NUMERICAL INVESTIGATION OF FORMATION OF INHOMOGENEOUS DIFFUSION STRUCTURES IN NONLINEAR IONIZATION – RECOMBINATION KINETIC PROCESSES

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UDC 538.56

Electron and ion transfer in a low-temperature plasma and a semiconductor plasma in some conditions involves the formation of distinctly inhomogeneous structures. A possible reason for this process, which is investigated numerically in this paper, is the nonlinearity in the ambipolar diffusion equation due to three-particle electron recombination.

In the isothermic ambipolar diffusion approximation $[(|N_e - N_i|)/N_e \ll 1]$ the equations of ionization–recombination kinetics for unsteady electron (e) and ion (i) transfer have the form [1]

$$\frac{\partial N_e}{\partial t} - \frac{\mu_i D_e + \mu_e D_i}{\mu_e + \mu_i}\frac{\partial^2 N_e}{\partial x^2} = \alpha_i N N_e - \alpha_r N_e^3,$$
$$\frac{\partial N_e}{\partial t} + \frac{\mu_i D_e + \mu_e D_i}{D_e - D_i}\frac{\partial (N_e E_x)}{\partial x} = \alpha_i N N_e - \alpha_r N_e^3. \tag{1}$$

In dimensionless form Eqs. (1) are

$$\frac{\partial u}{\partial \tau} - \frac{\partial^2 u}{\partial \xi^2} = \varphi (u - u^3); \tag{2}$$

$$\frac{\partial u}{\partial \tau} + \frac{\varphi - 1}{\varphi}\frac{\partial (uF)}{\partial \xi} = \varphi (u - u^3), \tag{3}$$

where

$$u = N_e/N_e(\infty);\ \tau = t/t^*;\ \xi = x/x^*;\ F = E_x/E_x^*;\quad \varphi = \frac{\mu_e + \mu_i}{2\mu_i};$$
$$t^* = \left(\frac{2\mu_i \alpha_r N_e^2(\infty)}{\mu_e + \mu_i}\right)^{-1};\quad x^* = \left(\frac{D_e}{\alpha_r N_e^2(\infty)}\right)^{1/2};\quad E_x^* = \left(\frac{e x^*}{kT}\right)^{-1},$$

and the other symbols have their usual meaning [2]. We note only that u is the electron concentration N_e, expressed relative to $N_e(\infty)$, corresponding to the established homogeneous steady state, when ionization is completely compensated by recombination: $N_e(\infty) = (\alpha_i/\alpha_r)^{1/2}$.

Since we will be considering only the problem of concentration distribution, Dirichlet boundary conditions

$$u(\xi = 0,\ \tau) = u_0 = \text{const},\ u(\xi = \delta,\ \tau) = u_\delta = \text{const}$$

on the finite interval (0, δ) will be imposed for Eq. (2).

The initial conditions

$$u(\xi,\ \tau = 0) = u^*(\xi),$$

for which we use a linear, rectangular, or sinusoidal distribution, are coupled with the boundary conditions

$$u^*(\xi = 0) = u_0,\ u^*(\xi = \delta) = u_\delta$$

to simplify the calculation algorithm.

To obtain the specific relations $u(\xi, \tau)$ we used the scalar pivot method [3] with a nonlinearity approximation on the right-hand side of Eq. (2) by the quasilinearization method [4], when the value of u^3 on the i-th step for the coordinate and the (j+1)-th step for time is given by the expression

$$(u_i^{j+1})^3 = (u_i^j)^3 + 3(u_i^j)^2(u_i^{j+1} - u_i^j).$$

The condition for convergence of the scalar pivot method for this problem is fulfilled when the time step $\theta < 0.5$. In the calculations the value of θ was taken as 0.05 and it was assumed that the solution becomes stabilized when $\tau \to \infty$, if the condition

Kiev. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 2, pp. 74–78, March–April, 1981. Original article submitted January 30, 1980.

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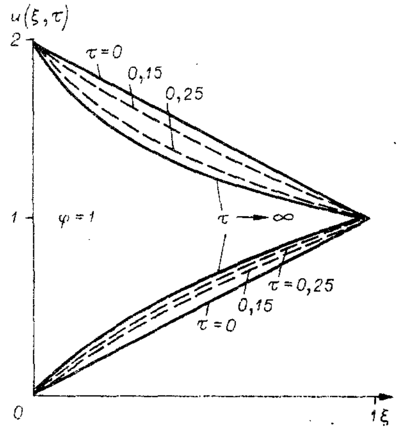

Fig. 1

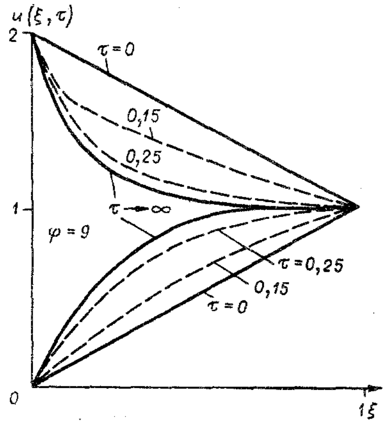

Fig. 2

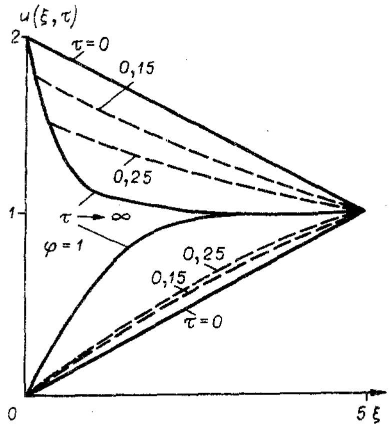

Fig. 3

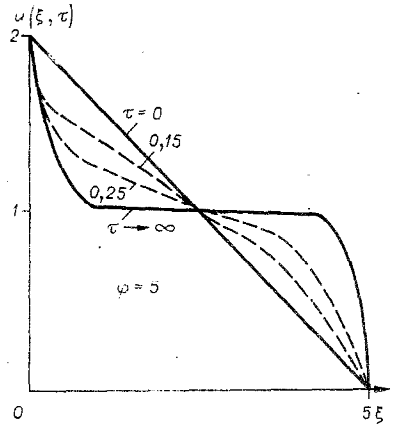

Fig. 4

$$\max_i |u_i^{j+1} - u_i^j| < 10^{-3}$$

is fulfilled.

Numerical calculations of the establishment regimes showed that the spatial distribution of electron concentration is distinctly inhomogeneous, and the form of the established distribution does not depend so much on the form of the initial distribution, that is mainly determined by the boundary values. We first consider the establishment process for a linear initial distribution (Figs. 1-4). Here and in the other figures the continuous lines represent the initial ($\tau = 0$) and steady ($\tau \to \infty$) states, while the dashed lines represent the intermediate states.

The presented relations show that a distinctly inhomogeneous electron concentration distribution is formed with the passage of time. The degree of inhomogeneity, a possible quantitative index of which is the maximum

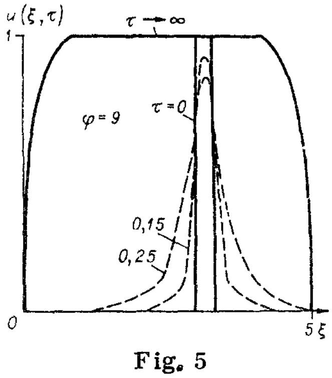

Fig. 5

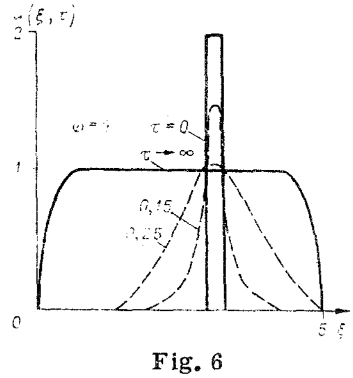

Fig. 6

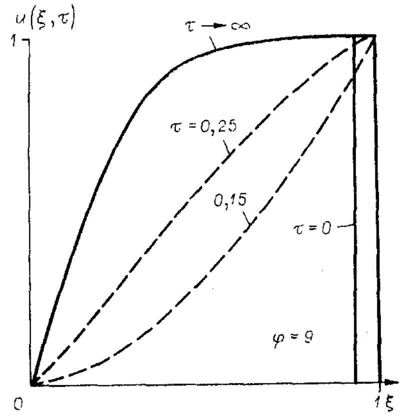

Fig. 7

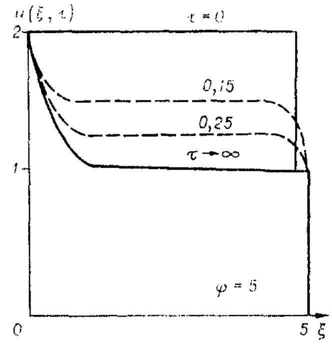

Fig. 8

modulus of the derivative $\partial u/\partial\xi$, increases monotonically with increase in the parameter φ (Fig. 2) and width of the segment (Fig. 3), if δ lies in the interval ~ (0-5). A further increase in δ has practically no effect on the slope of the function $u(\xi, \tau \to \infty)$.

It is essential to note that the degree of inhomogeneity of the electron concentration profile when $u_0 = 1$ is greater, the more u_0 differs from the steady homogeneous state, and reaches a maximum when the steady state is attained.

For the steady state, following [2], we can obtain the relation

$$\partial u/\partial\xi = \sqrt{(\varphi/2)}(1 - u^2) + A, \quad A = \text{const.} \tag{4}$$

If we bear in mind the data presented in Figs. 1-3, and put $\partial u/\partial\xi\,(u = 1) \equiv 0$, then $A = 0$ and the maximum modulus of the derivative $\partial u/d\xi$, which is attained at point $\xi = 0$ due to the smoothness of the function $u(\xi, \tau \to \infty)$, increases with increase in u_0 when $u_0 > 1$ and with reduction of u_0 when $u_0 < 1$.

Similar properties characterize the establishment of the steady inhomogeneous profile from the initial linear profile, if a value $u_0 > 1$ is assigned at one end of the interval, and $u_\delta < 1$ at the other (Fig. 4). In the center of the interval a plateau is formed, the width of which is greater, the greater the parameter φ and the interval width δ.

Another series of calculations was carried out for problems of spreading of a narrow plasma layer of thickness h ($h \ll \delta$) with zero boundary conditions at points $\xi = 0$ and $\xi = \delta$ (Figs. 5, 6). As Figs. 5 and 6 show, the narrow rectangular electron concentration distribution is transformed into a convex profile, and during stabilization there may be oscillations at the maximum of the function $u(\xi, \tau)$, if $\max u^*(\xi) < 1$. When $\max u^*(\xi) > 1$ the maximum of the distribution $u(\xi, \tau)$ tends monotonically to unity.

Using Eq. (4), we can establish the relation between the maxima of the function $u(\xi, \tau \to \infty)$ and the values of the derivatives at points $\xi = 0$ and $\xi = \delta$:

$$\frac{\partial u}{\partial\xi}(\xi = 0, \tau \to \infty) = \frac{\partial u}{\partial\xi}(\xi = \delta, \tau \to \infty) = \sqrt{\frac{\varphi}{2}}\, u^2_{\max}(\xi, \tau \to \infty),$$

from which follows the symmetry of the particle flow on the walls in the steady state.

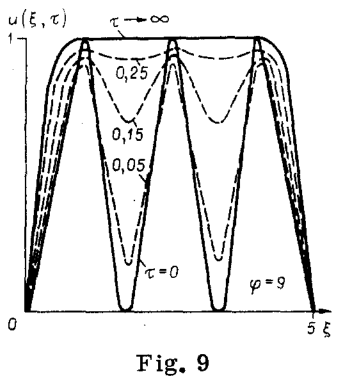

Fig. 9

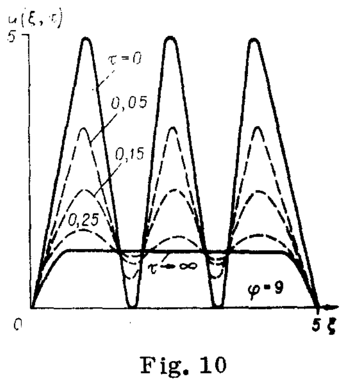

Fig. 10

Spreading regimes for some other types of rectangular distribution are shown in Figs. 7 and 8. It is apparent that the steady state for such regimes coincides with those shown in Figs. 1-4.

It follows from the data discussed above that the inhomogeneous distribution of electrons where they are localized close to the ends of the interval $(0, \delta)$ when u_0 or $u_\delta > 1$ and delocalized at the same points when u_0 or $u_\delta < 1$ begins to appear at the very start of the establishment process, and increases steadily towards the end of the transient process.

We also made a numerical investigation of the smoothing out of the electron concentration in a stratified inhomogeneous plasma (Figs. 9, 10). The results of the calculations indicated that the filling of the troughs is a monotonic process, irrespective of whether $\max u^*(\xi) \leq 1$ or $\max u^*(\xi) > 1$, and corresponds to the first stage of establishment of the convex concentration profile for the nonlinear chemical kinetic processes examined in [5]. As distinct from [5], however, no spatial oscillations are observed in the considered system, although when $\max u^*(\xi) \leq 1$ local oscillations at the peaks are possible (see Fig. 9). For establishment processes when $\max u^*(\xi) > 1$ there are no oscillations at the peaks.

We note in conclusion that the reason for the electron localization and delocalization effects in the considered diffusion processes, like the reason for formation of inhomogeneous thermal structures in media with nonlinear bulk absorption [6-9], is the change in the mechanisms of generation of charged particles when the sign of the source on the right-hand side of Eq. (2) is changed by passage across the boundary of the homogeneous steady state $u = 1$.

We express our thanks to N. Kh. Érkenov for valuable recommendations on the development of the algorithm of the numerical calculation.

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