ELECTRICAL DIRECT CURRENT DISCHARGES IN AIR AT ATMOSPHERIC PRESSURE: THE EFFECT OF ELECTRODE HEATING ON THE DISCHARGE CHARACTERISTICS

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Microplasma discharges in air, at atmospheric pressure, are simulated using a one-dimensional (1D) hybrid physics model. The model includes charged and neutral species conservation with detailed gas-phase chemistry, a self-consistent solution of the electric field, electron and neutral gas temperatures, and an external circuit model. In addition, conjugate heat transfer in both the cathode and the anode is considered. Special attention is given to the conjugate heat transfer and its effects on the gas temperature and discharge characteristic predictions, such as the current–voltage characteristics (CVCs). A classical shape for the CVCs of a discharge is obtained, with all observable sections: a glow discharge, an abnormal glow discharge, and an arc. Dependences of the electrode surface temperatures on the discharge current density are obtained. For each point of the CVC, all basic parameters of the electrical discharge, including a temperature field in the electrode gap in the metal electrodes, are obtained.

1 Introduction

In the last few decades, atmospheric pressure discharges in the air have been the subject of much research. The interest has been motivated by a wide spectrum of possible technological applications, including surface treatment of various materials (e. g., biological tissues), coating deposition by thermal spraying, plasma-chemical technology [1–3], and chemical analysis [4]. For investigating and improving the overall performance of the devices based on discharges in the atmosphere, it is necessary to obtain an accurate understanding of the physical processes taking place. Of special interest are the stationary discharges of direct current (DC) — glow discharge and an arc — which, in view of their simplicity and ease of realization, are a touchstone for new ideas and diagnostics in the physics of gas-discharge plasma.

It is known that the existence of small interelectrode intervals (of the order of tenths of a millimeter) is necessary for the stability of a discharge at atmospheric pressure. This is the reason why such discharges are sometimes called microdischarges [4]. Various methods for controlling gas-discharge plasma for long interelectrode intervals have been developed in order to achieve stable direct current discharges. These include the laminar flow of gas [5, 6] and the creation of acoustic flows (streaming) in a discharge chamber [7, 8]. Microdischarges, as well as sufficiently extensive discharges with various control methods, are labour consuming and difficult for experimental diagnostics [9]. In such cases, the behavior and properties of the discharge are usually assessed according to CVCs. The qualitative behavior of CVCs is well known for a wide range of discharge currents, with clearly distinguishable sections corresponding to normal and abnormal glow discharges, to the transition of a glow discharge into an arc and to a direct arc discharge [10].

Numerical modeling methods in plasma physics are tools for researching the discharge of a DC at atmospheric pressure [11–13]. A comparison of experimental CVCs of discharges with those obtained by accurate modeling of physical processes is an important tool and can also supply data on discharges. Generally, when modeling electrical discharges, the electrode temperature is considered to be constant. However, under real conditions (even in the case of cooling), the temperature of the electrode surface in contact with the plasma differs from the given. This affects the temperature field in the interelectrode interval and, therefore, influences the density of the neutral particles, which leads to a change in the coefficients of the inelastic processes and also to a change in the distribution of the charged particles in the plasma. When the discharge current increases, moving along the discharge CVC curve from the abnormal glow discharge to the arc, the electrode temperatures grow significantly, particularly that of the cathode. This undoubtedly leads to an increase in thermionic emission from the cathode and affects the discharge characteristics.

Thus, the study of electrical microdischarges in atmospheric air, taking into account the self-consistent heating of electrodes induced by processes occurring in regions near to the electrodes and the flow of heat from the plasma, as well as the investigation of the effects of heated electrodes on the discharge characteristics, including its CVCs, are extremely important problems in modern physics and in the technology of gas-discharge processes [14].

The purpose of the present work is to model microdischarges in air at atmospheric pressure for a wide range of discharge currents, taking into account conjugate heat transfer between electrodes and discharge plasma.

2 Model Description

First, it is necessary to carry out a self-consistent calculation, including a description of the basic parameters of the electrical discharge and taking into account gas heating and a description of the temperature field in the metal electrodes. For this purpose, the calculation domain was divided into three subdomains: metal cathode, interelectrode space, and metal anode.

In the interelectrode domain, equations were solved describing a gas-discharge plasma, while in the cathode and anode domains, a heat balance equation was solved. At the boundary between the electrical discharge and the electrodes, the boundary conditions that describe the heating mechanisms of the electrode surfaces produced by processes occurring in the electrical discharge were set. The equations that describe each of the computational domains (plasma, cathode, and anode) and the corresponding boundary conditions are considered in the following.

2.1 Modeling the discharge domain

Air is a multicomponent molecular gas characterized by a vast set of elementary processes occurring on varied spatial and time scales. This is why the choice of a plasma-chemical model depends on the formulation

Set of plasma-chemical reactions

No.	Process	Reaction constant, k_j, cm^6s^{-1}
1	$e + O_2 \rightarrow 2e + O_2^+$	Convolution of EEDF with cross section
2	$e + 2O_2 \rightarrow O_2 + O_2^-$	$1.4 \cdot 10^{-29} \left(\frac{300}{T_e}\right) \exp\left(\frac{700(T_e - T_g)}{T_e T_g}\right)$
3	$e + O_2 + N_2 \rightarrow N_2 + O_2^-$	$1.07 \cdot 10^{-31} \left(\frac{300}{T_g}\right) \exp\left(\frac{1500(T_e - T_g)}{T_e T_g}\right)$
4	$e + O_2^+ \rightarrow O_2$	$2 \cdot 10^{-7} \left(\frac{300}{T_g}\right)^{1/2}$
5	$O_2 + O_2^- \rightarrow e + 2O_2$	$8.6 \cdot 10^{-10} \exp\left(-\frac{6030}{T_g}\right)\left(1 - \exp\left(-\frac{1570}{T_g}\right)\right)$
6	$O_2^+ + O_2^- \rightarrow 2O_2$	$2 \cdot 10^{-7} \left(\frac{300}{T_g}\right)^{1/2} \left(1 + 10^{-18} N \left(\frac{300}{T_g}\right)^2\right)$

of the problem. In this problem, to describe a classical DC electrical discharge, taking into account heating of the electrodes and their influence on the parameters of the discharge, a description of elementary processes can be considered in the context of the formation of positive and negative ions.

In this work, air was considered as a mixture of nitrogen and oxygen (77% N_2 and 23% O_2). Here, the present authors applied a set of plasma-chemical reactions developed in other work [15], which considered only positive and negative molecular ions O_2^+ and O_2^- of air and 6 reactions containing these ions (see the table).

The exclusion of nitrogen in the set of ions presented for the stationary electrical discharge was possible because of both the large speeds of recharge and the conversions of N_2^+ and N_4^+ ions into O_2^+ ions [16].

In the chain of conversion and charge-exchange reactions ($N_2^+ + N_2 + N_2(O_2) \rightarrow N_4^+ + N_2(O_2)$, $N_4^+ + O_2 \rightarrow 2N_2 + O_2^+$, and $N_2^+ + O_2 \rightarrow N_2 + O_2^+$), N_2^+ and N_4^+ ions produce O_2^+ ions. At atmospheric pressure, this occurs on a time scale on the order of 1 ns, which is much shorter than the time to establish a glow discharge and arc.

To perform a numerical simulation, a fluid model of electrical discharge was formulated [12]. It is based on the density balance equations for electrons, positive and negative ions and on electrons heat balance equation which takes into account not only the volume processes but also the spatial transfer by conduction and the Poisson equation for finding a self-consistent electric potential. The mobility and diffusion coefficients for electrons, as well as some constants of the inelastic processes involving them, are calculated by convolving the electron distribution function $f(w, T_e)$, with the cross section $\sigma(w)$. In this work, the electron distribution function $f(w, T_e)$ is assumed Maxwellian, because electrical discharge is calculated in a wide range of discharge currents, including currents corresponding to the arc discharge. In this case, the electron–electron collisions start to dominate, this leads to Maxwellization electron energy distribution function (EEDF).

2.2 Modeling the cathode domain

To account for cathode heating and for determination of the cathode temperature field, the following heat balance equation was considered:

$$\rho_c c_c \frac{\partial T}{\partial t} = \nabla \left(\lambda_c(T_c) \nabla T_c \right) \tag{1}$$

where ρ_c is the mass density of the cathode material; c_c is the cathode heat capacity; and λ_c is the cathode thermal conductivity. The boundary conditions for Eq. (1) to the cathode surface from the plasma region ($x = 0$) were determined as follows:

$$nQ|_{x=0} = n \left(Q_i + Q_g + Q_{\mathrm{TF}} + Q_e \right) .$$

Here, the heat flux Q_i to the cathode was caused by two mechanisms: (i) heat flux due to the ion kinetic energy, mainly acquired on the path length in the cathode fall, U_{CF}; and (ii) heat flux due to ion recombination on the walls. When an ion hits a wall, it extracts an electron and recombines while releasing the rest of its internal energy (ionization energy). The ion needs energy equal to the material work function W_c in order to extract an electron from the cathode and it is assumed that the rest of the energy is deposited on the cathode. Thus, Q_i is determined as follows:

$$Q_i = q_e \sum_s \Gamma_s \left(U_{\mathrm{CF}} + U_s - W_c \right)$$

where U_s is the oxygen ionization potential.

The main mechanism for the cathode heating due to energy transfer from the hot gas (plasma) to the cathode region is determined by the density of the heat flow:

$$Q_g = -\lambda(T)\nabla T\,. \tag{2}$$

Due to thermionic emission, the cathode is cooled and the flux density is determined as follows:

$$Q_{\mathrm{TF}} = -q_e \Gamma_c W_c\,.$$

It should be noted that some of the electrons have left the cathode through emission due to elastic collisions with neutral gas particles, which can change their movement to the opposite direction. Thus, if their power is sufficient to reach the cathode surface, they also contribute to its heating. The heat flux density in this case will be determined by the formula:

$$Q_e = q_e \Gamma_e \left(\frac{5}{6}\,\overline{\varepsilon} + W\right)\,.$$

For Eq. (1), to impose conditions on the outer walls of the cathode to maintain a constant temperature, it is necessary that

$$T_c|_{\mathrm{out}} = T_0\,.$$

2.3 Modeling the anode domain

To account for anode heating and to determine the temperature field, the heat balance equation was considered, similar to Eq. (1):

$$\rho_a c_a \frac{\partial T}{\partial t} = \nabla\left(\lambda_a(T_a)\nabla T_a\right) \tag{3}$$

where ρ_a is the mass density of the anode material; c_a is the anode heat capacity; and λ_a is the anode thermal conductivity. The boundary conditions for Eq. (3) to the anode surface from the plasma region ($x = L$) were determined as follows:

$$nQ|_{x=L} = n\left(Q_g + Q_{\mathrm{ea}} + Q_{\mathrm{ia}}\right)\,.$$

Here, the term Q_g is defined similarly to Eq. (2); Q_{ea} is the heat flow associated with the electrons energy that make up the discharge current and the electron neutralization on the anode surface; and Q_{ia} is the heat flow associated with the energy of negative air ions that make up the discharge current.

3 Results of Numerical Simulation

During the modeling, it was supposed that the cross-section sizes of the electrodes were much bigger than the interelectrode interval, which was taken equal to 0.1 mm. Therefore, it is possible to consider a 1D geometry. In addition, it was assumed that the lengths of the cathode and the anode were identical and both equal to 10 mm.

As a result of a series of numerical experiments, the basic characteristics of an electrical discharge were determined for a wide range of discharge currents, including the temperature fields of both the interelectrode interval and the metal electrodes.

Figure 1 demonstrates the dependence between the reduction of voltage in the interelectrode interval and the current density — a CVC with all of the characteristic sections: the classical glow discharge (point A), the abnormal glow discharge (from point A to point B), the transitive section between the glow discharge and the arc (the decreasing curve from point B to point D), and the nonequilibrium arc

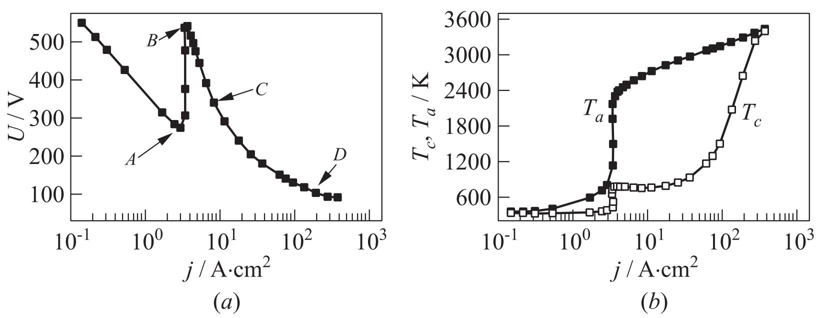

Figure 1 Dependences of the reduction of voltage in the discharge interval (a) and of the cathode surface temperature (b) on the current density in the cathode

discharge (from point D and beyond to the right). The dependence of the temperature on the cathode and anode surfaces for various discharge current densities is also shown in Fig. 1.

In the regions of normal (point A) and abnormal (point B) glow discharges, it can be seen that there is a sharp growth in the cathode temperature up to values of 2500 K. Then, there is a nearly linear growth of the cathode surface temperature, depending upon the current density on a half-logarithmic scale, up to values corresponding to the melting point (3695 K) of the metal cathode (tungsten) during arc discharge. It is worth noting the interesting behavior of the anode surface temperature, i.e., its dependence on the current density. The first growth in temperature is observed on the abnormal branch of the CVC up to values of the order of 800 K; then, on the transition section from the abnormal glow discharge to the arc, a weak minimum in the behavior of the dependence between anode temperature and current density as well as a sharp growth from approximately 100 A/cm^2 up to values corresponding to the melting point (3695 K) of the anode (tungsten) can be seen.

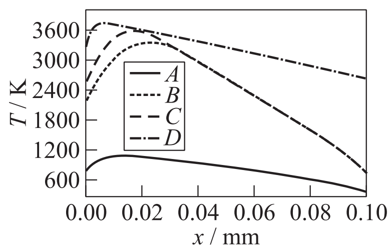

Figure 2 Temperature distribution of heavy particles in the plasma (ions and neutral particles) for various points of the discharge CVCs

Figure 2 shows the temperature distributions of heavy particles in plasma — ions and neutral particles — for various points of the CVC of the discharge. It is evident that the temperature has a maximum near the cathode region of the discharge and that the increase in current density leads to a growth in the maximum values of temperature of the heavy components of the plasma.

In Fig. 3, the distributions of the main parameters of the electrical discharge for various points of the CVC are shown. It is clear that when the current density increases, the discharge quasi-neutral region grows and, at the same time, the plasma concentration increases.

An interesting peculiarity is observed in the behavior of electron concentration in the anode region during transition to the arc discharge: it stops decreasing and starts growing.

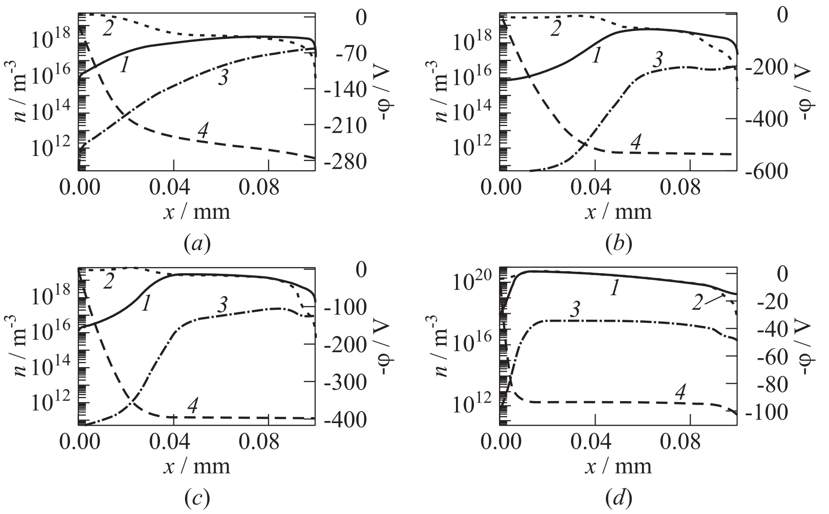

Figure 3 Distribution of charged particle density (*1* — n_c; *2* — n_p; and *3* — n_m) and the potential (*4*) for different points on the discharge CVCs

4 Concluding Remarks

In this work, the behavior of microdischarges at atmospheric pressure has been studied for a wide range of discharge currents, taking into account effect of conjugate heat transfer between electrodes and plasma. A classical shape for the CVCs of a discharge has been obtained with all observable sections: glow discharge, abnormal glow discharge, and an arc. The achieved results could be useful both for basic studies of microdischarges at atmospheric pressure and for the creation and optimization of devices whose working environment is a gas-discharge plasma.

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