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FORMATION OF SHOCK WAVES IN FLOW OF CHARGE CARRIERS IN SEMICONDUCTORS

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A hydrodynamic model of the physics of semiconductors is studied numerically. It is shown that the solution of the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode has a shock wave. This problem is solved using an iterative method. An economical conservative semi-implicit difference scheme is developed for search of a numerical solution.

Introduction. At present, hydrodynamic models have found wide application in modeling transport of charge carriers (electrons or holes) in semiconductors. These models treat the motion of charge carriers as a charged fluid flow. Gas-dynamic models [1] containing conservation laws for the number of particles, momentum, and energy, Poisson's equations for electric potential, and the Fourier law for specific heat flux have been used most widely. These models, however, have some disadvantages. In particular, they ignore the anisotropy of pressure.

In the present paper, we study stationary solutions of the one-dimensional gas-dynamic model of [2], which allows for the anisotropy of pressure. We consider the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode, which models electron flow in a silicon diode consisting of three regions with different doping densities. This model problem describes the heating of free electrons inside the semiconductor, and, therefore, it is widely used in testing hydrodynamic models in the physics of semiconductors [1].

From the mathematical point of view, the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode is a boundary-value problem for a system of ordinary differential equations. In the present paper, numerical solutions of this problem are sought by an iterative method. As the evolution equations, we consider the hydrodynamic model of [2], which, for the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode, is written as the following system of conservation laws:

$$\boldsymbol{U}_t + \boldsymbol{J}(\boldsymbol{U})_x = (\boldsymbol{G}(\boldsymbol{U})T(\boldsymbol{U})_x)_x + \boldsymbol{F}(x, \boldsymbol{U}). \tag{1}$$

Here t and x are the time and spatial variable, $\boldsymbol{U} = (u_1, u_2, u_3)^*$, $\boldsymbol{J} = (j_1, j_2, j_3)^*$, $j_i = j_i(\boldsymbol{U})$, $\boldsymbol{G} = (g_1, g_2, g_3)^*$, $g_i = g_i(\boldsymbol{U})$, $\boldsymbol{F} = (f_1, f_2, f_3)^*$, and $f_i = f_i(x, \boldsymbol{U})$. The asterisk denotes transposition.

To find an approximate stationary solution of system (1), we construct an economical conservative semi-implicit difference scheme. The numerical experiment performed showed that the solution of the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode includes a shock wave. The result obtained in the present work is qualitatively different from results of numerical studies of gas-dynamic models ignoring the anisotropy of pressure (see, for example, [1, 3]).

Hydrodynamic Model. Electron flow in semiconductors is traditionally described using a hydrodynamic model that includes:

— The law of conservation of the number of particles

$$n_t + (nv)_x = 0; \tag{2}$$

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— The law of conservation of momentum

$$(nv)_t + \left(n\left(v^2 + \frac{K_\beta T}{m_{\text{eff}}}\right)\right)_x = -n\left(\frac{eE}{m_{\text{eff}}} + \frac{v}{\tau_1}\right); \tag{3}$$

— The energy conservation law

$$\left(n\left(v^2 + \frac{3K_\beta T}{m_{\text{eff}}}\right)\right)_t + \left(nv\left(v^2 + \frac{5K_\beta T}{m_{\text{eff}}}\right) + \frac{2Q}{m_{\text{eff}}}\right)_x = -\frac{2envE}{m_{\text{eff}}} - \frac{n}{\tau_2}\left(v^2 + \frac{3K_\beta}{m_{\text{eff}}}(T - T_0)\right); \tag{4}$$

— The Poisson's equation for electric potential

$$\Phi_{xx} = \frac{e}{\varepsilon_s}(n - N(x)). \tag{5}$$

Here n is the electron density (the number of free electrons in unit volume), v is the electron velocity, T is the electron temperature, K_β is Boltzmann's constant, Q is the specific heat flux, Φ is the electric potential, $E = -\Phi_x$ is the electric intensity, T_0 is the temperature of the molecular lattice of the semiconductor, e is the elementary charge, $m_{\text{eff}} = m_r m_e$ is the effective mass of an electron, where m_e is the mass of an electron and m_r is a correction factor, $\varepsilon_s = \varepsilon_r \varepsilon_0$ is the permittivity in silicon, ε_0 is the permittivity in vacuum, $\varepsilon_r = 11.7$ is a correction factor for silicon, $N(x)$ is the doping density as a function of x, and τ_α are the relaxation times. The relaxation times (10^{-12} sec) from [4] are used:

$$\tau_\alpha = a_\alpha + b_\alpha(\mathcal{E} - 1) + c_\alpha \exp[-d_\alpha(\mathcal{E} - 1)] \qquad (\alpha = 1,\ 2,\ 3),$$

where a_α, b_α, c_α, and d_α are constants and $\mathcal{E} = m_{\text{eff}} v^2/(2K_\beta T_0) + 3T/(2T_0)$. We note that Eqs. (2)–(5) are written for the case where the only charge carriers are electrons.

To close system (2)–(5), we use the Fourier law. Anile and Pennisi [2] proposed the Fourier law that takes the anisotropy of pressure into account:

$$Q = \frac{5}{2} K_\beta \tau_3 n T\left(v\left(\frac{1}{\tau_1} - \frac{1}{\tau_3}\right) - \frac{K_\beta T_x}{m_{\text{eff}}}\right). \tag{6}$$

Here it is necessary to explain the term "anisotropy of pressure" as applied to a one-dimensional gas-dynamic model. Anile and Pennisi [2] studied an extended multidimensional hydrodynamic model in which the heat flux Q is a sought function, and the pressure is anisotropic. In [2], the extended hydrodynamic model is used to obtain the Fourier law for closure of the gas-dynamic model [in the case of the one-dimensional model, the Fourier law has the form (6)]. The gas-dynamic model with the Fourier law (6) describes the charge transport in semiconductors more adequately than the gas-dynamic model with the Fourier law

$$Q = -5K_\beta^2 \tau_3 n T T_x/(2m_{\text{eff}}), \tag{7}$$

that is derived directly from the Boltzmann equation ignoring the anisotropy of pressure [1].

We consider an n^+–n–n^+ ballistic diode consisting of three regions with different doping densities: n^+-region, n-region, and n^+-region. The doping density is $N(x) = N^+$ in the n^+-region and $N(x) = N$ in n-region. Within the framework of the model from [2], the electron flow in the (n^+–n–n^+) ballistic diode is described by the stationary forms of Eqs. (2)–(4), the Poisson's equation (5), and the Fourier law (6). At the ends of the diode, we impose the following boundary conditions [1]:

$$n = N^+, \quad T = T_0 \quad \text{for} \quad x = 0, \qquad x = l; \tag{8}$$

$$\Phi = \frac{K_\beta T_0}{e} \ln \frac{N^+}{n_i} \quad \text{for} \quad x = 0, \qquad \Phi = \frac{K_\beta T_0}{e} \ln \frac{N^+}{n_i} + V_b \quad \text{for} \quad x = l/ \tag{9}$$

Here l is the width of the (n^+–n–n^+) diode, n_i is the natural electron concentration, and V_b is the bias voltage in the diode.

We seek the electron flow in the (n^+–n–n^+) ballistic diode for $t \to \infty$ as the limit of the solution of Eqs. (2)–(6) subject to boundary conditions (8) and (9) and a certain specified initial condition at the initial time $t = 0$.

For simplicity, we convert to dimensionless quantities:

$$x' = \frac{x}{l}, \qquad t' = \frac{C_0 t}{l}, \qquad n' = \frac{n}{N^+}, \qquad v' = \frac{v}{C_0}, \qquad T' = \frac{T}{T_0},$$
$$Q' = \frac{Q}{m_{\text{eff}} C_0^3 N^+}, \qquad \Phi' = \frac{e\Phi}{K_\beta T_0}, \qquad E' = \frac{elE}{K_\beta T_0}, \tag{10}$$

where $C_0^2 = K_\beta T_0 / m_{\text{eff}}$. Below, the primes at dimensionless physical variables are omitted.

Equation (5) in the dimensionless quantities (10) takes the form

$$\Phi_{xx} = \beta(n - \rho(x)), \tag{11}$$

where $\beta = e^2 l^2 N^+ / (\varepsilon_s K_\beta T_0)$, $\rho(x) = N(x)/N^+$ is a piecewise-constant function: $\rho(x) = 1$ at $0 \leqslant x \leqslant l_+$, $1 - l_+ \leqslant x \leqslant 1$ and $\rho(x) = \delta$ at $l_+ < x < 1 - l_+$, where l_+ is the width of the n^+-region, and δ is the ratio of the doping density $N(x)$ in the n-region to the value of $N(x)$ in the n^+-region ($\delta = N/N^+$, $0 < \delta < 1$). Boundary conditions (9) can be written as

$$\Phi = \Phi_0 \quad \text{for} \quad x = 0, \qquad \Phi = \Phi_0 + \hat{V}_b \quad \text{for} \quad x = 1, \tag{12}$$

where $\Phi_0 = \ln(N^+/n_i)$ and $\hat{V}_b = eV_b/(K_\beta T_0)$.

Treating Eq. (11) as an ordinary differential equation for the unknown function Φ with boundary conditions (12), we obtain

$$\Phi = \Phi_0 + \hat{V}_b x + \beta(x-1)\int_0^x \zeta(n - \rho(\zeta))\, d\zeta - \beta x \int_x^1 (1-\zeta)(n - \rho(\zeta))\, d\zeta. \tag{13}$$

Differentiating (13) with respect to x, we have

$$E = -\hat{V}_b - \beta \int_0^x (n - \rho(\zeta))\, d\zeta + \beta \int_0^1 (1-\zeta)(n - \rho(\zeta))\, d\zeta. \tag{14}$$

Thus, it is assumed that in the problem of a n^+-n-n^+ ballistic diode in Eqs. (3), (4), the electric intensity E is a specified function of the electron density n and the space variable x.

In view of this, we formulate a mixed problem whose solution in the limit $t \to \infty$ describes the electron flow in the (n^+-n-n^+) ballistic diode. For $t \to \infty$, we seek a stationary solution of the system

$$\boldsymbol{U}_t + \boldsymbol{J}_x = (\boldsymbol{G}T_x)_x + \boldsymbol{F}, \tag{15}$$

that satisfies the boundary conditions

$$n = 1, \quad w = (m^2 + 3)/2 \quad \text{for} \quad x = 0, \quad x = 1 \tag{16}$$

under the specified initial condition

$$\boldsymbol{U}\big|_{t=0} = \boldsymbol{U}_0(x). \tag{17}$$

Here

$$\boldsymbol{U} = \begin{pmatrix} n \\ m \\ w \end{pmatrix}, \qquad \boldsymbol{J} = \boldsymbol{J}(\boldsymbol{U}) = \begin{pmatrix} m \\ 2(w + m^2/n)/3 \\ m(m^2/n + 5\tau_3(2w - m^2/n)/(3\tau_1))/(2n) \end{pmatrix},$$

$$\boldsymbol{F} = \boldsymbol{F}(E, \boldsymbol{U}) = \begin{pmatrix} 0 \\ -nE - m/\tau_1 \\ -mE - (w - 3n/2)/\tau_2 \end{pmatrix}, \quad m = nv, \quad w = n(v^2 + 3T)/2,$$

$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{U}) = \begin{pmatrix} 0 \\ 0 \\ 5nT\tau_3/2 \end{pmatrix}, \qquad T = (2w - m^2/n)/(3n).$$

With allowance for transformation to the dimensionless quantities (10), system (15) is a vector form of Eqs. (2)–(4), and boundary conditions (16) are obtained from boundary conditions (8).

After transformation to the dimensionless quantities, the relaxation times τ_α take the form

$$\tau_\alpha = \hat{\tau}\Big\{a_\alpha + b_\alpha\Big(\frac{w}{n} - 1\Big) + c_\alpha \exp\Big[-d_\alpha\Big(\frac{w}{n} - 1\Big)\Big]\Big\} \qquad (\alpha = 1,\ 2,\ 3), \tag{18}$$

where $\hat{\tau} = (C_0/l)\cdot 10^{-12}$ sec. With allowance for (14), it is assumed that the right term $\boldsymbol{F}$ on the right side of system (15) is a function of x and $\boldsymbol{U}$ [$\boldsymbol{F} = \boldsymbol{F}(x, \boldsymbol{U})$]. Thus, system (15) relates only components of the vector $\boldsymbol{U}$, i.e., as noted above, the hydrodynamic model (2)–(6) can be written in the form of system (1).

We note that the value of the electric potential on the left boundary Φ_0 does not influence the solution of the mixed problem (15)–(17). From (14) it follows that among the parameters included in boundary conditions (9), only the bias voltage V_b exerts an influence on the solution of the mixed problem (15)–(17).

Difference Model. It is known that in solutions of nonlinear systems of conservation laws there can be strong discontinuities even at smooth initial data. Therefore, it is not improbable that the solution of the problem of an (n^+–n–n^+) ballistic diode has discontinuities. Thus, the solution of system (15) should be understood in a generalized sense.

The vector function $\boldsymbol{U} = \boldsymbol{U}(t, x)$ is a generalized solution of system (15) if for any rectangle $(\alpha, \beta) \times (a, b)$, the vector function $\boldsymbol{U}(t, x)$ is a solution of the integral equation

$$\int_a^b \boldsymbol{U}(\beta, x)\,dx - \int_a^b \boldsymbol{U}(\alpha, x)\,dx + \int_\alpha^\beta \boldsymbol{J}(\boldsymbol{U}(t, b))\,dt - \int_\alpha^\beta \boldsymbol{J}(\boldsymbol{U}(t, a))\,dt$$

$$= \int_\alpha^\beta \boldsymbol{G}T_x(t, b)\,dt - \int_\alpha^\beta \boldsymbol{G}T_x(t, a)\,dt + \int_a^b \int_\alpha^\beta \boldsymbol{F}(x, \boldsymbol{U}(t, x))\,dt\,dx. \tag{19}$$

Equation (19) describes solutions of system (15) with discontinuous physical variables, in particular, with possible discontinuities in the distributions of the electron density n and the electron velocity v.

In the region $D = \{(t, x) | t \geqslant 0,\ 0 \leqslant x \leqslant 1\}$, we introduce the grid $D^\Delta_{h_k} = \{(t_i, x_k) | i = 0, 1, \ldots;\ k = \overline{0, K}\}$, where $t_i = i\Delta$, $x_0 = 0$, $x_k = x_{k-1} + h_k$, $x_K = 1$, Δ is the step in time t, and h_k is the step of the space variable x between the nodes (t_i, x_{k-1}) and (t_i, x_k) of the grid.

We approximate (15) by the conservative difference scheme

$$\boldsymbol{U}_k^{i+1} = \boldsymbol{U}_k^i - \frac{2\Delta}{h_{k+1} + h_k}(\boldsymbol{J}^i_{k+1/2} - \boldsymbol{J}^i_{k-1/2})$$

$$+ \frac{2\Delta}{h_{k+1} + h_k}\Big(\boldsymbol{G}^i_{k+1/2}\frac{\xi T_k^{i+1}}{h_{k+1}} - \boldsymbol{G}^i_{k-1/2}\frac{\xi T_{k-1}^{i+1}}{h_k}\Big) + \Delta \boldsymbol{F}(\boldsymbol{U}^i_k, E^i_k). \tag{20}$$

Here

$$\boldsymbol{J}^i_{k+1/2} = ((\min(0, \lambda^3_{k+1/2}) - \min(0, \lambda^1_{k+1/2}))\boldsymbol{J}^i_{k+1} + (\max(0, \lambda^3_{k+1/2}) - \max(0, \lambda^1_{k+1/2}))\boldsymbol{J}^i_k$$

$$-\frac{1}{2}(\lambda^3_{k+1/2}|\lambda^1_{k+1/2}| - \lambda^1_{k+1/2}|\lambda^3_{k+1/2}|)\xi \boldsymbol{U}^i_k)/(\lambda^3_{k+1/2} - \lambda^1_{k+1/2}),$$

$$E^i_0 = -\hat{V}_b + \beta\Big\{\sum_{k=1}^K \frac{h_k}{2}((1 - x_k)n^i_k + (1 - x_{k-1})n^i_{k-1}) - l_+ - (1 - 2l_+)\frac{\delta}{2}\Big\},$$

$$E^i_k = E^i_{k-1} + \beta h_k(\rho_k - (n^i_k + n^i_{k-1})/2),$$

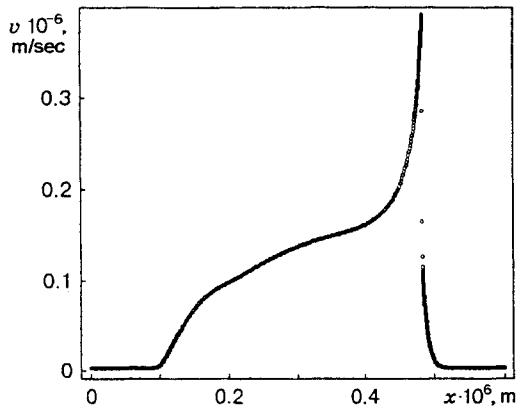

Fig. 1

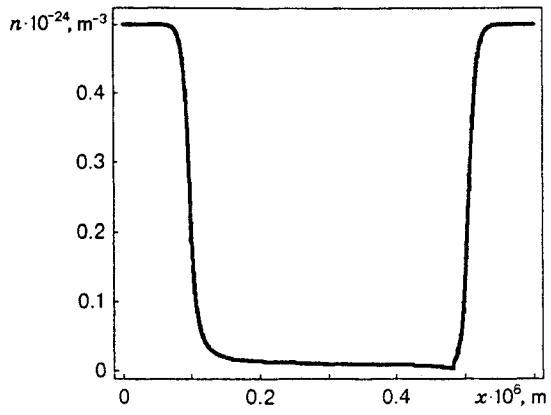

Fig. 2

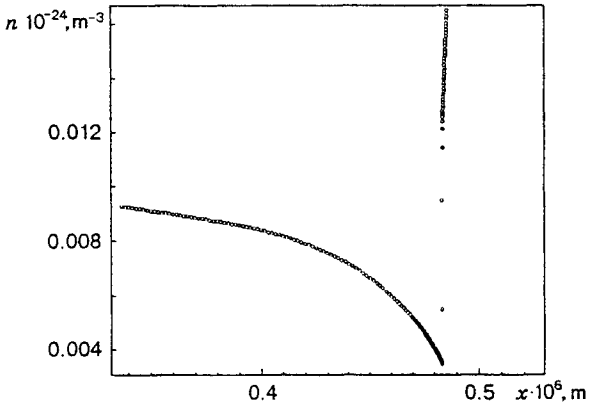

Fig. 3

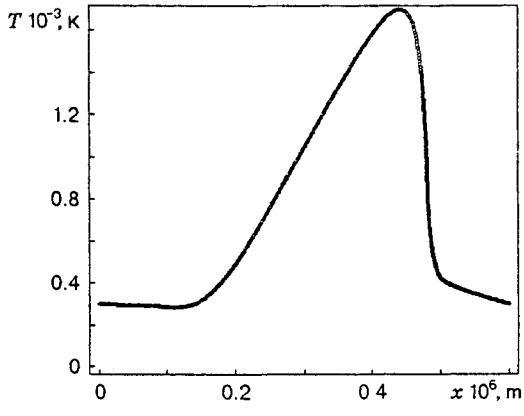

Fig. 4

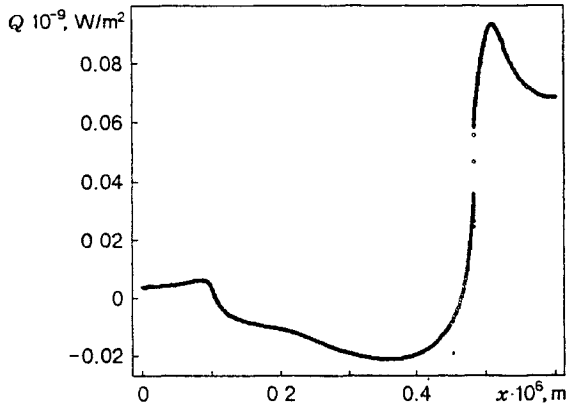

Fig. 5

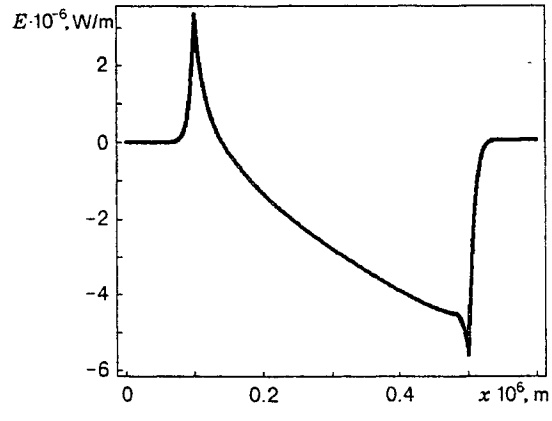

Fig. 6

$G^i_{k+1/2} = G((U^i_{k+1} + U^i_k)/2)$, $J^i_k = J(U^i_k)$, $T^i_k = T(U^i_k)$, $\lambda^1_{k+1/2}$ is the least eigenvalue and $\lambda^3_{k+1/2}$ is the largest eigenvalue of the matrix $A_{k+1/2} = A((U^i_{k+1} + U^i_k)/2)$, $A(U) = \partial J/\partial U$ is the Jacobi matrix, U^i_k are the values of the solution of the scheme (20) at the node (t_i, x_k) of the grid $D^{\Delta}_{h_k}$, $\rho_k = \rho(x_k)$, $\xi = \psi - I$ is a difference operator, I is an identical operator, ψ is a translation operator, and $\psi U^i_k = U^i_{k+1}$. The eigenvalues $\lambda^j_{k+1/2}$ of the matrix $A_{k+1/2}$ can be found from the general formulas for roots of the third-order polynomial. The characteristic equation $\det(A(U) - \lambda I) = 0$ has the form

$$y^3 + \frac{5}{3}v\left(\omega - 1 + \frac{3}{2}æT\right)y^2 - \frac{5}{3}T(\omega + æv^2)y - \frac{5}{2}æ vT^2 = 0, \tag{21}$$

where $y = v - \lambda$, $\omega = \tau_3/\tau_1$, $æ = (\tau_1\gamma_3 - \tau_3\gamma_1)/\tau_1^2$, and $\gamma_\alpha = \hat{\tau}(b_\alpha - c_\alpha d_\alpha \exp[-d_\alpha(w/n - 1)])$. Since it is difficult to obtain an explicit formula for the roots λ^j of polynomial (21), it is suggested that the numerical fluxes $J^i_{k+1/2}$ from [5] be used. They can be obtained without knowledge of the eigenvectors of the Jacobi matrix $A(U)$. The recurrence formulas for E^i_k are obtained from (14) by replacing the integrals by approximate values using the trapezoid rule.

The scheme (20) is semi-implicit and it approximates (15) with first-order accuracy. As shown by numerical experiments, for the present scheme to be stable, it is necessary that the step in time Δ be proportional to the step of the space variable $h = \min_k h_k$, i.e., $\Delta/h = \text{const}$. We note that to ensure stability in explicit schemes, it is necessary that the relation $\Delta/h^2 = \text{const}$ hold. The scheme (20) is economical, i.e., the number of operations required to find the grid function in a new time layer is proportional to the number of nodes of the grid $D^{\Delta}_{h_k}$ in one time layer. In addition, because the scheme (20) is conservative, its solution converges to the generalized solution of system (15), i.e., to the solution of Eq. (19).

Results of Numerical Experiments. Numerical experiments were performed for the following values of the physical parameters. The effective electron mass m_{eff} has a correction factor $m_r = 0.26$. The width of the $(n^+\text{-}n\text{-}n^+)$ diode is $l = 6 \cdot 10^{-7}$ m and the width of the n^+-region is $l_+ = 10^{-7}$ m. The doping density is $N(x) = 5 \cdot 10^{23}$ m^{-3} in the n^+-region and $N(x) = 2 \cdot 10^{21}$ m^{-3} in the n region. The temperature of the molecular lattice of the semiconductor is $T_0 = 300$ K. The bias voltage is $V_b = 1$ V. The relaxation times τ_1, τ_2, and τ_3 determined in (18) have the constants

$$\begin{aligned} &a_1 = 0.1153, \quad b_1 = -0.0068, \quad c_1 = 0.4988, \quad d_1 = 1.5137,\\ &a_2 = 0.4076, \quad b_2 = 0.0075, \quad c_2 = 3.1546, \quad d_2 = 1.4833,\\ &a_3 = 0.077, \quad b_3 = -0.0033, \quad c_3 = 0.2879, \quad d_3 = 1.0053. \end{aligned}$$

The numerical experiments showed that the greatest errors in the numerical solution arise near $(n^+\text{-}n)$ transitions. In view of this, the grid $D^{\Delta}_{h_k}$ was made finer in the $(n^+\text{-}n)$ transition regions and in the shock-wave region. The numerical experiment was conducted on the grid $D^{\Delta}_{h_k}$ with the steps

$$\begin{gathered} h_k = \alpha h, \qquad k = 1, \ldots, \tilde{K};\\ h_k = \beta h - \gamma(k - \tilde{K} - 1), \qquad k = \tilde{K} + 1, \ldots, 2\tilde{K};\\ h_k = h, \qquad k = 2\tilde{K} + 1, \ldots, 2(K_+ - \tilde{K});\\ h_k = h + \gamma(k - 2K_+ + 2\tilde{K} - 1), \qquad k = 2K_+ - 2\tilde{K} + 1, \ldots, 2K_+ - \tilde{K};\\ h_k = \alpha h, \qquad k = 2K_+ - \tilde{K} + 1, \ldots, 2K_+ + 5\tilde{K};\\ h_k = \beta h - \gamma(k - 2K_+ - 5\tilde{K} - 1), \qquad k = 2K_+ + 5\tilde{K} + 1, \ldots, 2K_+ + 6\tilde{K};\\ h_k = h, \qquad k = 2K_+ + 6\tilde{K} + 1, \ldots, 4K_+ + 2\tilde{K};\\ h_k = h + \gamma(k - 4K_+ - 2\tilde{K} - 1), \qquad k = 4K_+ + 2\tilde{K} + 1, \ldots, 4K_+ + 3\tilde{K};\\ h_k = \alpha h, \qquad k = 4K_+ + 3\tilde{K} + 1, \ldots, K. \end{gathered}$$

Here $\beta = \alpha - 1$, $\gamma = (\beta - 1)h/(\tilde{K} - 1)$, $K = 4(K_+ + \tilde{K})$, $K_+ = (2 + \alpha/2)\tilde{K}$, and $h = 1/(12\alpha\tilde{K})$. The

parameters α and $\tilde{K}$ had the values $\alpha = 30$ and $\tilde{K} = 30$ and the number of partitions was $K = 2160$. The grid $D^{\Delta}_{h_k}$ was constructed so that its nodes were at points of the $(n^+\text{-}n)$ transitions.

The distribution of the electron velocity v is given in Fig. 1. A strong discontinuity is observed before the right $(n^+\text{-}n)$ transition. The distribution of the electron density n is given in Figs. 2 and 3, and Fig. 3 illustrates the presence of a strong discontinuity in the density distribution n. Thus, a stationary shock wave is observed in the $(n^+\text{-}n\text{-}n^+)$ ballistic diode. The distribution of the electron temperature T is given in Fig. 4 and the distribution of the specific heat flux Q is shown in Fig. 5. The values of Q_k are determined from the discrete form of Eq. (6) with $(T_x)_k = s_k \min(|\xi T_k|/h_{k+1}, |\xi T_{k-1}|/h_k)$, where $s_k = \operatorname{sign}(\xi T_k)$ if $|\xi T_k| \leqslant |\xi T_{k-1}|$, and, otherwise, $s_k = \operatorname{sign}(\xi T_{k-1})$. Figure 6 gives the distribution of the electric intensity E determined from (14) by replacing the integrals by approximate values using the trapezoid rule.

Conclusion. The numerical solution given in Figs. 1–6 is qualitatively different from the numerical solution of the problem of an $(n^+\text{-}n\text{-}n^+)$ ballistic diode within the framework of the gas-dynamic model with the Fourier law (7) ignoring the anisotropy of pressure, which was obtained, for example, in [1, 3] for the same physical parameters. The results of [1, 3] indicate that in the ballistic diode, the electron density n and electron velocity v are continuous despite the characteristic peak of the velocity v before the right $(n^+\text{-}n)$ transition. [It should be noted that in [3], as in the present paper, the numerical solution of the problem of a $(n^+\text{-}n\text{-}n^+)$ ballistic diode was obtained using an iterative method.]

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