Capacitive coupled RF discharge: modelling at the local statement of the problem

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Abstract. In this paper a mathematical model of capacitively coupled RF discharge at atmospheric pressure is constructed, a method of numerical realization of the model is developed, and the numerical calculations are carried out. Comparison of the results of the numerical experiments with the data of other authors, in particular, with the experimental data, is demonstrated as well a model adequacy as effectiveness of the numerical method. A results of calculations of the model problem at pressure of 760 Torr, frequency of generator of 13.76 MHz and interelectrode distance of 20mm, in local approximation are presented.

1. Introduction

Low-temperature non-equilibrium plasma is widely used in various fields of science and technology [1-7]. Low-temperature plasma is applied for material treatment aimed to increase service life and reliability of machine-building products, to create light-weight and service-strong polymeric composite materials, polyethylene-plastic materials, nanodispersed metal powders and compounds, etc. Various types of discharges are used to create plasma and important role in this process is assigned to RF-discharges, and particularly, to CCRF-discharges. Argon as the plasma gas is often usedin the plasma systems. Analysis of the literature revealed a number of disadvantages that are inherent to the using models of the capacitively coupled RF (CCRF) discharges at high pressures. As a rule, a simplified scheme of plasma chemical reactions in the drift-diffusion approximation is taken into account. This scheme is quite adequate for argon at low pressure and contains a reaction for electrons, atomic ions, neutral and excited atoms.

However, studies of microwave discharges showed that the ratio of concentrations of atomic and molecular ions depends on the gas temperature [8]. The present work is a continuation of previously published [9,10]. Our calculations for simplified kinetic scheme which is typically used at low pressures have shown that there is a significant change of the gas temperature in the interelectrode space at atmospheric pressure, and the boundary conditions of the first kind (i.e. the gas temperature at the boundary is constant and equal to the temperature of the electrodes) while a gas temperature in the interelectrode space is practically constant at low pressures. Changes of the gas temperature profile in the interelectrode space is less pronounced at the third kind boundary conditions (i.e. with free heat exchange). As a result, we include the molecular ion and argon dimerto the kinetic scheme.

2. Mathematical model

We have constructed a self-sustained mathematical model, which is described a capacitive coupled RF discharge between two plane-parallel electrodes, one of them is grounded and the other is connected to
RF generator, wherein the interelectrode distance is smaller than the electrode size. In this case the electric field is close to the potential field and the discharge is uniform along the electrode. It allows us to use one-dimensional approximation [11]. Estimates of the time and the distance of the electrons losses of an energy acquired from the electric field, are showed that a local approximation can be used for the simulation of an RF discharge at atmospheric pressure, when the parameters of the electron components of the plasma (such as diffusion coefficients, mobility, the average energy, constants of the plasma-chemical reactions, etc.) depend on the local value of the reduced electric field (ratio $E/N$ of the electric field $E$ to the concentration of heavy particles $N$) [12].

Self-sustained model of the CCRF discharge at atmospheric pressure in the local approximation contains the balance equations for electrons, metastable atoms, molecular and atomic ions, the kinetic equations for argon dimer and neutral atoms, the Poisson equation for the electric field potential, as well as stationary atomic heat equation ion gas with the boundary conditions of heat transfer, calculated on the average for the period of oscillation of the field parameters. Rate coefficients for processes taking place in electron impact depends on the local value of the reduced electric field and the degree of ionization taking into account electron-electron collisions. A simplified diagram of argon atom wherein the 4 lowest nearby electronically excited states is described as the single level excited atoms of density. The following plasma-chemical reactions is considered in the model:

$$
\begin{align*}
\text{Ar}^+ + e &\rightarrow \text{Ar} + e + \text{Ar}^*; \quad \text{Ar}^* + e \rightarrow \text{Ar} + h\nu; \\
\text{Ar}^+ + \text{Ar}^* + e &\rightarrow \text{Ar} + \text{Ar} + e; \quad \text{Ar} + \text{Ar} + 2\text{Ar}^* \rightarrow 2\text{Ar} + \text{Ar}^*; \quad \text{Ar}^* + \text{Ar}^* \rightarrow \text{Ar} + \text{Ar} + \text{Ar}^*; \\
\text{Ar} + \text{Ar} + 2\text{Ar}^* &\rightarrow \text{Ar} + \text{Ar} + \text{Ar}^*; \quad \text{Ar}^* + \text{Ar}^* + e \rightarrow 2\text{Ar} + \text{Ar}^*; \\
\text{Ar} + \text{Ar} + \text{Ar}^* + e &\rightarrow \text{Ar} + \text{Ar} + \text{Ar}^*; \quad \text{Ar} + \text{Ar} + \text{Ar}^* + e \rightarrow \text{Ar} + \text{Ar} + \text{Ar}^*.
\end{align*}
$$

Constants of the processes are taken from [13-20].

3. Numerical method for solving the problem

The mathematical model is described by a system of boundary and initial-boundary problems, which are characterized by several features complicating a numerical solution: different time scales of variation of the main characteristics of the steady discharge; the presence of large gradients of the density of charged particles, the electric field and the electron temperature near the electrodes; the system is nonlinear, both on separate equations and as whole. Existing methods of nonlinear problems solving (see, e.g., [21-26]) were unusable in this case. Therefore, we used an approximate method for solving nonlinear system of boundary and initial-boundary problems, which is considered in this paper. The metod is based on a preliminary finite-dimensional approximation of the problem by using finite-difference schemes with a subsequent application for its implementation of the iterative process.

The finite-difference approximation of the convection-diffusion equations of charged particles is constructed by an integro-interpolation method with a method of directed differences to approximate first-order derivative terms. An implicit Euler scheme was used to solve the Cauchy problems. A Newton linearization is used to approximate the quadratic nonlinearities in the right side of the equations. Density flows for the ion and electron gas are calculated by the Scharfetter-Gummel scheme [27].

The numerical algorithm is based on moving the non-linearity in coefficients (diffusion coefficients, the mobility and the constants of plasma-chemical reactions) to the low layer. The linearization of the system is carried out by the method of the Seidel type. The linearization of the heat equation for the atom temperature was carried out by Jacobi method, in which the initial approximation is the value of the atomic-ion temperature on the previous period. The calculations were carried out until the steady state of the full charge balance in the interelectrode space is reached, i.e., charges which is brought to the electrode by electrons and positive ions for the period of the field oscillation are exactly compensated.

4. The results of numerical experiments

The numerical simulation is carried out by a software package based on the Matlab. Numerical calculations performed at atmospheric pressure, interelectrode distance of 2 mm, and frequency of the
high-frequency generator of 13.56 MHz is compared with results of [18] and is showed a good correspondence. Additionally, the model problem was solved at atmospheric pressure, the interelectrode distance of 20 mm, and the RF generator frequency of 13.56 MHz. It is found that in the last case the gas temperature is about 2000 K in the discharge center and about 930 K near the electrodes. This difference between the gas temperature amounted to 53.5%, is effected to significantly on the charged particles densities in the interelectrode space. The densities is more convex at 20 mm than at 2 mm. The most significant changes are observed in the distribution of molecular positive argon ions. The graph of argon molecular positive ions is substantially constant at the distance is 2 mm, while there is a local maximum of ones near of the electrode at the distance of 20 mm, and the local minimum is observed in the center of discharge area. The ratio of the minimum of the density of molecular positive argon ions to the maximum ones is about 0.43, i.e, the molecular ions density falls more than 2 times in the middle of the discharge gap. At the same time, there is the preservation of quasi-neutrality of the plasma in the ambipolar field. The ratio of dimer to the excited atoms also changes: the maximum is about 0.78 at the distance 2 mm, while ones is about 0.38 when the distance is 20 mm. Thus, if the dimers density at the distance of 2 mm can be assumed constant, while ones is decreased at 20 mm, when the gas temperature is maximum.

5. Conclusion

The mathematical model of low-temperature CCRF plasma in argon, eliminating the drawbacks of existing models is constructed. The model includes drift–diffusion equations for electron and ions, Poisson’s equation for the potential of the electrical field, balance equations for metastables and grounded state atoms as well as a steady state equation for atomic-ion gas conductivity. A numerical method is proposed for model solution. The solution for the model with non-ideal conductor is obtained. The results of simulations are shown that in case of a significant gas heating as well at higher pressures, as in the case of large interelectrode distances at low pressures, the processes of formation and destruction of particles, and consequently influences on the distribution and balance of charged (electrons, atomic and molecular ions) and excited particles in the discharge gap.

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