Solution of the problem of interaction between capacitive coupled radio-frequency discharge and a sample

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Abstract. The numerical study of interaction between the capacitive coupled radio frequency (CCRF) discharge and materials is performed. A nonlinear problem, which includes initial-boundary value problems for electron, ion, neutral atom, metastable atom, gas temperature and Poisson's equation is solved. A harmonic voltage on the loaded electrodes and Ohm's law for the sample is assumed. A results of calculations of the model problem at pressure p=760 Torr, frequency of generator f=13.76 MHz in local approximation are presented.

1. Introduction

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 [1-4]. Mathematical models, which allow calculating main parameters of RF-discharges is created and solved numerically in order to improve operational modes of the equipment. Models in 0D, 1D, 2D and 3D approximation can be used to simulate discharges [5-8], however, 1D models is allowed describing the physics of the processes in a discharge at low cost providing that they describe the discharge adequately. Plasma parameters change when treated specimen is inserted into the discharg. Sometimes changes of parameters of the sample by plasma is studied without studying variation of the discharge characteristics (see [9, 10], for example). Statistical simulation is also used for plasma processes researches [11-15]. This work was aimed to study influence of the sample located on an electrode on the parameters of plasma of a CCRF (13.56 MHz) discharge in argon at atmospheric pressure

2. Setting of the problem

Herein we compare results obtained for two models. Ones describes capacitive coupled radio-frequency discharge between two parallel plate electrodes, one of which is grounded and the other is connected to a CCRF-generator (Model N1). The second model describes situation, when the sample located on the grounded electrode (Model N2).

Both models are described in frame of the following physical hypothesis. Electrical field is close to the potential one and the discharge is uniform along the electrodes that allow us to use 1D model [16].

The electron energy dissipation at atmospheric pressure is significantly less than the field period, while plasma parameters change in time with the field frequency. The length of electron energy relaxation at atmospheric pressure is significantly less than the dimensions of the computational domain, therefore we can use local approximation for plasma simulation. In this approximation parameters of electronic component of the plasma depend on local value of a reduced electrical field E/N [17].

A simplified diagram of argon atom wherein the 4 lowest nearby electronically excited states is described as the single level excited atoms of density nm. Such diagram is reasoned by efficiently mixing of these levels at the electron impact [18,19].

It is assumed that the ideal gas is occurred in a discharge chamber, therefore where P is pressure, is Boltzmann's constant, is atom temperature, N is density of argon atoms in the ground state.

Let us introduce the *Ox* axis at the normal direction to the surface of electrodes, in this case coordinates $x=0$, $x = b$ and $x=a$ corresponds to the grounded electrode, loaded electrode and to the sample surface, respectively. Here b is distance between electrodes, a is thickness of the sample. Domain $0 < x < a$ in the second model is occupied with the sample. Therefore boundary conditions are formulated at the points $x = a(r-1)$ and $x=b$, where r is the model number hereinafter.

Processes in CCRF discharge are described by the following problems.

2.1. Convection– diffusion equation for electrons

$$\frac{dn_e}{dt} + \frac{d}{dx}\left(-D_e \frac{dn_e}{dx} - \mu_e n_e E\right) = R_1 n_e N + R_2 n_m^2 + R_3 n_m n_e - R_4 n_e n_+ -$$
$$-R_5 n_e^2 n_+, \quad a(r-1) < x < b, \quad t > 0$$

The boundary conditions depend from the electric field directions:

$$\begin{cases} G_e = -\gamma G_+, & \text{if the field is directed to the electord or the sample} \\ & (E \leq 0 \text{ at } x = a(r-1), \quad E > 0 \text{ at } x = b) \\ \frac{dG_e}{dx} = 0, & \text{if the field is directed from the electrod or the sample} \\ & (E > 0 \text{ at } x = a(r-1), \quad E \leq 0 \text{ at } x = b) \end{cases}$$

Here n_e, n_+, n_m are densities of electrons, ions and metastable, respectively, $G_e = -D_e\, dn_e/dt - \mu_e n_e E$, $G_+ = -D_+\, dn_+/dt + \mu_+ n_+ E$ are densities of electron and ion flows, μ_e μ_+ are mobility of electrons and ions, D_e, D_+ are electron and ion diffusion coefficients, γ is secondary electron emission factor E is electric field intensity, $(E = -\partial\phi/\partial x)$, φ is electric field potential. Here in after $R_i, i=1\ldots9$, are factors of plasma chemical reaction velocities (table 1) (Ar+e→Ar$^+$+2e; Ar*+Ar*→Ar+Ar$^+$+e; Ar*+e→Ar$^+$+2e; Ar$^+$+e→Ar+h$_v$; Ar$^+$+2e→Ar+e; Ar+e→Ar*+e; Ar*→Ar+h$_v$; Ar*+Ar→2Ar; Ar*+e→ Ar+e). [20-26].

2.2. Convection–diffusion equation for ions

$$\frac{dn_+}{dt} + \frac{d}{dx}\left(-D_+ \frac{dn_+}{dx} + \mu_+ n_+ E\right) = R_1 n_e N + R_2 n_m^2 + R_3 n_m n_e - R_4 n_e n_+ -$$
$$-R_5 n_e^2 n_+, \quad a(r-1) < x < b, \quad t > 0$$

The boundary conditions are anologues

$$\begin{cases} \frac{dG_+}{dx} = 0, & \text{if the field is directed to the electord or the sample} \\ & (E \leq 0 \text{ at } x = a(r-1), \quad E > 0 \text{ at } x = b) \\ G_+ = 0, & \text{if the field is directed from the electrod or the sample} \\ & (E > 0 \text{ at } x = a(r-1), \quad E \leq 0 \text{ at } x = b) \end{cases}$$

2.3. Poisson's equation for the electric field potential φ

$$-\frac{d^2\phi}{dx^2} = \frac{q_e}{\varepsilon_0}(n_+ - n_e), \quad a(r-1) < x < b, \quad t > 0$$

where q_e is the electron charge, ε_0 is the electrical constant, ω is the angular frequency of electric field. with boundary conditions for the model No.1

$$\begin{cases} \phi = V_a \sin(\omega t), & \text{on the loaded electrod } (x = b) \\ \phi = 0, & \text{on the grounded electrod } (x = 0) \end{cases}$$

And for model No.2

$$\begin{cases} \phi = V_a \sin(\omega t), & \text{on the loaded electrod } (x = b) \\ i = -\sigma \; d\phi/dx, & \text{on the sample} (x = a) \end{cases}$$

where V_a – is the amplitude of the driven potential, σ – specific conductivity of the sample, $i = q_e(G_+ - G_e) + \varepsilon_0 \, dE/dt$ – total current density

2.4. Balance equation of metastable atom

$$\frac{dn_m}{dt} - \frac{d}{dx}\left(D_m \frac{dn_m}{dx}\right) = R_6 N n_e - R_2 n_m^2 - R_3 n_m n_e - R_7 n_m - R_8 N n_m -$$

$$-R_9 n_m n_e, a(r-1) < x < b, \quad t > 0$$

where D_m is full heat-transfer coefficient of the sample, T_w is electrode cooling water temperature.

3. Results of calculations

To solve non-linear systems of boundary value problems and initial-boundary value problems we used the approximation method based on preliminary finite dimensional approximation with use of the difference scheme and furtherly applying iteration process for its implementation. Difference approximation for the convection equations of charged particle diffusion is derived with use of integro-interpolation method. Drift terms are approximated by using upwind differences as in [27-29]. The research papers [30-35] are dedicated to the methods to solve non-linear problems of continuum mechanics, which describe two-layer iteration methods including methods implying nonlinearity lowering to lower layer.

Calculation was performed for the following values: γ=0.01; σ=0.01 cm; P=760 Torr, V_a=100 B, k_{full} =0.5 W/(m²·K). Simulation is showed that placing of the sample with finite thermal conductivity on an electrode bring in asymmetry the discharge and shift the gas temperature maximum to the sample (see fig.1, fig. 2) that results in changes and asymmetry of other processes.
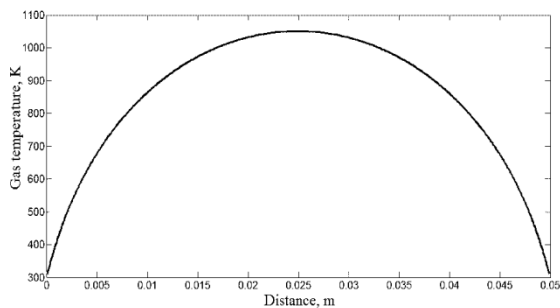

Figure1.distribution of gas temperature between electrodes for the first model.
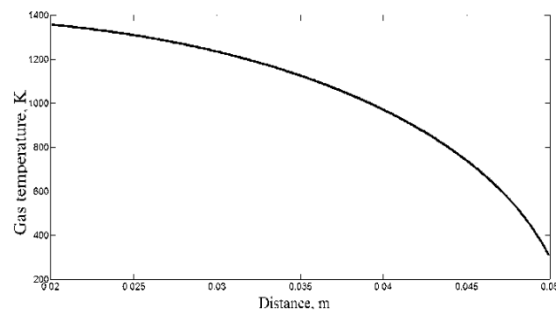
Figure 2. distribution of gas temperature between the sample and the electrode for the second model.

Due to strong dependence of molecular and atomic ions densities on the value of gas temperature and the significant difference the last ones, the kinetic scheme (table 1) shall complicate by processes with dimers and molecular ions [22].

4. Conclusion

The article describes the model of interaction between CCRF discharge and a sample, which allows calculating the characteristics of CCRF-in the interval between the sample and the powered electrode. 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. It is established that placing the sample with finite conductivity on an electrode result in asymmetry in discharge characteristics.

Acknowledgments

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