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Modeling the dielectric barrier micro-discharge in argon at atmospheric pressure

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Abstract. Dielectric barrier micro-discharge in argon at atmospheric pressure is simulated. Spatial and temporal discharge parameters are presented.

1. Introduction

The non-thermal plasma of gas discharges at high pressure for many years is of great interest to scientists, as an object for the study of fundamental plasma phenomena [1], and from the point of view of the many practical applications. Discharge plasma combines a low temperature of heavy particles and high temperature of electrons.

Various types of bits in which non-equilibrium plasma is supported at the present time are the subject of study by many research groups. The main reasons for this fact are the low cost of equipment for creation of these discharges, and ease of their use. This causes a wide range of applications of such systems – various radiation sources, the generation of ozone, plasma displays, surface treatment, treatment of industrial and exhaust (or destruction of harmful pollutants in the atmosphere), sterilization of medical instruments and products, disinfection of food products and packaging and plasma in biomedicine.

Typically, DC discharges under these conditions are not sustainable [for example, see 1]. Therefore, currently being developed various methods to control the parameters of the plasma DC discharges [2]. Another way to obtain a stable discharge in atmospheric pressure is to change the conditions of burning, in particular the transition to a non-stationary discharge - a barrier, pulsed, high-frequency, microwave discharges [1, 3-6] and others. One of the most common types of these discharges is a dielectric barrier discharge (DBD), in which one or both of the metal electrodes are covered with a dielectric layer. Dielectrics accumulate charges on the surface during the current pulse. These currents in turn create a self-induced field in the gas gap, which suppresses the discharge until the current density exceeds a threshold value.

Despite the low cost of equipment for creation of sources DBD discharges now there is still a problem for their stable operation and optimization. Therefore, at the present time good instrument to predict the parameters of DBD is numerical simulation. Various methods of modeling discharges were considered earlier by the authors in [2,7-8].
2. Model description

The model included balance equations for the densities of charged (electrons, ions) and the excited particles \( n_k \), the electron energy density \( \varepsilon_n \), and the Poisson equation for the potential \( \varphi \). The stationary state was determined by solving the time-dependent equations. The fluxes of charged (electrons, ions) \( \Gamma_k \) and electron energy flux \( Q \) were given in the drift-diffusion form. The complete system of balance equations is

\[
\frac{\partial n_k}{\partial t} + \nabla \cdot \Gamma_k = \sum_j c_{k,j} R_j, \\
\frac{3 \varepsilon_n}{2} + \nabla \cdot Q = -q_e \Gamma_e \cdot E + \frac{3}{2} \varepsilon_n (T_e - T) + \sum_j \Delta \varepsilon_j R_j, \\

\Gamma_k = -D_k \nabla n_k + z_k \mu_k \varepsilon_n k, \quad Q = -D_e \nabla n_e - \mu_e \varepsilon_n e.
\]

Where \( q_e \) – is the electron charge, and \( \varepsilon_0 \) – is the permittivity of free space, \( Z_k \) – is a charge particle grade \( k \), \( E \) – is the electric field intensity, \( \delta = 2m_e / M_a \) – is the ratio of the electron mass \( m_e \) to the mass of an atom of gas \( M_a \), \( v_{ea} \) – is the rate of elastic electron-atom collisions, \( T_e = (2/3)n_e / n_e \) – is the electron temperature.

The right-hand side of equation (1) is defined by reactions in the discharge. Each reaction gives a positive contribution to the function of the source, if it is formed corresponding to the type of particle and the negative contribution, if that kind of particle disappears. In this expression \( j \) – is the index of the reaction (of 32 plasma-chemical reactions taken into account), \( c_{k,j} \) – is the number of particles of type \( k \) resulting in a reaction of the type \( j \) (both positive and negative). Reaction rate \( c_{k,j} \) is determined by constants corresponding processes \( k_j(T_e) \) and they are proportional to the product of the concentrations of the reactants: \( R_j = k_j(T_e) \cdot \prod_{k=1}^{N} n_k \) where \( N = 2 \) for the reactions between the two types of particles, \( N = 3 \) – for the reactions between three varieties of particles.

The first term on the right side of the first equation (2) corresponds to the Joule heat in the electric field of the electrons and neutral particles of gas, respectively. The second term in (2) describes the energy exchange in elastic collisions of electrons with neutral gas particles. The third term in (2) describes the inelastic energy losses of the electron gas, which \( \Delta \varepsilon_j \) – is the energy lost (or acquired if \( \Delta \varepsilon_j < 0 \)) the electrons in this reaction, and \( R_j \) – is the reaction rate, which is determined by a constant corresponding inelastic process \( R_j = k_j(T_e) \cdot n_e \cdot n_n \) where \( n_n \) – is the sort of neutral particles.

Discharge model is a hybrid, because for electron coefficient of mobility \( \mu_e \), \( \mu_e \) and diffusion \( D_e \), \( D_e \), as well as some constants processes with their participation, calculated by the convolution of the EDF \( f(w, T_e) \), resulting from the decision of the local Boltzmann equation with a cross section of the corresponding process as follows

\[
k_j(T_e) = \sqrt{2q_e/m_e} \int_0^{\infty} f(w, T_e) \sigma(w) w dw.
\]
Here, the index j constants of processes proceeds only by the reactions 11 [9]. When we found the EDF in the kinetic equation takes into account the heating of electrons in the longitudinal electric field and change their energy due to the elastic, inelastic collisions and electron-electron collisions.

The calculations were made for argon using a kit comprising 32 plasma-chemical reactions [9], and taking into account the three effective excited atomic level $^1\text{Ar}^*$, $^3\text{Ar}^*$, $^3\text{Ar}^*$ and two excimer level $^3\text{Ar}_2^*$, $^1\text{Ar}_2^*$, three kinds of ions $^1\text{Ar}^+$, $^3\text{Ar}^+$, $^3\text{Ar}^+$, Ion mobility $\mu_i$ was taken from [9], and the diffusion coefficients $D_i$ were calculated by the Einstein relation [9].

Boundary conditions were set at the cathode ($z = 0$) and the anode ($z = L$) to the density of charged particles, the electron energy density and potential:

$$\mathbf{n} \cdot \mathbf{\Gamma}_e|_0 = \nu_e \bar{n}_e / 2 - \gamma \mathbf{n} \cdot \mathbf{\Gamma}_k, \quad \mathbf{n} \cdot \mathbf{\Gamma}_e|_L = \nu_e \bar{n}_e / 2,$$

where $\gamma = 0.1$ – is the secondary emission coefficient, $\nu_e \bar{n}_e = \sqrt{8k_B T_e / \pi m_e}$ and $\nu_{i,th} = \sqrt{8k_B T_e / \pi M}$ – are the electron and ion thermal velocity, respectively, $V_0$ – is the voltage amplitude, $w = 2\pi n$ – is cyclic frequency, $\nu$ – is frequency.

Surface charge accumulation is added to the dielectric surfaces that are adjacent to the gap where the plasma forms by way of the following boundary condition:

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s,$$

where $\rho_s$ – is the surface charge density, which is computed by solving the following distributed ODE on the surfaces:

$$\frac{d \rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i - \mathbf{n} \cdot \mathbf{J}_e,$$

where $\mathbf{n} \cdot \mathbf{J}_i$ – is the normal component of the total ion current density at the wall, and $\mathbf{n} \cdot \mathbf{J}_e$ – is the normal component of the total electron current density at the wall.

3. Results

Modeling of barrier micro-discharge parameters was carried out in the framework of a one-dimensional geometry of the discharge Fig.1. The magnitude of the discharge gap, the distance between the inner surfaces of the dielectrics $L = 2$ mm, the thickness of the dielectric barriers $d = 1$ mm and relative permittivity coefficient $\varepsilon = 10$.  

**Fig. 1.** The scheme of one-dimensional geometry of the DBD. 1 is left-electrode; 1-2, 3-4 are dielectrics; 2-3 is the discharge gap; 4 is right electrode.

The left electrode is grounded and the other is energized $V_{rf}$. In our calculation we assumed: $V_0 = 2$ kV, $v = 50$ kHz. Atmospheric pressure is expected.

As a result of numerical experiments for the conditions we observed a pulse current to half the period applied to the discharge voltage. It occurs with increasing the potential drop across the gap to
reach the breakdown voltage, and is accompanied by a sharp decrease in the voltage drop across the barriers. It is due to the neutralization of the surface charge of the dielectric barriers to the flow of current (Fig. 2). In Fig. 3 shows the space-time dependence of the electron concentration in the discharge gap. It is seen that when the $t = 40$ mks character of the distribution parameters in time begins to repeat. The maximum concentration of charged particles observed in moments of current pulses.

Fig. 2. Time dependence of the voltage across the electrodes and the discharge current.

Fig. 3. The space-time dependence of the electron density in the discharge gap.

Fig. 4. a) The density distribution of charged particles in the discharge gap, b) the electric field and potential distributions at the time $t = 45$ mks.

The pattern of distribution of basic parameters of the barrier micro-discharge at times when the current reaches the maximum value at the different polarity of the applied voltage are shown in Fig. 4-5. It can be seen that there is some similarity distributions with distributions in DC glow discharge. In both cases, there are layers of a positive charge near dielectric. A large space charge occurs near the negative electrode. Following the positive charge layer there is a maximum concentration of charged particles with a minimum of the electric field (the region of negative glow NG). It is worth noting that while there is an interesting phenomenon – a reversal of the sign of the electric field. The main ions in the high density of charged particles (NG) are $Ar^+$ and $Ar_{2}^+$. 
The following is the second point of the treatment field (transition region between the dark space (FDS) and positive column (PC). It is followed by a region with a uniform distribution of plasma parameters (PC) with a characteristic small maximum concentration of the charged particles and a minimum of electric field. In this lengthy plasma region $Ar_2^+$ and $Ar_3^+$ are the main ions. In the transition from a uniform distribution of the discharge parameters in a PC to a small space charge of the positive electrode is observed reversal of the sign of electric field.

![Graph](image)

Fig. 5. a) The density distribution of charged particles in the discharge gap, b) the electric field and potential distributions at the time $t = 50$ mks.

4. Conclusions

Thus, in the simulation result was obtained spatial-temporal distribution pattern parameters of dielectric barrier micro-discharge at atmospheric pressure. It has been shown that there is a current pulse at half period the voltage supplied to the discharge for the conditions of the discharge and the account number of plasma chemical reactions occurring in the discharge. Graphs the distribution of the main DBD parameters are presented in moments of current pulses with different polarities. It is shown that the distribution pattern similar to the distributions in DC glow discharge. It was found a reversal of the sign of the electric field. The described model of allows us to describe the main parameters of DBD plasma at atmospheric pressure and it is a useful tool in predicting their basic properties under various external conditions.

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