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Numerical investigation of a high-pressure gas medium pre-ionization by runaway electrons

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Abstract. A comparative simulation of the generation and acceleration of runaway electrons in the discharge gap during the initiation of the discharge by nanosecond and subnanosecond pulses is carried out. We used a numerical model based on the PIC-MCC method. Calculations were carried out for N₂ 6 atm pressure. Numerical simulation of a formation process of the electron avalanche initiated by an electron field-emitted from the top of the cathode microspike was carried out taking into account the motion of each electron in the avalanche. Characteristic runaway electron trajectories, runaway electron energy gained during the motion through the discharge gap, times required for runaway electrons to reach the anode were calculated. We compared our results with calculations using well-known differential equation of electron acceleration using braking force in Bethe approximation. We solved this equation also for braking force based on real (experimental) ionization cross section. The reasons for the discrepancy in the calculation results are discussed.

1. Introduction

The generation of runaway electron beams in high-pressure gases, in particular, air, is one of the most interesting problems in gas discharge physics. The greatest success in the generation of runaway electrons at high pressure was achieved using nano- and subnanosecond accelerators [1]. Using this equipment M Yalandin and co-authors carried out a series of experiments on the generation of subnanosecond runaway electron beams in gases at atmospheric pressure [1-3]. V Tarasenko and co-authors [4-6] also used the equipment with similar parameters for generation of runaway electrons. For increasing the efficiency of electron transition to the runaway mode, the special designed cathodes were used in above-mentioned experiments [3-6]. These designs provide the amplification of electric field near the cathode surface. The region of the enhanced electric field can also be realized in a cathode layer.

Earlier, in [7, 8], we have shown the possibility of transferring of electrons into the runaway mode at the final stage of the formation of the cathode layer of a self-sustaining volume discharge, at pressures of ~ 1 atm. The results of [9] obtained for a uniform electric field in the gap show the generation of the runaway electrons at nitrogen pressures of up to 40 atm. In this case, the electrons can transfer into the runaway mode as a result of acceleration in the region of the enhanced electric field provided by the micro-spike on the cathode surface. In [10, 11], we showed a significant decrease
in the value of the electric field of the electron transferring into the runaway mode in the presence of a micro-spike in comparison with a homogeneous field. However, in these studies, the further acceleration of the runaway electrons in the discharge gap has not been calculated.

The aim of this work is to simulate the development of an electron avalanche that started from the top of the micro-spike on the cathode surface in the presence of runaway electrons, as well as to calculate the movement of runaway electrons through the discharge gap, taking into account the accompanying ionization processes.

2. Description of the model
The block diagram of our software which realizes PIC-MCC technique (Particle In Cell – Monte-Carlo Collisions) is shown in figure 1. The program took into account the gain of energy of each electron in avalanche when it moves between collisions and losses as a result of inelastic collisions. The nature of the collision (elastic, excitation of the vibration or electronic levels, ionization) was played out with the help of a random number generator. The program was written by us in C++. The necessary data on cross sections were taken from [12-17]. The program was tested for different values of a uniform electric field.

![Figure 1. Block diagram of the PIC-MCC module.](image)

Calculations were performed for two pulses of nanosecond and subnanosecond duration (figure 2) applied to the discharge gap corresponding to the experimental conditions [7, 18, 19]. The electrode configuration is shown in figure 3. The anode curvature radius was 1 cm. The cathode curvature radius was also 1 cm. In addition, for amplification the electric field, a cylinder of 2 mm diameter and 3 mm length was set at the top of the cathode. The cylinder was rounded by a hemisphere of a 1 mm radius. In the center of this hemisphere, we placed a micro-spike in the shape of a cone with a height of \( h = 10 \mu m \) and a base of 0.5 \( h \). To avoid singularities, the micro-spike top was rounded with the hemisphere of radius 0.01 \( h \). The discharge gap length \( d \) was 5 mm. The distribution of an electric field enhancement factor \( K_1 \) provided by the electrode geometry and configuration of the stationary electric field across the discharge gap determined by the electrode geometry are given in figure 4. The electric field enhancement factor is determined as \( K_1 = E/E_m \), where \( E \) is a local value of the electric field strength. \( E_m \) is an average value of the electric field strength over the discharge gap. It is
determined as $E_{m} = U/d$. Here $U$ is the voltage across the discharge gap, $d$ is the cathode-anode distance. The configuration of the electric field enhancement factor $K_2$ near the micro-spike with $h = 10 \, \mu m$ is given in figure 5. To calculate the $K_1$ and $K_2$ spatial distribution, Laplace equation was employed. The equation was solved numerically using the ANSYS software package. Since the micro-spike highness is two orders of magnitude less than the finger-shaped cathode radius, spatial scales of $K_1$ and $K_2$ distributions differs analogously. Therefore, to estimate the electric field enhancement factor near the micro-spike, it is quite correct to multiply $K_1$ and $K_2$. It was done in calculations.

**Figure 2.** Nanosecond (1) and subnanosecond (2) voltage pulses applied to discharge gap used in calculations.

**Figure 3.** The electrode configuration used in calculations.

**Figure 4.** Distribution of an electric field enhancement factor $K_1$ provided by the electrode geometry.

**Figure 5.** The distribution of the amplification factor of the electric field ($K_2$) for micro spike with height ($h$) of 10 $\mu m$. MS is the top of micro-spike

3. Results of calculations

We have carried out a series of calculations of the development of an electron avalanche initiated by a field-emission electron, which started from the top of the micro-spike. In the calculations, the average value of the electric field in the gap was determined as $E_{m} = U(t)/d$, where $U(t)$ is the voltage measured in the experiment at the gap (see figure 2). Note that the distortion of the electric field by electrons and ions in the avalanche was not taken into account due to the low concentration of charged particles.
Calculations have shown that when the voltage on the gap reaches a value of 100 kV (that is, about 70% of the value of the pulse breakdown voltage), the electrons located in the high-energy part of the energy distribution function begin to outrun the main part of the electrons in the avalanche. Some of these high-energy electrons get a statistical opportunity to transfer into the runaway mode. Flying through the gap and accelerating in the electric field, the runaway electron produces a series of ionization. As a result of these ionizations, slow electrons are formed. They move at the drift speed and show the flight path (track) of the runaway electron. Typical tracks of the motion of runaway electrons for nanosecond pulse are shown in figure 6.

![Figure 6](image1.png)

**Figure 6.** Variants of the trajectories (tracks) of the movement of runaway electrons that started under the same conditions in the case of nanosecond pulse. The letter "a" denotes an avalanche. For clarity, the size of the avalanche has been doubled. (C) – cathode, (A) – anode.

![Figure 7](image2.png)

**Figure 7.** Variants of the trajectories of the movement of runaway electrons in the case of subnanosecond pulse.

Tracks 1-4 correspond to different variants of the movement of runaway electrons that have outrun electron avalanches. In the experiment, these variants may correspond to different micro-spikes. For better clarity, the tracks are built on the concept of the presence (black color) or absence (white color) of electrons in a space cell. At the beginning of each track there is an avalanche of slow electrons,
indicated by the letter "a". The 1-3 tracks show the trajectories of RAES having been accelerated by the electric field and having successfully reached the anode. The analysis of the obtained results showed that the trajectory on average could be inscribed in a cylinder with a base area of about 1 mm$^2$ and a height from the cathode to the anode. Herewith, a weakly conductive column of ionized gas is formed in the discharge gap. The column comprises of many micro-channels whose total glow is seen as a volumetric discharge.

**Figure 8.** Energy of runaway electrons vs distance from the cathode ($z = 0$) ($z = 5$ – anode) for nanosecond (a) and subnanosecond (b) pulses. Curves 1-3 in (a) and 1-2 in (b) – corresponds of different trajectories of runaway electrons calculated by PIC-MCC method. Curves 4 in (a) and 3 in (b) – trajectories calculated using equation in [20] with Bethe formula. Curves 5 in (a) and 4 in (b) – trajectories calculated using equation in [20] with real ionization cross section [16].

The 4-th track corresponds to the electron having transitioned into the runaway regime but having abruptly changed the trajectory due to some “catastrophic collision” and having stopped acceleration. Such a collision leads, as a rule, to the emission of an X-ray quantum. However, we did not consider the occurrence and propagation of such a quantum in our calculations. That is “catastrophic collision” only shows the possibility of X-ray quantum generation. It should be noted that the probability of a trajectory with “catastrophic collisions” is quite high in the near-cathode region. These trajectories were not of interest to us from the point of view of the solved problem, and therefore only one example is shown in figure 6 (Track 4). However, X-ray quanta generated as a result of “catastrophic collisions” move in arbitrary directions and improve the homogeneity of an ionization process.

A similar situation was carried out for a subnanosecond pulse (figure 7). This figure does not show trajectories with “catastrophic collisions”, although they occurred in the case of a subnanosecond pulse, but with less probability. In general, the tracks in the case of a subnanosecond pulse have parameters similar to the case of a nanosecond pulse.

Despite the significant differences in the trajectories of the runaway electrons, the integral characteristics of the acceleration of these electrons are similar. Figure 8 shows the dependences of the energies of the runaway electrons on the $z$ coordinate. Figure 8 (a) corresponds to nanosecond pulse. Figure 8 (b) corresponds to subnanosecond pulse. Curves 1-3 in (a) and 1-2 in (b) – corresponds of different trajectories of runaway electrons.

We compared our results with calculations using well known differential equation of electron acceleration using braking force in Bethe approximation [20].

$$\frac{dE}{dt} = \left( \frac{2e}{m} \right)^{1/2} \left[ E(z,t) - F(e) \right],$$

(1)
\[
\frac{dz}{dt} = \left(\frac{2e}{m}\right)^{1/2},
\]

(2)

where \(E(z, t)\) is space and time distribution of electric field in the gap corresponding to nanosecond and subnanosecond voltage pulses (figures 2 and 4), \(\varepsilon\) is runaway electron energy, \(m\) is mass of electron, \(e\) is elementary charge. Braking force \(F(\varepsilon)\) is defined as:

\[
F(\varepsilon) = \frac{2\pi e^4 ZN}{\varepsilon} \ln \left(\frac{\varepsilon}{J}\right),
\]

(3)

where \(N\) is number density of neutral molecules, \(J\) is ionization energy.

We solved the system (1), (2) numerically. The result is shown in figure 8 a, curve 4 and in figure 8 b, curve 3. For comparison, we also solved this system for braking force, which calculated using experimental ionization cross section \((\sigma(\varepsilon))\) [16], because an ionization is the main energy loss for runaway electrons.

\[
F(\varepsilon) = JN\sigma_1(\varepsilon).
\]

(4)

The result is shown in figure 8 a, curve 5 and in figure 8 b, curve 4. It can be seen that the calculation using the Bethe formula gives underestimated values of the electron energy, and using the real ionization cross-section, inflated values are obtained. This is explained by the fact that the Bethe formula gives overestimated energy losses, and the solution of the system (1), (2) using the experimental ionization cross-section implicitly assumes the movement of an electron in a straight line, which reduces its energy losses.

4. Conclusion
The calculations carried out allow us to draw the following conclusions.

A field-emitted electron initiates an electron avalanche. From this avalanche, it is possible the exit of runaway electrons, which can further accelerate in the gap, producing ionization in it along the trajectory of their movement.

The combination of such trajectories can create a homogeneous pre-ionization of the gap, which provides the glowing of the discharge in a volumetric form.

We compared our results with calculations using well-known differential equation of electron acceleration using braking force in Bethe approximation and braking force based on real (experimental) ionization cross section. In the first case, the energy losses are overestimated, in the second case, the energy losses were underestimated.

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