MATHEMATICAL MODELING OF PLASMA IN A GLOW DISCHARGE OF SPHERICAL GEOMETRY

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UDC 537.525

The problem of determination of the parameters of a stationary glow discharge is considered in the general statement. The coupled system of nonlinear equations includes the balance equation with regard for diffusion processes for electrons and ions and the Poisson equation for the electric potential. The problem is considered in the spherical and – for comparison – planar geometries. The boundary conditions were determined by the electric current density at the boundaries of the discharge gap; the electron temperature was considered constant. The nonlinear coupled boundary-value problem is solved by using the method of continuation with respect to a parameter. The influence of diffusion processes and the geometry of the gas discharge on its properties are analyzed.

1. Introduction

The theory of gas-filled diodes represents one of the fundamental ones in the physics of gas discharges and low-temperature plasmas. At the same time, glow discharges are widely used in various technological processes related to a surface modification of constructional details and elements. Though the glow discharge is characterized with higher power losses in the discharge gap as compared to the arc one, it has a doubtless advantage concerning a possibility of the maximal localization of the technological action of a discharge in the anomalous mode on a treated surface. In this case, its effectiveness is reached locally due to the formation of the region of proper cathode potential drop between the plasma and the surface of a detail [1].

A characteristic peculiarity of low-pressure low-temperature plasma is the difference between the electron temperature T_e and that of a heavy component T_a. The principal role in the balance of charged particles is played by the processes of electron-impact ionization as well as diffusion processes that, together with the drift shift of charged particles under the action of an external field, determine the physical parameters of the discharge and the conditions of its existence. The characteristic temperature difference, $T_e \gg T_a$, also essentially influences the development of diffusion processes.

Considerable mathematical difficulties in the determination of parameters of gas-discharge plasma arising in the general statement with regard for the diffusion of charged particles compel to use a simplified statement of the problem. As a rule, the glow-discharge theory considers the cathode region in the planar geometry and the plasma of the positive column in the axisymmetric geometry as a practically independent region. As for the positive column region, with regard for the quasineutrality of plasma and the assumption $T_e(r) = \text{const}$, this essentially simplifies the system of equations reducing it to the equation of electron balance, where the determining role is played by their losses due to the diffusion to walls [2]. In spite of the mathematical simplicity of such an approach, it has a rather limited value, though allowing one to determine T_e and the relative radial distribution of the electron concentration $N_e(r)$. Indeed, in addition to the exclusion of the cathode region from the consideration, such a statement of the problem also excludes the possibility of both the quantitative estimation of the potential drop across the discharge gap and the determination of absolute values of N_e due to the uncertainty of the boundary conditions for the flows of charged particles, especially in the case of the current running under conditions of the accompanying gradient of N_e (which can take place in a nonplanar geometry).

The numerical calculations of plasma parameters were initiated by works [3,4]. Recently, a significant success has been achieved in this field [5–12]. However, the numerical modeling of processes mainly concerns either discharges with no regard for diffusion [3–5, 10–12] or short non-stationary discharges, where the positive column region is practically absent [6–9]. Not in the least place, this is related to the requirement of self-consistency of the discharge parameters, namely the correspondence between the specified currents and the potential drop across the discharge gap. In the case of the stationary coupled nonlinear boundary-value problem, it is extremely difficult to coordinate these parameters in the solution.

It is known [9] that, in glow discharges of the planar geometry, the role of diffusion processes becomes evident at pressures of 1 Torr and lower. It is the pressure region that is characteristic of the processes of surface modification in the glow discharge (0.01–1 Torr in [13]). The investigation of the role of diffusion processes in glow discharges on the basis of numerical modeling is related to the characteristic methodical problem conditioned by the so-called "mesh diffusion": it arises when using the difference schemes of calculations somewhat distorting the character of physical processes [5–9].

The influence of the spherical geometry on the character of processes in a glow discharge is hard to predict as compared to the planar one. In the former case, the densities of current, drift and diffusion flows decrease along the radius of the system, which creates additional gradients of the concentration of charges particles; respectively, the effectiveness of the ionization processes and the electric field distribution can change.

Thus, since the glow discharges with electrodes, whose geometry often is close to the spherical one, are widely used in technological processes [13], it is necessary to develop the corresponding methods for calculation of the physical and technological parameters of discharges just in the spherical geometry. In the present paper, the comparative determination of the parameters of stationary glow discharges of the spherical and planar geometries is performed.

2. Problem Statement and Solution Technique

Aiming at the modeling of one of the modes of experimental investigations [13], we consider that the discharge is maintained between two concentrically enclosed spheres; moreover, the surface of the internal sphere represents the cathode, whereas that of the external one – the anode. In the spherical coordinate system, the balance equation for the concentration of charged particles with regard for the symmetry of the problem has a form

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 J_e\right) - \alpha(E)|J_e| = 0, \qquad (1)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 J_i\right) - \alpha(E)|J_e| = 0, \qquad (2)$$

$$J_e = -\mu_e N_e E - D_e \frac{dN_e}{dr}, \qquad (3)$$

$$J_i = \mu_i N_i E - D_i \frac{dN_i}{dr}, \qquad (4)$$

where J_e and J_i stand for the densities of the electron and ion flows, respectively, ($J = e\,(J_i - J_e)$ is the electric current density in the discharge); N_e, N_i denote their concentrations; E is the electric field strength in the discharge; D_e, μ_e, D_i, and μ_i are the diffusion and mobility coefficients of electrons and ions, respectively; $\alpha(E)$ is the first Townsend coefficient.

In order to close the system of equations (1), (2), one should add the Poisson equation for the electrostatic potential to them,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\varphi}{dr}\right) = \frac{e}{\varepsilon_0}\left(N_e - N_i\right), \quad E = -\frac{d\varphi}{dr}, \qquad (5)$$

where e is the electron charge, and ε_0 is the dielectric constant.

The boundary conditions for problem (1), (2), (5) are as follows:

$$J_e = -\gamma J_i,\ eJ_e = \gamma J_K/(1+\gamma),\ \varphi = 0, \qquad (6)$$

$$J_i = 0,\ eJ_e = J_A,\ \varphi = V, \qquad (7)$$

at the cathode and the anode, respectively; here, J_K, J_A are the current densities at the cathode and the anode; γ denotes the coefficient of electron secondary emission from the cathode; and V is the voltage drop across the discharge gap.

The search for the solution of the coupled nonlinear boundary-value problem with nonlinear boundary conditions represents a rather complicated task from the viewpoint of computational mathematics. In addition, the existence conditions of stationary glow discharges critically depend on both the relation between the concentrations of charged particles and the electric field in the whole discharge gap. This fact imposes essential limitations on their initial approximations and the methods of linearization of the initial problem in the sense of the "physicity" of the approximation. The last circumstance practically requires to search for a self-consistent solution of the nonlinear boundary-value problem.

In order to find the solution of problem (1), (2), (5)–(7), the method of continuation of the solution with respect to a parameter [14] (the so-called quasilinearization method) was used. The search for the first approximation is performed in the assumption [3,4,9–12] that the role of diffusion is inessential and can be neglected. In this case, the relation for the electron and ion flows will include only the drift components:

$$J_e = \mu_e N_e E, \quad N_e = J_e/\mu_e E, \tag{8}$$

$$J_i = \mu_i N_i E, \quad N_i = J_i/\mu_i E. \tag{9}$$

In a similar manner, the equation for the electric potential will be reformulated for the electric field strength with regard for relations (8), (9):

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 E\right) = \frac{e}{\varepsilon_0}\left(\frac{J_i}{\mu_i E} - \frac{J_e}{\mu_e E}\right). \tag{10}$$

It is worth noting that the boundary-value problem (1), (2), (5)–(7) is formulated with respect to the electron and ion flows and represents a boundary-value problem for first-order equations. Its solution can exist only for a certain value of the parameter, which is presented here by the value of the electric field strength at one of the points of the boundary. The solution of the nonlinear boundary-value problem with differential first-order equations is found within the "shooting" method, by changing the value of the electric field strength at the anode. After solving the boundary-value problem for the flows, let's reformulate the initial problem (1), (2), (5)–(7) in accordance with the method of continuation of the solution with respect to a parameter with regard for the diffusion terms:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\left(-\mu_e N_e E - D_e\frac{dN_e}{dr}\right)\right) -$$

$$-\alpha(E)\left|-\mu_e N_e E - D_e\frac{dN_e}{dr}\right| = 0, \tag{11}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\left(\mu_i N_i E - D_i\frac{dN_i}{dr}\right)\right) -$$

$$-\alpha(E)\left|-\mu_e N_e E - D_e\frac{dN_e}{dr}\right| = 0, \tag{12}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 E\right) =$$

$$= \frac{e}{\varepsilon_0}\left(\frac{J_i}{\mu_i E} - \frac{J_e}{\mu_e E} - \lambda\left(\frac{D_i}{\mu_i E}\frac{dN_i}{dr} - \frac{D_e}{\mu_e E}\frac{dN_e}{dr}\right)\right), \tag{13}$$

where λ denotes some formal parameter of the method. Supposing that the drift component of the flows in the cathode region is much higher than the diffusion one due to a large absolute value of the electric field, the boundary conditions take the form

$$e\mu_i N_i E = J_K/(1+\gamma),$$

$$e\mu_e N_e E = \gamma J_K/(1+\gamma),\ \varphi = 0, \tag{14}$$

$$\mu_i N_i E - D_i\frac{dN_i}{dr} = 0,\ -\mu_e N_e E - D_e\frac{dN_e}{dr} = J_A/e,$$

$$\varphi = V \tag{15}$$

at the cathode and the anode, respectively. The boundary conditions for the electric potential are determined from the solution of problem (1), (2), (10) with respect to the flows. At the first step, the gradients of the electron and ion concentrations that appear in the Poisson equation (13) are determined, with the use of the found flows, from the solution of the following system of differential equations:

$$J_e = -\mu_e N_e E - D_e\frac{dN_e}{dr}, \tag{16}$$

$$J_i = \mu_i N_i E - D_i\frac{dN_i}{dr}, \tag{17}$$

with the initial conditions (14).

According to the method of continuation with respect to a parameter, we assume that the solution of the problem at $\lambda = 0$ is known. In the given case, it is the solution of problem (1), (2), (10) for the flows. At $\lambda = 1$, problem (11)–(15) is identical with the initial one (1), (2), (5)–(7). After differentiating with respect to the parameter, the nonlinear boundary-value problem (11)–(15) is presented in the form of a collection of linear boundary-value problems for the derivatives of the unknown functions with respect to the parameter λ. For their solution at each step, one uses the method of their reduction to a number of Cauchy problems that can be integrated with the help of the implicit Euler method of the second order of accuracy. After solving the linear boundary-value problems for the derivatives with respect to the parameter, the values of the unknown functions are found by means of the integration of the latter over λ.

In the case of solving the nonlinear coupled boundary-value problem (1)–(7), the method of continuation with respect to a parameter has certain

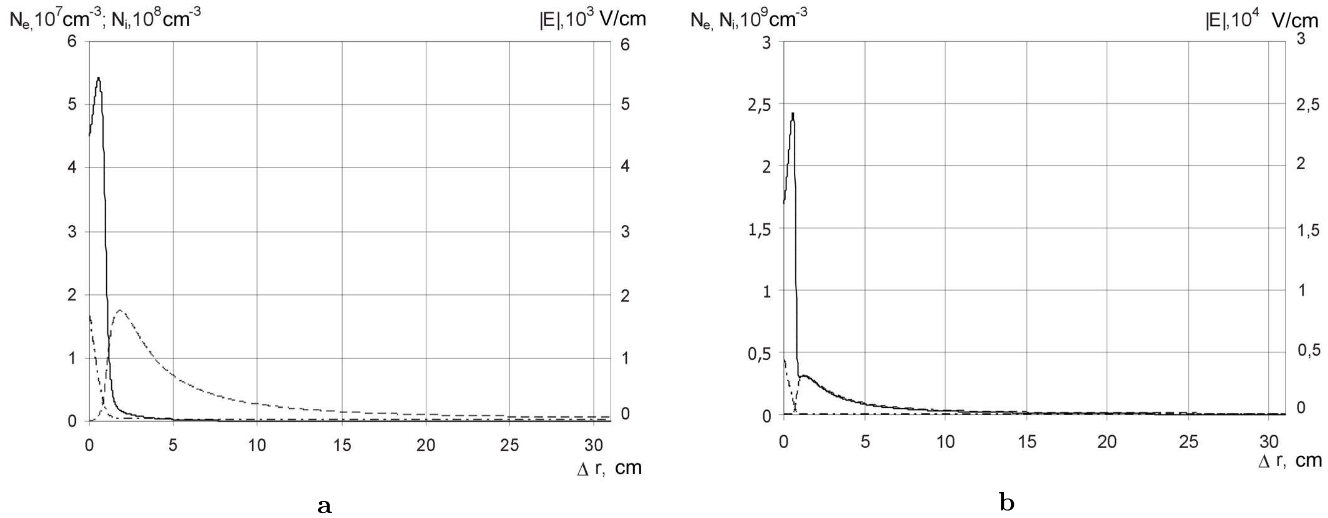

Fig. 1. Spatial distribution of the concentration of ions (solid curve), electrons (dashed curve) and the electric field strength (dash-dotted curve) in the spherical geometry ($r_K = 2$ cm): a – $I = 10^{-2}$ A, b – $I = 10^{-1}$ A

advantages as compared with the difference schemes proposed in [7]. First of all, it is the absence of the so-called "mesh diffusion," whose presence in difference schemes results from the approximation of differential operators by finite differences [6]. This fact allows us to estimate more correctly the influence of diffusion on the characteristics of a glow discharge. In addition, the change of the order of the method in difference schemes also conditions a change of the global matrix of the system of algebraic equations, which the initial boundary-value problem is reduced to. Thus, the only possible way to control the convergence of the process considered in works [6–10] is a change of the difference mesh length. At the same time, the method of reduction of the linearized boundary-value problem to the system of Cauchy problems gives, in our case, a possibility to regulate the accuracy of calculations not only changing the difference mesh length but also choosing the order of the scheme of integration of the Cauchy problems. The latter possibility can shorten (depending on the choice of the scheme) the time of calculations in the case of a permanent mesh in the process of successive approximations to the solution of the initial nonlinear boundary-value problem.

3. Analysis of Numerical Results

In the calculations for a glow discharge in the plasma-forming medium of molecular nitrogen, we assumed the following relation for the first Townsend coefficient [2,6,16]:

$$\alpha = 12p \exp\left(-342p/|E|\right), \ \text{cm}^{-1}, \tag{18}$$

where p is the pressure (Torr), E is the electric field strength (V/cm). The diffusion coefficients were determined as

$$D_e = \mu_e kT_e/e, \quad D_i = \mu_i kT_i/e, \tag{19}$$

(k is the Boltzmann constant) with the following values of the physical parameters [5]: $\mu_e = 4.4 \times 10^5 p^{-1}$ cm^2·Torr/(V·s), $\mu_i = 1.44 \times 10^3$ cm^2·Torr/(V·s), $T_i = T_a = 300$ K, $T_e = 11600$ K. The temperature T_e was estimated using the technique presented in [2] with regard for the spherical geometry of the discharge region [15]. The coefficient of electron secondary emission from the cathode amounts to $\gamma = 0.02$ in the same way as in [2–4].

We considered the following values of parameters of the problem in the spherical geometry: $p = 1.1$ Torr, $r_K = 2$ cm, $R = 33$ cm are the radii of the internal (cathode) and the external (anode) spheres of the gas-filled diode, respectively. The calculations were performed for two values of the discharge current intensity $I = 10^{-2}$ and $I = 10^{-1}$ A (respectively, the current density $J(r) = I/4\pi r^2$ at the cathode amounted to 0.2 and 2 mA/cm^2, which fits the interval of calculations carried out in [3,7]).

Some results of calculations are presented in Figs. 1–4. For the convenience of comparison with the case of planar geometry, the distances from the cathode Δr are marked out at the abscissa axes of the figures. In

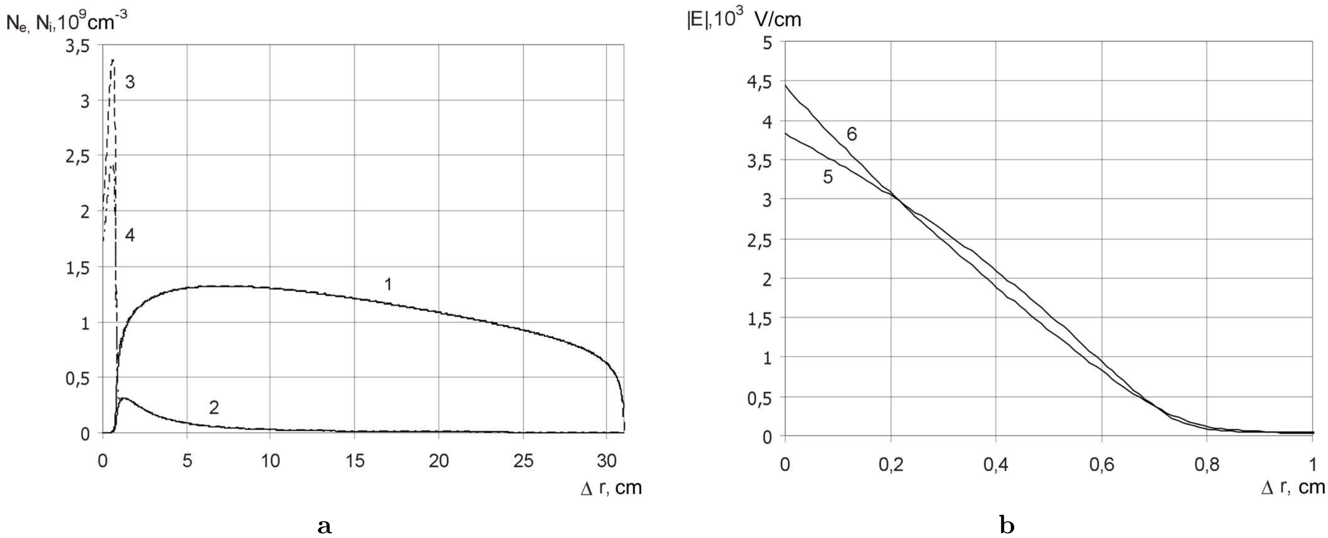

Fig. 2. Spatial distribution of the concentration of electrons (*1, 2*), ions (*3, 4*) and the electric field strength in the neighborhood of the cathode potential drop (*5, 6*) in the "planar" geometry (r_K = 100 cm) (*1, 3, 5*) and in the spherical geometry (r_K = 2 cm) (*2, 4, 6*) ($I = 10^{-1}$A)

particular, Fig. 1 gives the radial distribution of the ion and electron concentrations as well as the electric field strength in a spherical diode for the mentioned values of discharge currents. Here, we assume that the diffusion in the discharge gap can be neglected (that is, it is the solution of problem (1), (2), (10)).

The distributions of the electron and ion concentrations with regard for diffusion processes were also determined. However, for the chosen pressure $p = 1.1$ Torr, the additional influence of diffusion on the drift electron flow doesn't exceed 10% even in the narrow cathode region of the maximal gradient of $N_e(r)$; beyond its limits, it doesn't exceed 1%. For ions, the influence of diffusion can be neglected. That's why their influence isn't reflected in the mentioned figure. In what follows, we characterize only the changes of the voltage across the discharge gap conditioned by diffusion processes (see Fig. 3). It is worth noting that the role of diffusion must be more essential in the case of a decrease of the pressure in the spherical diode.

It is worth noting that we neglected the diffusion flows in the cathode layer in the boundary conditions (14) at the cathode. On the other hand, as follows from the presented dependences, the latter can influence the distribution of the concentrations of charged particles in the boundary region of the cathode layer and the positive column.

In order to separate the influence of the geometry of a discharge gap on the properties of the glow discharge, we also performed calculations for the planar geometry. This case is characterized with the same system of initial equations, but the cathode radius is assumed to be r_K = 100 cm. This point minimizes the role of the electrode curvature at least as concerns the processes in the cathode region. From the results presented in Fig. 2,*a*, it follows that the latter case is characterized by a considerable increase of the concentration of charged particles in the cathode region and especially in the positive column. It is essential that, in both cases, an approximately linear dependence of the electric field in the cathode region on the spatial coordinate (Fig. 2,*b*) is conserved, which well corresponds to the basic assumptions of the classic theory of glow discharges [2].

Respectively, the "planar" geometry of the glow discharge is characterized by a lower potential drop across the discharge gap than that in the case of the spherical geometry (Fig. 3). In contrast, taking into account the diffusion processes results in the increase of the potential drop across the discharge gap as follows from the same figure by the example of the discharge current of 10^{-2} A. However, in the case of the planar and spherical geometries, the cathode potential drop is not essentially changed in contrast to the field distribution in the positive column region, whereas the role of diffusion processes is mainly reduced to a change of the cathode drop.

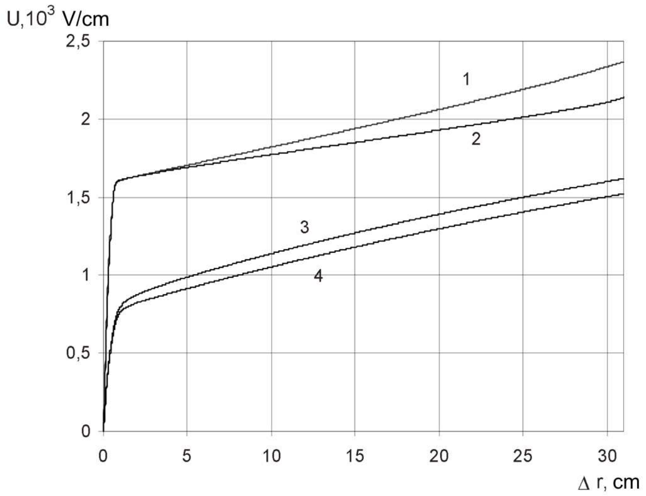

Fig. 3. Spatial distribution of the potential drop across a discharge gap in the spherical geometry ($r_K = 2$ cm, $I = 10^{-1}$A) (*1*), in the "planar" geometry ($r_K = 100$ cm, $I = 10^{-1}$A) (*2*), in the spherical geometry with regard for diffusion (*3*), and in the spherical geometry with no regard for diffusion (*4*) ($r_K = 2$ cm, $I = 10^{-2}$A)

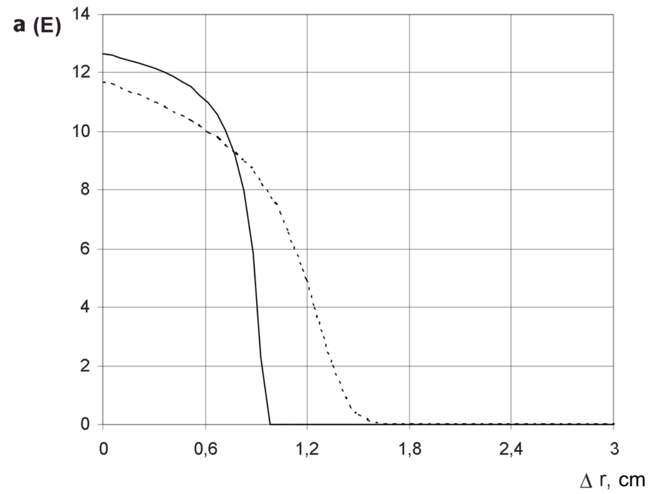

Fig. 4. Spatial distribution of the first Townsend coefficient in the neighborhood of the cathode potential drop in the spherical geometry: solid curve – $I = 10^{-1}$ A, dashed curve – $I = 10^{-2}$ A; $r_K = 2$ cm

For the sake of illustration, Fig. 4 also shows the distributions of the first Townsend coefficient. It is worth noting that, beyond the limits of the cathode layer, its values fall practically up to zero. This is valid for the modes with regard for diffusion and without it. In the positive column region, the influence of ionization with regard for the Townsend coefficient becomes much lower than that of the volume ionization in the positive column plasma [2,16] for the considered values of the electron temperature, which can condition a partial distortion of the real picture of the field and concentration distributions.

Attention is attracted to the appearance of a local maximum in the ion distribution (Fig. 1,*a* and 2,*a*). It also corresponds to the results of work [10], where it was explained by a considerable nonlinearity of the first Townsend coefficient (see Fig. 4).

The results obtained in this paper concerning the observed behavior of the low-temperature plasma of a glow discharge and the variation of the voltage across the electrodes depending on the discharge current agree with the basic tendencies of experimental investigations [13,15]. At the same time, the authors didn't pose the problem to achieve the quantitative coincidence between the experimental results and those of numerical modeling at the given stage, because, as for the parameter most convenient for comparison – discharge voltage, they are determined in one way or another by the choice of the Townsend and the secondary ion-electron emission coefficients. The investigation of the validity of choosing these parameters wasn't a task of this work.

4. Conclusions

The problem of determination of the parameters of a stationary glow discharge is considered in the general statement. The influence of the discharge geometry and diffusion processes on the physical parameters of the discharge is investigated. The obtained numerical results testify to the influence of diffusion on the characteristics of the discharge mainly in the region of the cathode layer. However, the investigations are performed at such a pressure of the plasma-forming gas (1.1 Torr), where its influence on diffusion processes isn't too essential. First of all, it is done from the considerations of the separation of the influence of the geometry of a glow discharge on its parameters. That's why the problem was considered in the spherical geometry and its solution was compared with that for the planar geometry. The results of modeling of gas discharges obtained in the given paper can be used for the estimates of real technological processes running in setups for the ion-plasma surface treatment in glow discharge modes.

In conclusion, it is worth noting certain cautions. The main disadvantage of the described approach to the mathematical modeling of a glow discharge of the spherical geometry lies in the fact that, despite the mathematical complexity of the given problem, its solution is, however, of semiempirical character. Indeed, the temperature is determined here with the use of the assumption $T_e(r)$ = const which is not quite evident in the spherical geometry and is formally borrowed from a similar problem for a long cylindrical tube. In addition, the requirement of self-consistency of the magnitudes of the discharge current and the voltage drop across the discharge gap results in the underspecification of the boundary-value problem with respect to either the currents or the voltage. This uncertainty can be overcome by "fitting" one of the boundary conditions from certain physical considerations, in other words, supposing the initial boundary-value problem dependent on a parameter presented, for example, by a boundary value of some of the unknown functions. After that, one should "optimize" the latter at each step of the solution in the sense of the strict fulfillment of other boundary conditions.

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Translated from Ukrainian by H.G. Kalyuzhna

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ПЛАЗМИ ЖЕВРІЮЧОГО РОЗРЯДУ В СФЕРИЧНІЙ ГЕОМЕТРІЇ

В.А. Жовтянський, Ю.І. Лелюх

Р е з ю м е

Розглянуто задачу визначення параметрів стаціонарного жевріючого розряду в загальній постановці. Зв'язана система нелінійних рівнянь включає рівняння балансу з урахуванням дифузійних процесів для електронів та йонів, а також рівняння Пуассона для електричного потенціалу. Задачу розглянуто у сферичній та, для порівняння, в плоскій геометрії. Граничні умови визначалися густиною електричного струму на межах розрядного проміжку; електронна температура вважалася сталою. Нелінійна зв'язана гранична задача розв'язувалась методом продовження за параметром. Проаналізовано вплив дифузійних процесів та геометрії газового розряду на його властивості.