2D fluid model of the one dielectric barrier discharge in the needle-plane configuration

S.V. Avtaeva[1], S.K. Kodanova [2], A.I. Kenzhebekova [2], T.S. Ramazanov[2]

[1] *Novosibirsk State University, Department of Applied Physics, Pirogova str. 2, Novosibirsk, 630090, Russia*
[2] *Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Al-Farabi 71, Almaty, 050040, Kazakhstan*

Time dependent characteristics of the one dielectric barrier discharge of alternating voltage in nitrogen at atmospheric pressure in the needle-plane configuration were studied using the 2D fluid model. Characteristic feature of the discharge is presence of a dielectric barrier near surface of the plane electrode for the conduction current. That leads to formation of a positive surface charge on the dielectric surface, which value changes during a voltage cycle. Other characteristic feature is presence of a strong electric field near a needle electrode during greater part of the voltage cycle.

1. Introduction

The one dielectric barrier discharges in the needle-plane configuration have various applications, for example, sterilization, electronography, surface modification, getting new chemical materials and others. A needle is made from thin wire (diameter ~10^2-10^3μm) and frequently with a sharpen tip. Typical dimension of the discharge plasma is a few millimeters and a distance between a needle and a processed surface is 1-3 mm. The localized plasma is one of such discharge advantages and so an effect of the discharge impact can be spatially controlled in a desired area. Dielectric barrier discharges with dielectric layers on both electrodes are studied adequately, for example [1, 2]. At atmospheric pressure the DBDs usually exist in the filamentary form. Breakdown in micro discharges realizes due to streamer mechanism. At the same time, properties of one dielectric barrier discharges and current maintenance mechanism in the discharges are studied worse, in particular in the needle-plane configuration. This type of discharges is named in [3] the ac barrier corona as it combines features of both dielectric barrier and corona discharges. The discharge consists of two modes: a bright streamer placed in the centre and a barrier corona diffusion area of a concave form round the streamer [4]. The streamer rises at the needle and spreads towards to the cathode barrier. A starting-point of the positive corona places not precisely on the needle tip but a bit lower its and area of the corona discharge forms a cone shape around the streamer. Visual observations show in the discharge plasma bullets of a cone shape spread from the needle to the plane surface [5, 6]. In the paper properties of the one dielectric barrier discharge in nitrogen at atmospheric pressure in the needle-plane configuration were simulated using the 2D fluid model.

2. Model

The 2D fluid model of the dielectric barrier discharge is based on the continuity equations of electrons and positive ions N_2^+, N_4^+ and the balance equations of neutral species, linked among themselves by 14 reactions at the condition of the local field approximation, the Poisson equation and an equation for the external electric circuit. Considered reactions are presented in the Table.

The continuity equations of electrons and positive ions have the form

$$\frac{\partial n_e}{\partial t} = -\nabla\Gamma_e + S_e, \quad \Gamma_e = -\mu_e E n_e - D_e \nabla n_e \; ; \qquad (1)$$

$$\frac{\partial n_{+,i}}{\partial t} = -\nabla\Gamma_{+,i} + S_{+,i}, \; \Gamma_{+,i} = +\mu_{+,i} E n_{+,i} - D_{+,i}\nabla n_{+,i} \; ; \qquad (2)$$

where n_e, $n_{+,i}$ are densities of electrons and positive ions of *i*-th kind, accordingly; Γ_e, $\Gamma_{+,i}$ are the particle fluxes; $\mu_e(E/n)$, $\mu_{+,i}(E/n)$, $D_e(E/N)$, $D_{+,i}(E/n)$ are the mobility and diffusion coefficients; $E = -\partial\varphi/\partial z$ is the electric field strength; φ is scalar potential; n is the total density of the neutral species; S_e, $S_{+,i}$ are the inter-particle collision source term for electrons and positive ions, respectively.

The balance equations for neutral species have the form

$$\frac{\partial n_k}{\partial t} - \nabla(D_k \nabla n_k) = S_k \; ; \qquad (3)$$

Here n_k is density of neutral species of *k*-th kind; D_k is the diffusion coefficient of the species; S_k is the inter-particle collision source term for neutral species. $D_k \neq 0$ for nitrogen atoms and metastable molecules.

The electric field is determined by the Poisson equation

$$\nabla^2 \varphi = -\frac{e}{\varepsilon_0}\left(\sum_i n_{+,i} - n_n - n_e\right), \quad (4)$$

where e is the elementary charge and ε_0 is the vacuum permittivity.

The boundary conditions for electron flux towards the uncovered electrode and dielectric barrier are

$$\vec{\Gamma}_e \cdot \vec{n} = -a\mu_e \vec{E} \cdot \vec{n} n_e + \frac{n_e \upsilon_{T,e}}{4} - \sum_{i,k} b_{i,k}\gamma_{i,k}\vec{\Gamma}_{i,k} \cdot \vec{n}, \quad (5)$$

and for positive ion flux are

$$\vec{\Gamma}_{+,i} \cdot \vec{n} = a\mu_{+,i}\vec{E} \cdot \vec{n} n_{+,i} + \frac{n_{+,i}\upsilon_{Tg,i}}{4}, \quad (6)$$

where $\vec{n}$ is the normal vector pointing toward the wall, $\upsilon_{T,e}$ and $\upsilon_{Tg,i}$ are the average thermal velocities of electrons and ions, respectively. The number a=1 if the drift velocity of electrons $\vec{\upsilon}_{dr} = -\mu_e \vec{E}$ or positive ions $\vec{\upsilon}_{dr} = \mu_{+,i}\vec{E}$ is directed to the corresponding electrode, and a=0 otherwise. $\gamma_{i,k}$ is the coefficient of secondary emission of electrons emitted with energy ε_γ due to impacts of positive ions and metastable molecules upon the dielectric surfaces. Coefficient $b_{i,k}$ = 1 if the flux of corresponding species $\Gamma_{i,k}$ is directed to the electrode and $b_{i,k}$ = 0 otherwise.

The boundary conditions for electron and positive ions fluxes towards the plasma-gas boundary are

$$\vec{\Gamma}_e \cdot \vec{n} = 0, \quad \vec{\Gamma}_{+,i} \cdot \vec{n} = 0. \quad (7)$$

The boundary conditions for diffusion fluxes of the nitrogen atoms and metastable molecules towards the uncovered electrode and dielectric barrier are

$$\vec{n}(-D_{m,k}\nabla n_{m,k}) = \frac{n_{m,k}\upsilon_{T,g}}{4}, \quad (8)$$

and towards the plasma-gas boundary are

$$\vec{n}(-D_{m,k}\nabla n_{m,k}) = 0 \quad (9)$$

Boundary conditions for Poisson's equation on a dielectric surface are

$$\vec{n} \cdot \frac{\varepsilon_0 \varepsilon_b \varphi}{d_b} - \vec{n} \cdot \vec{D}_{gas} = \sigma_b, \quad (10)$$

$$\frac{\partial \sigma_b}{\partial t} = \sum_j q_j \cdot \vec{n} \cdot \vec{\Gamma}_j. \quad (11)$$

Here $\vec{n}$ is the normal vector pointing toward the wall; $\vec{D} = \varepsilon \cdot \vec{E}$ is the electric displacement, ε is relative permittivity of the dielectric, $\vec{E}$ is the electric field strength; σ_b are the surface charge density, accumulated on a surface of the dielectric layer; j is electrons and i sorts of positive ions, $\vec{\Gamma}_j$ is the charged species flux, q_j is the species charge.

For Poisson's equation, the potential at the plane grounded-side electrode is zero, that at the needle powered-side electrode is $U_s(t)$ and at the plasma-gas boundary is $\vec{n} \cdot \vec{D}_{gas} = 0$. (12)

Initial conditions are set in a form of the space-uniform distributions of the species densities and the mean electron energy and the absence of charge on the dielectric surface.

The transport coefficients of electrons and rate constants of the electron-related reactions are calculated as functions of the reduced electric field (*E/N*) after solution of the Boltzmann kinetic equation in the two-term approximation. Mobility and diffusion coefficients of nitrogen ions were taken from [7]. Diffusion coefficients of nitrogen atoms and molecules were calculated in accordance to the elementary kinetic theory of the rarefied gases.

Table. Considered reactions.

1. $e+N_2 \text{->} 2e+N_2^+$	2. $e+N_2^+ \text{->} N+N$
3. $e+N_4^+ \text{->} N_2+N_2$	4. $N_2^+ + 2N_2 \text{->} N_4^+ + N_2$
5. $N_4^+ + N_2 \text{->} N_2^+ + N_2 + N_2$	6. $e+N_2 \text{->} e+N_2(A)$
7. $e+N_2 \text{->} e+N_2(a')$	8. $N_2(A)+N_2(a') \text{->} e+N_4^+$
9. $N_2(a')+N_2(a') \text{->} e+N_4^+$	10. $e+N_2 \text{->} e+N+N$
11. $e+N_2(A) \text{->} 2e+N_2^+$	12. $e+N_2(a') \text{->} 2e+N_2^+$
13. $e+e+N_2^+ \text{->} e+N_2$	14. $e+N_2^+ + N_2 \text{->} N_2+N_2$

3. Results and discussion

Parameters of the one dielectric barrier discharge of an alternating voltage in nitrogen in the needle-plane geometry are calculated. The top uncovered electrode has the form of a hemispherical surface with radius of 0.5 mm. The bottom plane electrode with radius of 3 mm is covered by a dielectric layer with thickness of 1 mm and relative dielectric permittivity 6. On the discharge axis a distance between electrodes is 2 mm, length of the gas gap is 1 mm. The bottom plane electrode is grounded. The alternate voltage $U=U_0 \sin wt$ with frequency 20 kHz and amplitude 4 kV is applied to the needle electrode. Pressure of nitrogen is 1 atm. Calculations were carried out up to steady-state regime.

Formation of a conducting channel is characteristic feature of an initial stage of the discharge. During voltage growing the electric field increases. Because of a great curvature of the top electrode the electric field is concentrated at the top electrode and the mean electron energy near to the electrode quickly grows. Electrons collect in the area near uncovered electrode, which is being under positive potential. Positive charge gradually collects on the dielectric surface. The surface charge density is maximal on the discharge axis and falls at moving away the axis (fig. 1). When the electron temperature reaches about 4 eV, there is a breakdown of the gas gap and a conducting channel in diameter of about 0.2 mm appears. The electron density in a sheath near uncovered electrode increases and reaches about 10^{15} m^{-3}. The most part of the period the electric field is concentrated at the needle and the mean electron energy in this area essentially exceeds the energy in the central part of the discharge and at the dielectric surface. The maximal gradient of potential arises in the axis areas where the distance between the electrodes is the list; the greatest ion flux arises in the same area.

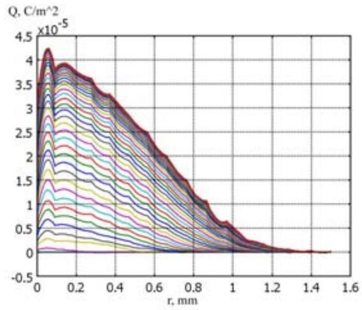
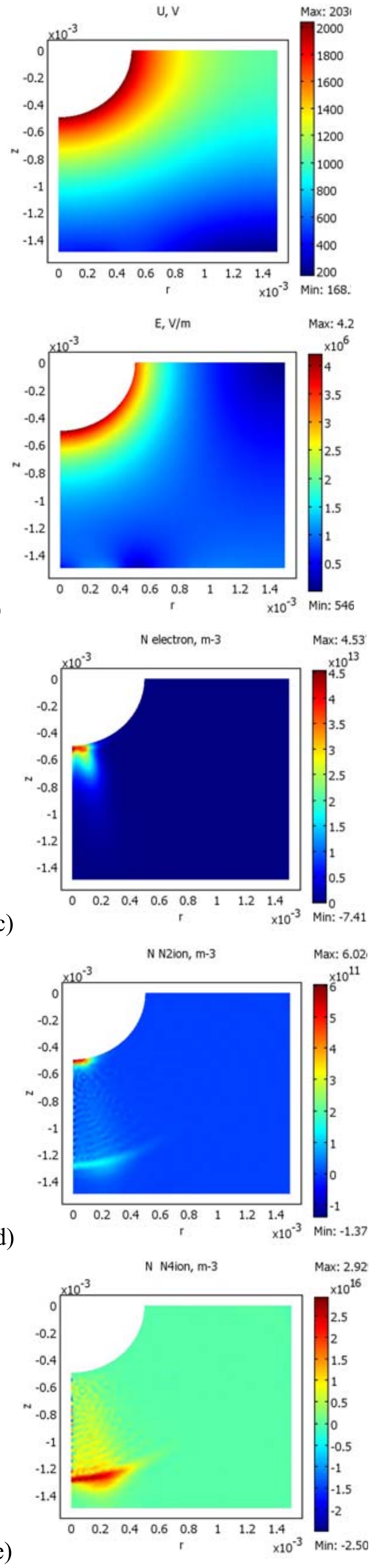


Fig 1. Surface charge distributions along the dielectric radius at various instants during a positive half-cycle of the needle voltage.

In the steady-state mode during a voltage positive half-cycle ions N_2^+ and N_4^+ drift towards dielectric on which surface the positive charge collects. Stratification of the ion fluxes (fig. 2d, e) and in the electric field distribution is observed. Having reached the dielectric surface, the wave of a positive charge closes a discharge gap, forming the channel of a positive space charge. Electrons are localized near to the top of uncovered hemispherical electrode (fig. 2c) where ionization takes place. On the dielectric surface representing a barrier to conduction current, the positive charge grows (fig. 1). This charge shields a field on the discharge axis near the dielectric surface. As a result the field in the central part of the discharge near the dielectric surface weaker in comparison with a field in surrounding peripheral areas. During this half-cycle the conduction current is basically carried by positive N_4^+ ions . The dielectric layer on the flat electrode surface represents a barrier to the conduction current, the current through dielectric is a displacement current.

During the negative voltage half-cycle the top uncovered electrode is under negative potential. Now positive ions localize near the small uncovered electrode, the area of a positive spatial charge of ~0.05 mm thickness is formed around it. In the area



a) b) c) d) e)

Fig. 2. Spatial distribution of a potential (a), an electric field strength (b), densities of electrons (c), N_2^+ (d) and N_4^+ (e) ions at 0.095T; T=0.05 ms; t= 0.00475 ms.

density of N_4^+ ions strongly exceeds density of N_2^+ ions. Electrons form a channel of the negative spatial charge, which begins on distance of about 0.05 mm from the uncovered electrode and terminates on the dielectric surface. Positive charge on the dielectric surface gradually decreases. However, this reduction occurs only in the area of 0.6 mm radius. During voltage increase densities of electrons and ions grow and reach a maximum. When the negative potential of the electrode starts to decrease, the field in the discharge gap also starts to fall, that is accompanied by reduction of electron and ion densities. Electrons carry the conduction current during this half-cycle. The current through dielectric layer still closes by the displacement current.

4. Conclusions

Processes proceeding in the DBD have complex character and are determined by a lot of factors. Characteristic feature of the discharge is presence of a dielectric barrier to conduction current near the plane electrode surface that leads to formation of the positive surface charge growing during the positive and decreasing during the negative half-cycle. Presence of the surface charge influences field distribution in the discharge gap and finally leads to restriction of the discharge area.

Other characteristic feature of the discharge is presence near the needle electrode of a strong electric field caused by electrode curvature during a greater part of the voltage period. In the area the ionization rate is great in comparison with its value in other areas of the discharge, therefore this area is a source of ions and electrons which then drift in electric field, creating discharge current.

5. References

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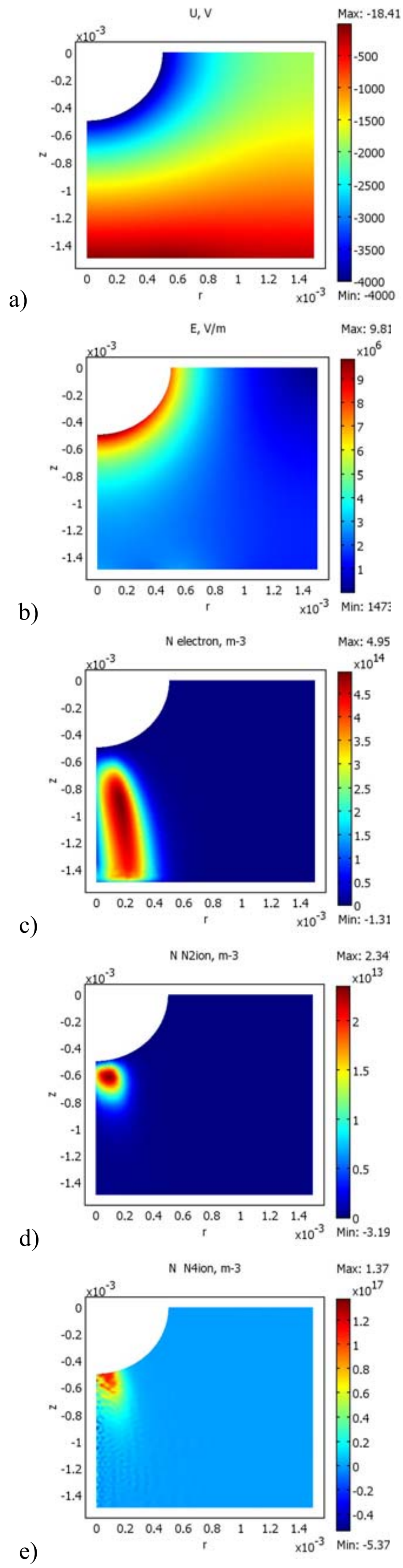

Fig. 3. Spatial distribution of a potential (a), an electric field strength (b), densities of electrons (c), N_2^+ (d) and N_4^+ (e) ions at 0.75T; T=0.05 ms; *t*= 0.0375 ms.