Study of ionization waves in a pulse discharge in argon

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Abstract. In the article we present the results of the investigation of the initial stage of nanosecond discharge formation in inhomogeneous pre-ionized argon of atmospheric pressure. The peculiarities of the cathode directed ionization wave development between two flat electrodes in argon of atmospheric pressure are presented.

1. Introduction

Nonequilibrium and unstable plasma of impulse volume discharge can be widely used in power gas lasers, in optical sources, plasma medicine etc. In spite of a number of articles devoted to impulse volume discharges a lot of issues connected with physics of impulse breakdown and mechanisms of the initial stages formation are not still fully investigated [1–8].

Our paper presents theoretical investigation of the ionization wave (IW) formation in a pure argon at atmospheric pressure with pre-ionization. IW develops in interelectrode gap between two parallel electrodes. Detailed description of the numerical domain is presented in [9].

2. Methods of investigation

The simulation was performed in a two-dimensional axisymmetric formulation. The computational model includes a particle balance equation for electrons, atomic and molecular ions, lower excited levels of Ar (1s5), Ar (1s4), Ar (1s3), Ar (1s2), highly excited levels of Ar (hl) (combining 2p, 2s, 3d, 3p in one level) and excimers (1). In total, more than 130 reactions were considered. The constants were taken from [10–14] and determined by the electron temperature, which was found by solving the equation for the electron energy. The self-consistent electric field was found from the Poisson equation. Neutral gas heating was not taken into account. The temperature of heavy particles in the counting process was assumed to be equal to the temperature of a neutral gas – 300 K.

\[
\frac{\partial n}{\partial t} + \nabla \cdot \Gamma = S
\]

\[
\Gamma = q n \mu E - \nabla (D n)
\]

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} n k_B T_e \right) + \nabla \cdot \mathbf{F} = \dot{Q}_e - \dot{Q}_a - \dot{Q}_m,
\]

\[
\mathbf{F} = \frac{5}{2} k_B T_e \Gamma_e - \nabla (\lambda_e T_e)
\]
\[ \lambda_e = \frac{5}{2} n_e D_e \]
\[ \nabla \cdot \mathbf{E} = \frac{e(n_{\text{Ar}^+} + n_{\text{Ar}_2^+} - n_e)}{\varepsilon_0} \]

where \( n_e, n_{\text{Ar}^+}, n_{\text{Ar}_2^+}, \Gamma, \mu, D \) – concentration of electrons, atomic and molecular ions, flow, mobility and diffusion coefficient of the respective plasma components, \( e \) – electron charge, \( k_B \) – Boltzmann constant, \( T_e, \lambda_e, D_e \) – temperature, thermal conductivity and electron diffusion coefficient, \( Q_E \) – electric field operation, \( Q_{el}, Q_{in} \) – elastic and inelastic electron energy losses, \( S \) – source of birth and death of the considered particles in the plasma, \( \mathbf{E} \) – electric field strength. For ions \( q = +1 \), for electrons \( q = -1 \), for excited particles \( q = 0 \).

It should be noted that diffusion fluxes for the concentrations and electron temperatures was taken in the form \( \mathbf{\Gamma}_{\text{diff}} = -\nabla(Dn) \) and \( \mathbf{F} = -\nabla(\lambda_e T_e) \) [15]. The mobility coefficients for ions and the diffusion coefficient of excited particles in their own gas were taken from [16].

The boundary conditions at the cathode for the potential, charged and excited particles (index \( i \) refers to atomic and molecular ions):

\[ \phi_e = 0, \quad \frac{\partial n}{\partial z} = 0, \quad \Gamma_e = -\gamma \sum_i \Gamma_i, \quad n^* = 0, \quad \frac{3}{2} k_u T_e = I - 2\varphi_w; \]

at the anode:

\[ \phi_a = 25 \text{kV}, \quad \frac{\partial n}{\partial z} = \frac{\partial T_e}{\partial z} = 0, \quad n_i = 0, \quad n_e = 0; \]

on the side faces of the computational domain:

\[ \frac{\partial \varphi}{\partial r} = \frac{\partial n}{\partial r} = \frac{\partial n^*}{\partial r} = \frac{\partial T_e}{\partial r} = 0, \]

where \( \gamma = 0.1 \) – second Townsend coefficient, \( I = 15.76 \text{eV} \) – argon ionization potential, \( \varphi_w = 4.5 \text{eV} \) – work output of the cathode. For ion-electron emission, the flux of both atomic and molecular ions to the cathode was taken into account.

The calculation was performed according to an explicit scheme with the second order of accuracy in time and space [17]. In the interelectrode gap, the grid was uniform with 2000 cells, along the radius – with thickening (150 cells). The initial concentration was set on the axis of the discharge gap by a Gaussian function with a maximum concentration of electrons and atomic ions \( 10^8 \text{cm}^{-3} \).

The pre-ionization electron and ion concentration in the gap is set as follows:

\[ n_e(x,y) = n_0 \exp \left(-\frac{(x-x_0)^2}{\sigma_x^2}\right) \exp \left(-\frac{(y-y_0)^2}{\sigma_y^2}\right) \]

Here \( \sigma_x, \sigma_y \) – the characteristic sizes of the pre-ionization area for different directions, \( x_0, y_0 \) – position of the pre-ionization area, \( n_0 = 10^8 \text{cm}^{-3} \).

3. The results of the researches and their investigation

Figures 1a and 1b show the characteristic distributions of uncompensated space charge \( (n_{\text{Ar}^+} + n_{\text{Ar}_2^+} - n_e) \) and electric field in the discharge gap, respectively, for different points in time. It should be noted that the formation of non-monotonic behavior of the space charge inside the discharge gap is the result of the development of two ionization waves, which move in opposite directions. On the outer side of the ionization front, the intensity is large, and inside it drops sharply, since a quasineutral plasma is formed there. But inside the region between the ionization waves, the field decreases at the initial moment of time (1–3), then increases (time moment 3–4), which is a consequence of the interaction of two regions with an uncompensated charge of opposite sign (in accordance with the space charge graph), which in turn leads to a non-monotonic behavior of the electric field, and as a result, the non-monotonic behavior of the ionization frequency areas.
Figure 1. Characteristic distributions of uncompensated charge \((n_{Ar} + n_{Ar^-} - n_e)\) (a) and the longitudinal component of the electric field strength (b) in the interelectrode gap the time points 1 – 1.5 ns; 2 – 2.0 ns; 3 – 2.5 ns and 4 – 3.0 ns \((U_0 = 25 \text{ kV}, p = 760 \text{ Torr})\).

At the initial moment of time, the longitudinal electric field \(E_x\) at the front of the ionization waves increases, and in the cathode-directed grows faster and reaches large values. At the time moment \(~ 3.0–3.5\) ns, \(E_x\) has passed through a maximum and falls in a cathode directed wave, while in an anode-directed wave it continues to grow monotone. Then, as waves approach the electrodes, the value of \(E_x\) in both waves decreases, while the decrease rate of anode-directed wave is much higher. For example, over a time interval of 3.5–4.0 ns, \(E_x\) in an anode-directed falls more than an order of magnitude, while in a cathode-directed, decreases by no more than 10%.

An analysis of the characteristic distributions of excited atoms (figure 2b) shows that the excited levels of \(\text{Ar} (1s2), \text{Ar} (1s4), \text{Ar} (1s5), \text{Ar} (\text{hl})\) are most intensively populated and when the ionization waves approach the electrodes, it is \(~ 10^{14} \text{ cm}^{-3}\), and the concentration of excimer molecules is the smallest and amounts to \(~ 10^{12} \text{ cm}^{-3}\) in the plasma column. The characteristic dependences for excited particles repeat the dependencies for electrons, since at the considered concentrations of electrons, excited particles and reaction rate constants (for electron energies of 2–7 eV – figure 2a), the characteristic transition time between the excited levels (through the collision between excited particles with electrons and neutral atoms) is much higher.

Figure 2. a) Characteristic electron temperature distributions at time points 1 – 1.5 ns; 2 – 2.0 ns; 3 – 2.5 ns; 4 – 3.0 ns; 5 – 3.5 ns and 6 – 4.0 ns \((U_0 = 25 \text{ kV}, p = 760 \text{ Torr})\). b) Distributions of concentrations of charged and excited particles at time 4.0 ns \((U_0 = 25 \text{ kV}, p = 760 \text{ Torr})\).

The velocity of the ionization waves can be determined by fixing the position of the maximum values for the field strength \(E_x\), temperature electrons \(T_e\) and concentration of electrons \(n_e\). All these estimations take the same results for the cathode-directed ionization wave which is about \(10^7–10^8 \text{ cm} \cdot \text{s}^{-1}\), at the time moment 4 ns. The concentration of electrons in the discharge gap, with the
exception of the cathode layer, lies in the range $\approx 10^{13}$–$10^{14}$ cm$^{-3}$, which agrees satisfactorily with the results of the experiment [6, 18], and the field strength is close to $10^5$ V·cm$^{-1}$.

4. Conclusion
The discharge formation occurs during the propagation of cathode and anode ionization waves which move in opposite direction. Anode wave reaches the electrode faster, but higher values for electric field strengths are achieved in cathode ionization wave. Characteristic values for the ionization wave velocity and electron concentration are in a good agreement with experiment.

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