0. \tag{18}$$

The system of equations considered (13), (14) is substantially nonlinear. Indeed, along with the strong nonlinearity of the EHP diffusion and heat conduction coefficients, as well as the right-hand sides of Eqs. (13), (14), the variables n and T in the system are coupled through the gradient terms, the right-hand sides, while in Eq. (14) – also through the time derivative. All this implies great difficulty on the numerical solution of the problem described even in the spatially one-dimensional case.

It must be noted that the systems of equations (3), (4), or (13), (14), resemble in some sense the nonlinear system

$$\frac{\partial X}{\partial t}=D_1\left\{\frac{\partial^2 X}{\partial x^2}+\frac{\partial^2 X}{\partial z^2}\right\}+F_1(X,\ Y,\ \lambda), \tag{19}$$

$$\frac{\partial Y}{\partial t}=D_2\left\{\frac{\partial^2 Y}{\partial x^2}+\frac{\partial^2 Y}{\partial z^2}\right\}+F_2(X,\ Y,\ \lambda), \tag{20}$$

being a classical object of studying dissipative structures [14, 15]; in particular, morphogenesis. The solution of the system of equations (13), (14) also leads to the manifestation of EHP stratification (dissipative structures) [16], as will be shown in the following investigation by the present authors, devoted to results and analysis of the numerical calculations.

However, the system under consideration (13), (14) is more complicated, and consequently so is the numerical solution, than the system (19), (20), since the variables in it are coupled not only nonlinearly through the functions F_1 and F_2, but they are also at the same time the object of applying the differentation operators.

One can rewrite the equations of the system (13), (14) in a form providing a smoother representation of the complicated numerical realization of the given problem. For this we introduce, along with the variables n and T, the new unknown quantities $\Phi = nT^{1+\alpha}$, $\Psi = nT^{2+\alpha}$. Following some transformations, Eqs. (13) and (14) can then be rewritten in the form:

$$\frac{\partial \Phi}{\partial t} = -\alpha\left(\frac{\Psi}{\Phi}\right)^{1+\alpha}\left\{\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial z^2}\right\}+\frac{2}{3}(1+\alpha)\left(\frac{5}{2}+\alpha\right)\times\left(\frac{\Psi}{\Phi}\right)^{\alpha}\left\{\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial z^2}\right\}+f_1(\Phi,\Psi), \quad (21)$$

$$\frac{\partial \Psi}{\partial t} = \frac{2}{3}(2+\alpha)\left(\frac{5}{2}+\alpha\right)\left(\frac{\Psi}{\Phi}\right)^{1+\alpha}\left\{\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial z^2}\right\}-(1+\alpha)\left(\frac{\Psi}{\Phi}\right)^{2+\alpha}\left\{\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial x^2}\right\}+f_2(\Phi,\Psi), \quad (22)$$

where

$$f_1(\Phi,\Psi) = -\alpha\left(\frac{\Psi}{\Phi}\right)^{1+\alpha}R(\Phi,\Psi)+\frac{2}{3}(1+\alpha)\left(\frac{\Psi}{\Phi}\right)^{\alpha}P(\Phi,\Psi);$$

$$f_2(\Phi,\Psi) = -(1+\alpha)\left(\frac{\Psi}{\Phi}\right)^{2+\alpha}R(\Phi,\Psi)+\frac{2}{3}(2+\alpha)\left(\frac{\Psi}{\Phi}\right)^{1+\alpha}P(\Phi,\Psi),$$

while $R(\Phi, \Psi)$ and $P(\Phi, \Psi)$ are determined from (5) and (6).

As seen from the right-hand side of Eq. (21), the system contains terms with negative diffusion, which can importantly affect the nature of the behavior of solutions of the problem (3)-(11). By the structure of the equations it follows that in some cases the inhomogeneities may not get smoothed, but, on the contrary, be enhanced. This fact finally imposes the requirement of careful choice of the algorithm of numerical solution of the problem.

1. Numerical Solution Algorithm of the One-dimensional Problem. We consider initially a spatially homogeneous model, in which one studies the distributions of EHP concentration N and the effective temperature Θ in a direction perpendicular to that of electron and hole injection (parallel to the plane of heterostructure layers). Before turning to its description it must be pointed out that the solution of one-dimensional problems is an important stage in the numerical simulation of high dimensionality problems. The study of one-dimensional models with less cost makes it possible to clarify the difficulties in the nuemrical solution, characteristic of the given problem as a whole, as well as the solution features, manifested both in the one-dimensional and in the multidimensional cases.

Thus, we investigate structures with a width of active i-region ℓ_z, small in comparison with the diffusion length $\ell_D = (D_\ell \tau_r)^{1/2}$ and the carrier cooling length $\ell_\varepsilon = ((5/2 + \alpha)D_\ell \tau_\varepsilon)^{1/2}$. In this case, assuming ℓ_x, $a_x >> \ell_z$, integration of the original two-dimensional equations (3) and (4) over dz with account of the boundary conditions (7), (8) leads to the following spatially one-dimensional equations:

$$\frac{\partial N}{\partial \tau} = \frac{\partial^2}{\partial X^2}[D(\Theta)N]+R(N,\Theta)+\frac{2J}{2l_z}, \quad (23)$$

$$\frac{3}{2}\frac{\partial(N\Theta)}{\partial \tau} = \frac{\partial}{\partial X}\left\{\varkappa(N,\Theta)\frac{\partial\Theta}{\partial X}+\Pi(\Theta)\frac{\partial}{\partial X}[D(\Theta)N]\right\}+P(N,\Theta)+\frac{2J\Delta}{2l_z} \quad (24)$$

with the boundary and initial conditions

$$\frac{\partial}{\partial X}[D(\Theta)N]\Big|_{X=\mp l_x}=0, \quad \varkappa(N,\Theta)\frac{\partial\Theta}{\partial X}\Big|_{X=\mp l_x}=0, \quad (25)$$

$$N(X)|_{\tau=0} = N_0+\delta N_0, \quad \Theta(X)|_{\tau=0} = \Theta_0+\delta\Theta_0, \quad (26)$$

where the quantities δN_0 and $\delta\Theta_0$ are perturbations of the initial homogeneous distributions of concentration N_0 and temperature Θ_0.

On the segment $[-\ell, \ell]$ we introduce the uniform grid $\omega_h = \{x_i = (i - 1)h; i = 1, \ldots, N; h = 2\ell/(N - 1)\}$, and in the variable t – the grid $\omega_\tau = \{t_k = k\tau, k = 0, 1, \ldots\}$. For a difference approximation of system (23)-(26) we use a purely implicit conservative difference scheme, which in the dimensionless variables (12) is

$$n_t = [D(\hat{T})\,\hat{n}]_{\bar{x}x} - \frac{\hat{n}-1}{\tau_r(\hat{T})} + 2I,$$

$$\frac{3}{2}(nT)_t = \left(\frac{5}{2}+\alpha\right)[D(\hat{T})\,\hat{n}\hat{T}]_{\bar{x}x} - \frac{\hat{n}(\hat{T}-1)}{\tau_\varepsilon(\hat{T})} + 2\delta I, \tag{27}$$

$$[D(\hat{T})\,\hat{n}]_{x,1} = 0, \quad [D(\hat{T})\,\hat{n}]_{\bar{x},N} = 0, \quad \hat{T}_{x,1} = 0, \quad \hat{T}_{\bar{x},N} = 0.$$

The standard notation of [17] has been used here.

The implicit difference scheme (27) is a system of nonlinear difference equations with strongly coupled variables. It must be noted that the use of separation algorithms to solve the equations of system (27) does not lead to success. Such an algorithm consists of two iterative processes: an "external" process in the nonlinearity (for example, an iterative Newton method), and an "internal" process, similar to Seidel's method, in which both linearized equations are solved separately under the assumption that the information on the other function is included in the preceding iteration. As shown by the calculations, in this case the "internal" iteration converges only for a sufficiently short step in time: $\tau \leq \tau_{\max} \sim h^2/\max_{\omega h} D(T)$.

We apply the Newton iteration method [18] to the system of nonlinear equations (27), leading to a system of linear equations in $\delta n^{(s+1)} = n^{(s+1)} - n^{(s)}$, $\delta T^{(s+1)} = T^{(s+1)} - T^{(s)}$ (here s is the iteration number) on a three-point scheme for the internal grid sites. This system is solved at each iteration by Newton's method [18].

2. Numerical Solution Algorithm of Two-Dimensional Models. In the solution region of problem (13)-(18) $G = \{-\ell \leq x \leq \ell, -1 \leq z \leq 1\}$ we introduce the uniform grid $\Omega_h = \{x_i = (i-1)h_x,\ 1 \leq i \leq N,\ h_x = 2\ell/(N-1);\ z_j = (j-1)h_z;\ 1 \leq j \leq M,\ h_z = 2/(M-1)\}$. The grid in the variable t is defined in the usual manner: $\Omega_\tau = \{t_k = k\tau,\ k = 0, 1, 2, \ldots\}$ [17]. As a difference approximation of problem (13)-(18) on the grid $\Omega = \Omega_h \times \Omega_\tau$ we use a purely implicit difference scheme, similar to (27). This scheme is also nonlinear. If for its solution we use an algorithm based on separating the equations of the system, then along with weak convergence of iterations for each of them it is necessary to solve two five-point difference equations for $\delta n^{(s+1)}$ and $\delta T^{(s+1)}$. Each of these equations is also solved by iterations. As shown by the review [19], for two-dimensional problems this method is practically nonreasonable on contemporary computers. By the considerations provided above it is suggested to use for numerical solution of the problem described a method in which the system of difference relations is treated as one matrix equation in the vector (n, T). We turn now to describing this algorithm. The difference scheme for the system (13)-(18) is represented in the form:

$$f^1_{ij}(\hat{n}, \hat{T}) = -\frac{\hat{n}_{ij} - n_{ij}}{\tau} + \frac{1}{h_x^2}[D(\hat{T}_{i+1j})\,\hat{n}_{i+1j} - 2D(\hat{T}_{ij})\,\hat{n}_{ij} +$$
$$+ D(\hat{T}_{i-1j})\,\hat{n}_{i-1j}] + \frac{1}{h_z^2}[D(\hat{T}_{ij+1})\,\hat{n}_{ij+1} - 2D(\hat{T}_{ij})\,\hat{n}_{ij} + D(\hat{T}_{ij-1})\,\hat{n}_{ij-1}] -$$
$$- \frac{(\hat{n}_{ij}-1)}{\tau_r(\hat{T}_{ij})} = 0,$$

$$f^2_{ij}(\hat{u}, \hat{T}) = -\frac{3}{2}\frac{\hat{n}_{ij}\hat{T}_{ij} - n_{ij}T_{ij}}{\tau} + \frac{(5/2+\alpha)}{h_x^2}[D(\hat{T}_{i+1j})\,\hat{n}_{i+1j}\hat{T}_{i+1j} -$$
$$- 2D(\hat{T}_{ij})\,\hat{n}_{ij}\hat{T}_{ij} + D(\hat{T}_{i-1j})\,\hat{n}_{i-1j}\hat{T}_{i-1j}] + \frac{(5/2+\alpha)}{h_z^2}[D(\hat{T}_{ij+1})\,\hat{n}_{ij+1}\hat{T}_{ij+1} -$$
$$- 2D(\hat{T}_{ij})\,\hat{n}_{ij}\hat{T}_{ij} + D(\hat{T}_{ij-1})\,\hat{n}_{ij-1}\hat{T}_{ij-1}] - \hat{n}_{ij}(\hat{T}_{ij}-1)/\tau_\varepsilon(\hat{T}_{ij}) = 0,$$
$$f^1_{i1} = [D(\hat{T}_{i2})\,\hat{n}_{i2} - D(\hat{T}_{i1})\,\hat{n}_{i1}]/h_z + I = 0,$$
$$f^1_{iM} = [D(\hat{T}_{iM-1})\,\hat{n}_{iM-1} - D(\hat{T}_{iM})\,\hat{n}_{iM}]/h_z + I = 0, \tag{28}$$
$$f^1_{1j} = [D(\hat{T}_{2j})\,\hat{n}_{2j} - D(\hat{T}_{1j})\,\hat{n}_{1j}]/h_x = 0,$$
$$f^1_{Nj} = [D(\hat{T}_{N-1j})\,\hat{n}_{N-1j} - D(\hat{T}_{Nj})\,\hat{n}_{Nj}]/h_x = 0,$$
$$f^2_{i1} = \left(\frac{5}{2}+\alpha\right)[D(\hat{T}_{i2})\,\hat{n}_{i2}\hat{T}_{i2} - D(\hat{T}_{i1})\,\hat{n}_{i1}\hat{T}_{i1}]/h_z + \delta I = 0,$$

$$f^2_{iM} = \left(\frac{5}{2} + \alpha\right)\left[D(\hat{T}_{iM-1})\,\hat{n}_{iM-1}\,\hat{T}_{iM-1} - D(\hat{T}_{iM})\,\hat{n}_{iM}\,\hat{T}_{iM}\right]/h_z + \delta I = 0,$$

$$f^2_{1j} = \hat{T}_{2j} - \hat{T}_{1j} = 0, \quad f^2_{Nj} = \hat{T}_{N-1j} - \hat{T}_{Nj} = 0.$$

We further apply the Newton iteration method to the system of nonlinear equations (28), leading to the system of linear equations

$$\sum_{Q\in Ш(P)} \left\{\frac{\partial f^{k(s)}}{\partial n(Q)}\,\delta n(Q)^{s+1} + \frac{\partial f^{k(s)}}{\partial T(Q)}\,\delta T(Q)^{(s+1)}\right\} + f^k(P)^{(s)} = 0, \tag{29}$$

where k = 1, 2 is the number of equation of system (28), P is the point of the grid Ω_h and Ш(P) is the pattern of grid equations (28) at site P (including five points of the "cross" if P is internal, and two points – if P is a boundary site of the grid). In the system (29) s is the number of Newton iteration. From (29) we find at each iteration the increments $\delta n^{(s+1)}$ and $\delta T^{(s+1)}$, then from the equations $n^{(s+1)} = n(s) + \delta n^{(s+1)}$, $T^{(s+1)} = T(s) + \delta T^{(s+1)}$ we determine the values of the required functions at iteration s + 1. The criterion of concluding the iteration process described can be, for example, the condition $\|\delta n^{(s+1)}\| \leq \varepsilon_1\|n^{(s)}\| + \varepsilon_2$, where the grid norm is defined as $\|y\| = \left(\sum_{i=1}^{N-1}\sum_{j=1}^{M-1} y^2_{ij} h_x h_z\right)^{1/2}$. As the initial approximation $T^{(0)}$ and $n^{(0)}$ we take the values of the effective EHP temperature and concentration at the preceding time layer.

To solve the system of five-point equations (29) we used a matrix method [20], being a generalization to the case of second-order matrices of the "α – β" iteration process [21, 22]. We write down this algorithm. For this purpose we represent the system (29) in the form

$$A_{ij}U_{i-1j} - C_{ij}U_{ij} + B_{ij}U_{i+1j} + \bar{A}_{ij}U_{ij-1} + \bar{B}_{ij}U_{ij+1} + F_{ij} = 0,$$
$$-C_{i1}U_{i1} + \bar{B}_{i1}U_{i2} = -F_{i1}, \quad -C_{1j}U_{1j} + B_{1j}U_{2j} = -F_{1j}, \tag{30}$$

$$-\bar{A}_{iM}U_{1M-1} + C_{iM}U_{iM} = F_{iM}, \quad -A_{Nj}U_{N-1j} + C_{Nj}U_{Nj} = F_{Nj}. \tag{31}$$

Here $U_{ij} = (\delta n_{ij}^{(s+1)}, \delta T_{ij}^{(s+1)})$ is the vector of unknown functions, F_{ij} is the vector of the right-hand sides, and A_{ij}, C_{ij}, B_{ij}, $\bar{A}_{ij}$, $\bar{B}_{ij}$ are second-order matrices, where, for example:

$$A_{ij} = \begin{Vmatrix} \frac{\partial f^{1(s)}_{ij}}{\partial n_{i-1j}} & \frac{\partial f^{1(s)}_{ij}}{\partial T_{i-1j}} \\ \frac{\partial f^{2(s)}_{ij}}{\partial n_{i-1j}} & \frac{\partial f^{2(s)}_{ij}}{\partial T_{i-1j}} \end{Vmatrix}, \quad B_{ij} = \begin{Vmatrix} \frac{\partial f^{1(s)}_{ij}}{\partial n_{i+1j}} & \frac{\partial f^{1(s)}_{ij}}{\partial T_{i+1j}} \\ \frac{\partial f^{2(s)}_{ij}}{\partial n_{i+1j}} & \frac{\partial f^{2(s)}_{ij}}{\partial T_{i+1j}} \end{Vmatrix}$$

We seek a solution of the matrix equation (30) with boundary conditions (31) in a form simultaneously satisfying the conditions:

$$U_{ij} = \alpha_{i+1j}\cdot U_{i+1j} + \beta_{i+1j}, \quad U_{ij} = \gamma_{i-1j}\cdot U_{i-1j} + d_{i-1j}, \tag{32}$$

$$U_{ij} = \bar{\alpha}_{ij+1}\cdot U_{ij+1} + \bar{\beta}_{ij+1}, \quad U_{ij} = \bar{\gamma}_{ij-1}\cdot U_{ij-1} + \bar{d}_{ij-1}, \tag{33}$$

where α, γ, $\bar{\alpha}$, $\bar{\gamma}$ are matrices of size 2 × 2, and β, d, $\bar{\beta}$, $\bar{d}$ are two-dimensional vectors. Substituting (32) into (30) and using matrix manipulations, we obtain nonlinear equations for the determination of α, β, γ, d:

$$\alpha_{i+1j} = \Psi^{-1}_{ij\alpha}\cdot B_{ij}, \ \alpha_{1j} = C^{-1}_{1j}\cdot B_{1j}, \ \Psi_{ij\alpha} = C_{ij} - \bar{A}_{ij}\cdot\bar{\alpha}_{ij} - A_{ij}\cdot\alpha_{ij} - \bar{B}_{ij}\cdot\bar{\gamma}_{ij},$$
$$i = 2, 3, \ldots, N-1; \ j = 2, \ldots, M-1;$$
$$\beta_{i+1j} = \Psi^{-1}_{ij\alpha}\cdot(F_{ij} + A_{ij}\cdot\beta_{ij} + \bar{A}_{ij}\cdot\bar{\beta}_{ij} + \bar{B}_{ij}\cdot\bar{d}_{ij}), \ \beta_{1j} = C^{-1}_{1j}\cdot F_{1j}, \tag{34}$$
$$\gamma_{i-1j} = \Psi^{-1}_{ij\gamma}\cdot A_{ij}, \ \gamma_{N-1j} = C^{-1}_{Nj}\cdot A_{Nj},$$
$$\Psi_{ij\gamma} = C_{ij} - B_{ij}\cdot\gamma_{ij} - \bar{A}_{ij}\cdot\bar{\alpha}_{ij} - \bar{B}_{ij}\cdot\bar{\gamma}_{ij},$$
$$d_{i-1j} = \Psi^{-1}_{ij\gamma}\cdot(F_{ij} + B_{ij}\cdot d_{ij} + \bar{A}_{ij}\cdot\bar{\beta}_{ij} + \bar{B}_{ij}\cdot\bar{d}_{ij}), \ d_{N-1j} = C^{-1}_{Nj}\cdot F_{Nj}.$$

Similarly, substituting (33) into (3) and applying matrix equations, we obtain equations for α, β, γ, d:

$$\bar{\alpha}_{ij+1} = \Psi^{-1}_{ij\bar{\alpha}} \cdot \bar{B}_{ij}, \quad \bar{\alpha}_{i1} = C^{-1}_{i1} \cdot \bar{B}_{i1}, \quad j = 2, \ldots, M-1; \; i = 2, \ldots, N-1;$$

$$\Psi_{ij\bar{\alpha}} = C_{ij} - \bar{A}_{ij} \cdot \bar{\alpha}_{ij} - A_{ij} \cdot \alpha_{ij} - B_{ij} \cdot \gamma_{ij},$$

$$\bar{\beta}_{ij+1} = \Psi^{-1}_{ij\bar{\alpha}} \cdot (F_{ij} + \bar{A}_{ij} \cdot \bar{\beta}_{ij} + A_{ij} \cdot \beta_{ij} + B_{ij} \cdot d_{ij}), \quad \bar{\beta}_{i1} = C^{-1}_{i1} \cdot F_{i1},$$

$$\bar{\gamma}_{ij-1} = \Psi^{-1}_{ij\bar{\gamma}} \cdot \bar{A}_{ij}, \quad \bar{\gamma}_{iM-1} = C^{-1}_{iM} \cdot \bar{A}_{iM}, \quad \Psi_{ij\bar{\gamma}} = C_{ij} - \bar{B}_{ij} \cdot \bar{\gamma}_{ij} - A_{ij} \cdot \alpha_{ij} - B_{ij} \cdot \gamma_{ij}, \tag{35}$$

$$\bar{\alpha}_{ij-1} = \Psi^{-1}_{ij\bar{\gamma}} \cdot (F_{ij} + \bar{B}_{ij} \cdot \bar{d}_{ij} + A_{ij} \cdot \beta_{ij} + B_{ij} \cdot d_{ij}), \quad \bar{d}_{iM-1} = C^{-1}_{iM} \cdot F_{iM}.$$

The system for finding the coefficients (34)-(35) is nonlinear, and is solved by iterations, while to find α, γ, $\bar{\alpha}$, $\bar{\gamma}$ one can confine oneself to an autonomous iteration process, not related to the calculation of β, d, $\bar{\beta}$, $\bar{d}$. The solution of the matrix equation (30) can then be found from one of Eqs. (32), (33) with account of boundary conditions (31).

To realize the described computational algorithms in the two-dimensional and one-dimensional statements we prepared a FORTRAN program, by means of which we solved the corresponding systems of equations.

In conclusion, it is desirable to stress once more the large computational difficulties arising in numerical simulation of processes in an electron–hole plasma. The algorithms considered, particularly concerning the spatially two-dimensional case, are still far from completion. Their further development and study are of interest not only from the point of view of obtaining specific applied results in the region under consideration, but also from the point of view of creating effective methods of computing systems of nonlinear equations of the diffusion type.

NOTATION

τ, characteristic time of pair collisions; τ_p, momentum relaxation time; τ_ε, energy relaxation time; ℓ_S, Debye screening length; ℓ_X and ℓ_Z, characteristic sizes of the active gegion; N and n, charge carrier concentrations; Θ and T, effective temperatures; $D(N, \Theta)$, diffusion coefficient; $\varkappa(N, \Theta)$, EHP thermal conductivity coefficient; $E(N, \Theta)$, EHP energy density; $\Pi(N, \Theta)$, energy transferred by a single electron (hole) to the flow; Θ_ℓ, lattice temperature; D_ℓ, diffusion coefficient at $\Theta = \Theta_\ell$; $R(N, \Theta)$, recombination term; $P(N, \Theta)$, relaxation term; $\tau_r(\Theta)$, $\tau_\varepsilon(\Theta)$, carrier lifetime and relaxation time; N_ℓ, EHP concentration in the absence of injection through the heterotransitions; a_X and a, sizes of injection contacts; J and I, injection current densities; Δ, δ, energies of injected carriers; X(x), Heaviside function; ℓ_D, diffusion length; ℓ_ε, cooling length; and X, x, Z, z, space coordinates.

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DESCRIPTION OF THE NEIGHBORHOOD OF THE PHASE EQUILIBRIUM LINE AND METASTABLE REGION WITH THE PARAMETERIC EQUATION OF SCALING THEORY

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The deficiencies of the parameteric equation of scaling theory in the neighborhood of the phase equilibrium line and in the metastable region are analyzed.

The equation of state obtained in the well-known parametric representation of the scaling theory [1, 2] is widely used in calculations in the critical region. The first approximation of this representation, the so-called linear model, is the most widely studied. In this model the pressure and heat capacity at constant volume are calculated as follows [1, 2]:

$$\Delta p = (1 + \Delta\rho)\,\Delta\mu(\rho,\ T) - |\Delta\rho|^{\delta+1} a(x) - A(T), \tag{1}$$

$$\frac{\rho C_v}{T} = \frac{M p_K}{T_K^2}\,[|\Delta\rho|^{-\alpha/\beta} f(x) - \mu''(\rho_K,\ T)\,\Delta\rho + B(T)], \tag{2}$$

$$\tau = r(1 - b^2\theta^2),\ \Delta\rho = kr^{\beta}\theta,\ \Delta\mu = |\Delta\rho|^{\delta} h(x). \tag{3}$$

Here we use the conventional notation in scaling theory. The scaling functions in (1) through (3) are determined in terms of the parameter θ:

$$h(x) = a\theta(1 - \theta^2)(k|\theta|)^{-\delta},\ f(x) = \frac{ak\gamma(\gamma - 1)}{2\alpha b^2}\,(k|\theta|)^{\alpha/\beta}. \tag{4}$$

In order to proceed further one must relate the scaling variable $x = \tau/|\Delta\rho|^{1/\beta}$ with θ and also with expression for the scaling function of the isothermal compressibility $f_z = [\delta h(x) - \beta^{-1} x h'(x)]^{-1}$. From (3) one easily obtains

$$x = (1 - b^2\theta^2)\,(k|\theta|)^{-1/\beta}, \tag{5}$$

$$f_z(x) = \frac{k}{a}\,(k|\theta|)^{\delta-1}\left[1 + \frac{2(\beta + \gamma) - 3}{1 - 2\beta}\,\theta^2\right]^{-1}. \tag{6}$$

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