NUMERICAL SIMULATION OF THE STRUCTURE OF A SPHERICAL GLOW DISCHARGE

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The problem of determination of parameters of a stationary glow discharge is considered in the general formulation. A system of coupled nonlinear equations includes the balance equation with regard for diffusion processes for electrons and ions, as well as the Poisson equation for the electric potential. The nonlinear boundary-value problem is solved by the modified parameter continuation method. A special attention is paid to the study of the dependence of discharge characteristics on the diffusion processes and constants in the first Townsend coefficient. The electron temperature is considered constant.

1. Introduction

The theory of a gas-filled diode is one of the fundamental ones in the physics of gas discharge and low-temperature plasma [1,2]. At the same time, glow discharges are widely used in various technological processes related to the modification of surfaces of structural elements and units. Their undeniable advantage is the possibility of the maximum localization of the technological action of an anomalous glow discharge on the surface of a processed metal product. This is reached by means of using the latter as a cathode of the anomalous glow discharge. In this case, the efficiency of a technological effect is achieved locally due to the formation of a near-cathode potential drop region between plasma and a treated product [3].

It is considered [4, 5] that the role of diffusion processes in a glow discharge becomes significant at pressures of 1 Torr and lower. This pressure region is typical of the processes of surface modification (0.1–1 Torr in [6]). However, the study of diffusion processes on the basis of numerical modeling encounters the specific methodical difficulty caused by the so-called "mesh diffusion" that appears if using finite difference mesh methods that somewhat distort the character of physical processes [4, 5, 7]. That is why, in the previous work [8], a stationary solution of the problem in a spherical region was searched within the method of reducing the linearized boundary-value problem to the system of Cauchy problems, which allowed us to significantly minimize the above-mentioned difficulty. A drawback of the approach used in [8] was the way of allowing for the effect of diffusion processes that was calculated in the form of perturbations of the diffusionless solution, which imposed significant constraints on the current density and the discharge gap length.

Developing the previous results in [9, 10], the present work substantiates the possibility of modeling a glow discharge with the use of the modified parameter continuation method that has no mentioned drawbacks and allows one to solve one-dimensional boundary-value problems of calculating the plasma parameters in the most general formulation. This approach is used for the detailed investigation of diffusion processes in nitrogen and argon plasmas of a spherical glow discharge. These gases are widely used in technological processes of surface modification.

2. Problem Statement and Solution Technique

Aiming at the simulation of one of the modes of experimental study [6], we suppose that a discharge is maintained between two concentric spheres. Moreover, the surface of the inner sphere is the cathode and that of the outer one is the anode. In the spherical system of coordinates, the balance equation for the concentrations of charged particles and the Poisson equation with re-

gard for the problem symmetry have the form

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 J_e\right) - \alpha(E) J_e = 0, \quad J_e = -\mu_e N_e E - D_e \frac{dN_e}{dr}, \tag{1}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 J_i\right) + \alpha(E) J_e = 0, \quad J_i = -\mu_i N_i E - D_i \frac{dN_i}{dr}, \tag{2}$$

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

$$E = -\frac{d\varphi}{dr}, \quad J = e\left(J_i + J_e\right), \tag{3}$$

where J_e and J_i are the electron and ion flux densities, respectively, N_e and N_i are their concentrations, J and E are the current density and the electric field intensity in the discharge, respectively, D_e, μ_e, D_i, μ_i are the diffusion and mobility coefficients of electrons and ions, $\alpha(E)$ is the first Townsend coefficient, e is the electron charge, and ε_0 is the dielectric constant. The representation of the current density in (3) that takes the absolute values of the electron and ion fluxes into account is chosen conventionally. It is determined by the convenience of a mathematical model of the process and is often used in the glow discharge physics [2, 11, 12].

The boundary conditions for problem (1)–(3) at the cathode and the anode are formulated as [7]

$$J_e = \gamma J_i, \quad eJ_e = \gamma J_K/(1+\gamma), \quad \varphi = 0, \tag{4}$$

$$N_i = 0, \quad eJ_e = J_A, \quad dN_e/dr = 0, \tag{5}$$

respectively, where J_K and J_A are the cathode and anode current densities, and γ is the coefficient of secondary emission of electrons from the cathode.

The nonlinear boundary-value problem (1)–(5) is solved, by using the modified parameter continuation method. Its essence is as follows. The initial approximation is found by solving the nonlinear Cauchy problem with regard for boundary condition (5) at the anode. After that, the residuals are determined as the difference between the obtained solution of the Cauchy problem at the cathode and the values of boundary conditions (4). On the following stage, the boundary condition (4) at the cathode is derived as the sum of the solution of the Cauchy problem and the residual multiplied by some formal parameter λ. At $\lambda = 0$, the problem is equivalent to the nonlinear Cauchy problem, whereas, at $\lambda = 1$, it coincides with the initial boundary-value problem (1)–(5). Thus, the boundary condition (4) takes the following form at each step of the parameter continuation:

$$eJ_i = eJ_i^0 + \lambda\left(J_K/(1+\gamma) - eJ_i^0\right),$$

$$eJ_e = eJ_e^0 + \lambda\left(\gamma J_K/(1+\gamma) - eJ_e^0\right), \quad \varphi = \varphi^0 - \lambda\varphi^0. \tag{6}$$

Here, the symbol "0" corresponds to the boundary values of the Cauchy problem solution at the cathode. After that, the interval [0, 1] for λ is divided into L sufficiently small parts according to the general ideas of the theory of parametric boundary problems [13]. The solution of the nonlinear boundary-value problem (1)–(3), (5), (6) is found for each value of the parameter λ by the linearization. The solution of the problem for the previous value of λ is used as the first approximation at each step.

In order to study the effect of diffusion processes, we also solved the problem in the diffusionless formulation with zero diffusion coefficients in initial equations (1)–(3).

The linearized boundary-value problems were solved, by applying the method of reducing to the system of Cauchy problems at each iteration. The latter are integrated with the help of a modified implicit Euler technique of the third order of accuracy [13]. At each parameter step, the process of successive approximations was considered to converge if the sum of the differences of the unknowns in a region with the norm l_2 was smaller than some preassigned quantity δ.

3. Analysis of Numerical Results

In the calculations performed for a glow discharge in the plasma-forming medium of molecular nitrogen, we assumed the following relation for the first Townsend coefficient [2, 4, 12]:

$$\alpha = Ap\exp\left(-Bp/|E|\right), \ \mathrm{cm}^{-1} \tag{7a,b}$$

where p is the pressure (Torr), and E is the electric field intensity (V/cm). The constants in expression (7) were chosen as A=12 and 8.8 (cm Torr)$^{-1}$, B = 342 and 275 V/(cm Torr) for cases a and b, respectively. By analogy, the calculations for the argon medium were performed for two representations of the first Townsend coefficient [2, 12]:

$$\alpha = 12p\exp\left(-\frac{180p}{|E|}\right), \ \mathrm{cm}^{-1} \tag{8a}$$

and

$$\alpha = 29.2p \exp\left(-26,6\sqrt{\frac{p}{|E|}}\right),\ \text{cm}^{-1}. \qquad (8b)$$

The diffusion coefficients were determined as $D_e = \mu_e kT_e/e$, $D_i = \mu_i kT_i/e$, where k is the Boltzmann constant, $\mu_e = 4.4 \times 10^5 p^{-1}$, $\mu_i = 1.44 \times 10^3 p^{-1}$ cm^2·Torr/(V·s) for nitrogen [4] and $\mu_e = 3.3 \times 10^5 p^{-1}$, $\mu_i = 1.16 \times 10^3 p^{-1}$ cm^2·Torr/(V·s) for argon, $T_i = T_a$ =300 K, and T_e =11600 K. The coefficient of secondary emission of electrons from the cathode $\gamma = 0.1$ [4, 5, 7].

The following values of the physical parameters of the problem were assumed: $p = 1.1$ Torr, $r_K = 1.5$ cm, and R = (11.5–25) cm, which stood for the inner (cathode) and outer (anode) radii of the spherical gas-filled diode, respectively. The electric current density at the cathode amounted to (4–35) mA/cm^2($J(r) = I/4\pi r^2$), which corresponded to the discharge current equal to (0.012–1) A at the chosen cathode radius.

Some results of calculations are depicted in Figs. 1–4. In order to simplify the comparison of the results obtained for different configurations of the discharge gap and different cathode radii, we give the distances from the cathode Δr at the X-axes. Figure 1 shows the radial distribution of the ion and electron concentrations for the nitrogen (Fig. 1,*a*) and argon (Fig. 1,*b*) media with and without consideration of the diffusion processes for various values of the cathode current density J_K = (4–35) mA/cm^2. Both for molecular nitrogen and for argon, the influence of diffusion prevails as compared to the drift component in a narrow region of the positive column that neighbors the near-cathode layer. It is significant that the role of diffusion processes grows with increase in the current density. In this region, one also observes a local minimum of the absolute value of the electric field intensity (Fig. 2,*b*). The role of diffusion processes in the transient region between the near-cathode layer and the positive column practically results in a decrease of the local maximum of the concentrations of charged particles necessary to conduct the specified current. Thus, the diffusion processes play an important role for the conduction of the electric current in the region of the smallest electric field, where the drift component of the velocity in the form accepted in the work becomes minimal.

The above-mentioned problem of the "mesh" or "computational" diffusion appears due to the finite-difference approximation of derivatives of the product of the unknown functions [4,5]. According to the cited works, the coefficient of "computational" diffusion corresponds

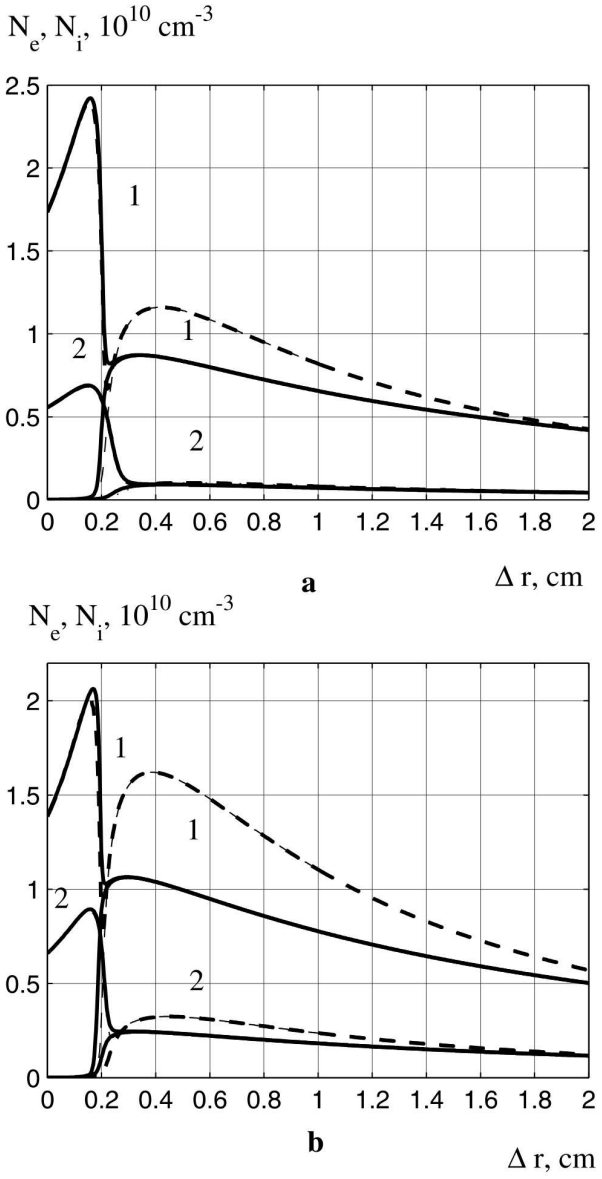

Fig. 1. Space distribution of the ion and electron concentrations in the near-cathode region with (solid curve) and without (dashed curve) taking the diffusion into account in nitrogen (*a*) and argon (*b*); (r_K = 1.5 cm, Δr = 10 cm, γ = 0.1, α in the form (7a) (*a*) and (8a) (*b*)): *1* – J_K = 4 mA/cm^2; *2* – J_K = 35 (*a*), 17 (*b*) mA/cm^2

to the substitution of the temperatures in the expression $D = \mu T$ by a half of the potential difference at one computation step h at a given point of the mesh,

$$D_c = \mu\Delta\varphi/2 = \mu Eh/2,$$

where μ is the mobility of some sort of charged particles and the temperature is measured in units of eV. A similar

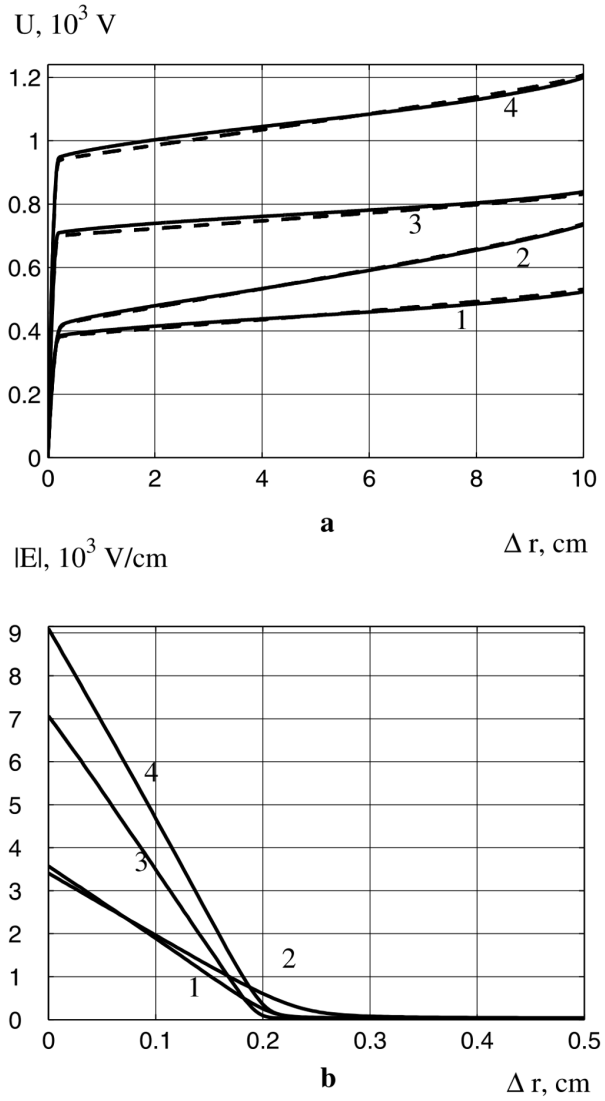

Fig. 2. Space distribution of the potential drop across the discharge gap (a) and the electric field intensity in the neighborhood of the cathode potential drop (b) with (solid curve) and without (dashed curve) taking the diffusion into account; (r_K = 1.5 cm, Δr = 10 cm, γ = 0.1 *1* – argon, J_K = 4 mA/cm^2, α in the form (8,*a*); *2* – nitrogen, J_K = 4 mA/cm^2, α in the form (7,*a*); *3* – argon, J_K = 17.5 mA/cm^2, α in the form (7,*a*); *4* – nitrogen, J_K = 35 mA/cm^2, α in the form (8,*a*)

problem arises in the case of finite difference mesh methods, where derivatives of different orders are approximated with the use of schemes with different numbers of points. It is worth noting that the technique of solving the one-dimensional boundary-value problems based on the reduction of the initial boundary-value problem to a sequence of Cauchy problems considerably minimizes the possibility of the appearance of the discussed difficulty due to the representation of the system of differential equations in the form of a first-order system. There is no doubt that any discretization of a problem generates an error of the discretization method together with the computational error caused by the computer capacity. However, the possibility of the appearance of additional "non-physical" terms in this problem formulation is absent for linear problems. The linearization of nonlinear boundary-value problems with respect to the unknown functions generates terms of this kind, but they are compensated by considering the solution from the previous approximation at each iteration. The latter procedure is actually a renormalization that follows from the linearization process itself. It is also worth emphasizing the advantage of the Runge–Kutta methods as compared with the mesh ones that consists in the independence of the chosen integration step on the mesh size and the possibility to apply integration schemes of various orders of accuracy without changing the mesh size.

Taking the diffusion processes into account practically does not result in a growth of the near-cathode potential drop in spite of a decrease of the concentrations of charged particles (Fig. 1 and 2,*a*), and it has no effect on the electric field intensity (Fig. 2,*b*). The difference of the potential drops across the discharge gap with and without considering the diffusion processes amounts to at most one per cent. In order to finally solve the problem of stability of the proposed method, we performed model calculations with the artificially reduced coefficients of electron and ion diffusion equal to 0.1 and 0.01 of the real values. The results of the numerical experiment testify to the rapid approach of the solution with decreased coefficients to the diffusionless one. As follows from a similar modeling described in [4], this would be impossible in the presence of "mesh diffusion", because the value of the latter would remain invariable at the insignificant (within one per cent) difference of the near-cathode potential drop.

It is worth emphasizing the effect of diffusion processes on the stability of the computational process. In particular, no stable solution was obtained for the diffusionless problem at the cathode current density J_K = 17 mA/cm^2 for argon and 35 mA/cm^2 for nitrogen and the 25-cm discharge gap. With increase in the cathode current density, the calculation process of the diffusionless problem lost stability even for discharge gaps less than 10 cm. At the same time, the problem with regard for diffusion processes was solved without significant computational burden at cathode current densities of 80 mA/cm^2

and discharge gap lengths exceeding 30 cm. The latter fact can also testify to the stabilizing role of diffusion processes in real low-pressure discharges.

Figure 3 presents the concentrations of charged particles as functions of the absolute values of the constants and the form of the functional dependence of the first Townsend coefficient in formulas (7) and (8). The increase of the absolute values of the constants in the expression for the first Townsend coefficient (7) results in the growth of the maximum values of $N_i(r)$ in the region of the near-cathode potential drop (Fig. 3,*a*). At the same time, the absolute values of the concentrations $N_e(r)$ and$N_i(r)$ decrease in the positive column region. Similar results (Fig. 3,*b*) can be observed by the example of argon in the case of the substitution of the functional dependence of the first Townsend coefficient by that falling more slowly ($1/|E|$ by $1/\sqrt{|E|}$) (8a, b), though the absolute value of $N_i(r)$ in the near-cathode layer is larger for coefficient (8a). It is worth noting that, as was checked separately, the near-cathode potential drop at the specified form of α is mainly determined by the constant A in formula (7). Indeed, taking into account that the maximum values of the electric field intensity are reached in the neighborhood of the cathode, the exponent at the cathode is minimal and therefore its value in (7) and (8) will tend to 1 under the infinite increase of the electric field intensity.

A decrease of the absolute value of the constants in the first Townsend coefficient will also result in the growth of the potential drop across the discharge gap (Fig. 4,*a*, curves *1* and *2*) and the widening of the near-cathode layer (Fig. 4,*b*). At the same time, the replacement of the functional dependence of the given coefficient by a smoother one gives rise to a decrease of the potential drop and a narrowing of the near-cathode region (Fig. 4, curves *3* and *4*).

The presented formulation of the problem of modeling a glow discharge corresponds to the conditions of the experimental study described in [6]. At the same time, a more detailed consideration is required to study the validity of the central symmetry condition for discharges of this type, as well as the hypothesis that the total current density decreases in the inverse proportion to the squared radius at the discharge gap length considering the presence of anode spots registered experimentally. That is why the results obtained from the numerical modeling allow one to estimate the effect of such factors as diffusion processes and the representation of the Townsend coefficient on the physical characteristics of the discharge. However, the numerical modeling carried out for this formulation of the problem yields a

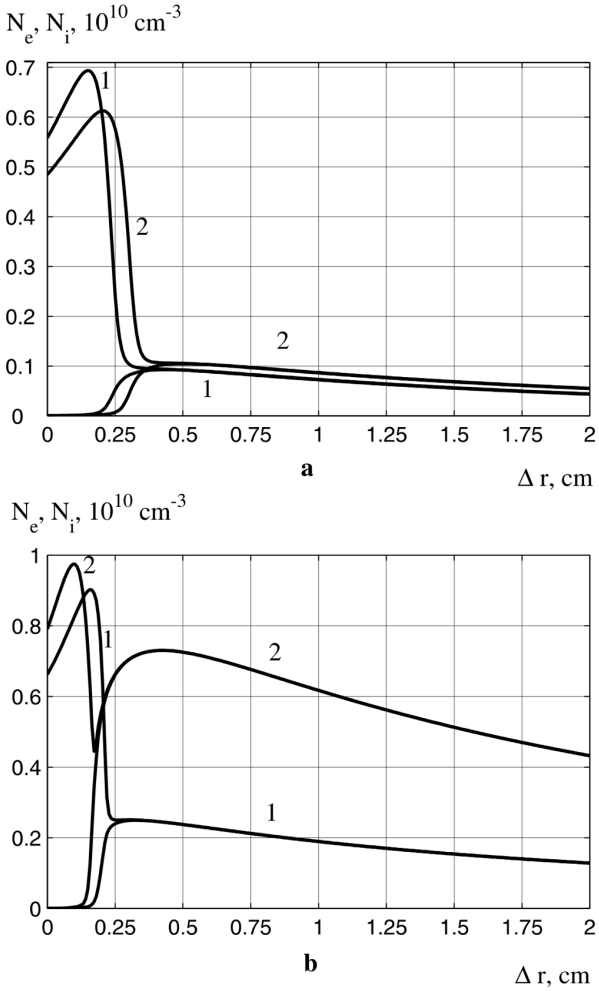

Fig. 3. Space distribution of the charged-particle concentration in the near-cathode region for various first Townsend coefficients in nitrogen (*a*) and in argon (*b*); (r_K =1.5 cm, Δr = 23.5 cm, γ= 0.1, J_K=4 mA/cm^2): *1* – α in the form (12,*a*) (*a*) and (8,*a*) (*b*); *2* – α in the form (12,*b*) (*a*) and (8,*b*) (*b*)

persistent overstatement of the potential drop across the discharge gap as compared with experimental data for the studied current and pressure ranges. It is also worth noting that, as follows from the above results, the potential drop is determined by the choice of the Townsend and secondary ion-electron emission coefficients [9]. The study of the validity of choosing these parameters was beyond the scope of this work. In addition, a separate consideration may be also required to analyze the problem of allowance for the so-called nonlocal effects caused by the fact that, at low pressures of the plasma-forming gas, the electric field can significantly change along the

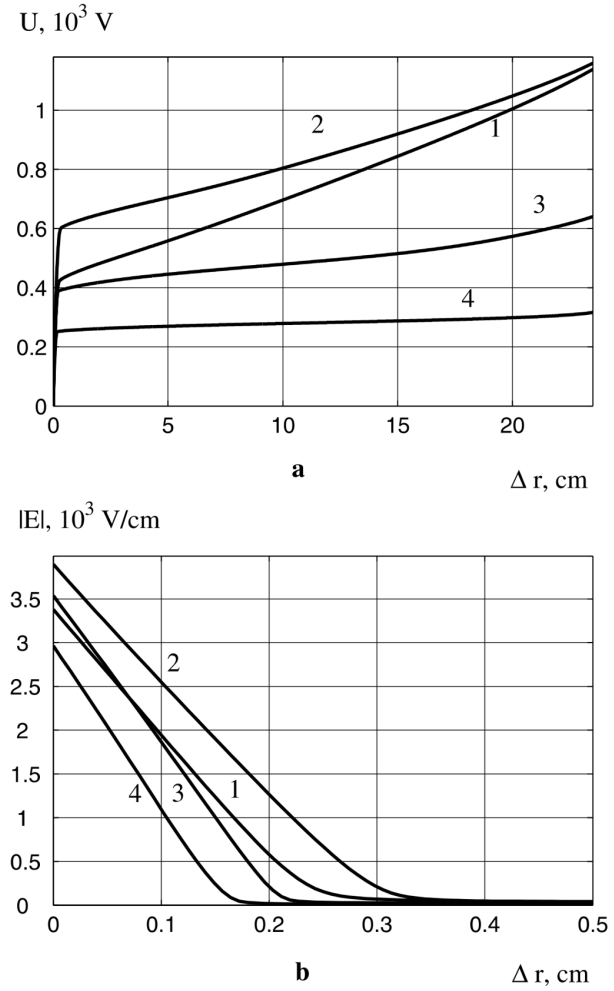

Fig. 4. Space distribution of the potential drop across the discharge gap (*a*) and the electric field intensity in the neighborhood of the cathode potential drop (*b*) for various first Townsend coefficients; (r_K =1.5 cm, Δr = 23.5 cm, γ= 0.1, J_K=4 mA/cm^2): *1* – nitrogen, α in the form (7,*a*); *2* – nitrogen, α in the form (7,*b*); *3* – argon, α in the form (8,*a*); *4* – argon, α in the form (8,*b*)

electron free path in the near-cathode discharge region [14].

It is also worth noting that the electron temperature was determined from the assumption $T_e(r) = \text{const}$, which is not quite evident for a spherical region. However, the allowance for the radial distribution of the electron temperature would complicate the initial system of equations. The aim of this work (besides the verification of the method of solving the connected nonlinear boundary-value problems of the glow discharge theory) was to study the effect of diffusion processes and the form of the functional dependence of the first Townsend coefficient on the physical parameters of the glow discharge. That is why, according to the logics of the cycle of works [4, 5, 7], we firstly decided to restrict ourselves to the assumption about its constancy, which corresponds to the absolute majority of publications devoted to this question. In what follows, it is expedient to investigate the influence of temperature effects on the characteristics of the glow discharge by means of including the energy equation to the system of coupled nonlinear equations.

4. Conclusions

We have considered the problem of determination of the parameters of a stationary glow discharge in the general formulation. The effect of diffusion processes on the physical parameters of the discharge is investigated. The obtained numerical results testify to the influence of the diffusion on the discharge characteristics in the positive column region that neighbors the near-cathode layer. It is established that the diffusion processes have a decisive effect on the stabilization of a discharge in the hydrodynamic approximation. The glow discharge characteristics at different values of the constants and functional dependences in the first Townsend coefficient are compared. In the author's opinion, the substantiation of the form of the functional dependence of the constants in the first Townsend coefficient must be the object of experimental studies due to their significant influence on the discharge parameters.

It is worth noting that the parameter continuation method of solving nonlinear boundary-value problems, which is proposed in the work on the basis of the general ideas of the parametric equation theory [13], allows one to make simple generalizations in the case of ordinary differential equations, by choosing the schemes and directions of the parameter motion in the course of solving the problem. This fact gives a possibility to optimize the computational process and to automatically correct its stability while solving the problem. It is worth emphasizing that, as was noted in the process of numerical modeling, this method manifests elements of the asymptotic convergence even in the simplest form without choosing the direction of the parameter integration [13].

The results of modeling the stationary gas discharges obtained in this work can be used to estimate the role of separate processes in real technologies of ion-plasma surface treatment in the glow discharge modes in argon and argon-nitrogen mixtures, as well as their optimization.

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ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ СТРУКТУРИ ЖЕВРІЮЧОГО РОЗРЯДУ СФЕРИЧНОЇ ФОРМИ

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 іонів, а також рівняння Пуассона для електричного потенціалу. Нелінійна гранична задача розв'язується модифікованим методом продовження за параметром. Особливу увагу приділено дослідженню впливу дифузійних процесів, а також залежності розв'язку від сталих першого коефіцієнта Таунсенда на характеристики розряду. Електронна температура вважається сталою.