Monte-Carlo simulation of the ionization processes for discharges in the left branch of the Paschen curve

A A Grishkov, Yu D Korolev and V A Shklyaev
Institute of High Current Electronics SB RAS, 2/3 Akademichesky Ave., Tomsk, 634055, Russia

E-mail: grishkov@to.hcei.tsc.ru

Abstract. The paper deals with the development of the simulation methods applied to the low-pressure discharges in which the reduced electric field \( E/p \) is extremely high and there exists a problem for the correct description of the ionization processes in the classical electron avalanches. Here we use the PIC/MC code xoopic for calculation of the impact ionization coefficient \( \alpha \), the electron drift velocity and the electron diffusion coefficient \( D \) in the electron avalanches in nitrogen. The range of calculations covers the ratio \( E/p \leq 1000 \text{ V(cm-Torr)}^{-1} \). The simulation method was tested on a simple analytical model of an electron avalanche and showed good agreement in low and moderate \( E/p \). It is shown that in conditions of high \( E/p \) the spatial distribution of electrons in the avalanche head based on the concepts of electron mobility during their drift motion and diffusion coefficient is not quite correct. The work confirmed that at the very low pressures pre-breakdown phenomena and the transition to the next stage of high-current breakdown cannot be based on ideas about classical electron avalanches.

1. Introduction
The subject of research in this paper is the development of methods for simulating ionization processes in the prebreakdown stage of low-pressure gas discharges. Speaking about low pressure we mean a fairly wide range of conditions with including the conditions where the free path of an electron for ionization can be comparable or even exceed the length of the interelectrode gap. This situation is typical for a number of modern technical devices, in particular, for generators of electron and ion beams in systems with a plasma cathode [1], for hydrogen thyratrons with a hot cathode as well as for the so-called thyratrons with a cold cathode which are often called pseudospark switches [2–6].

In the extreme case of very low pressures pre-breakdown phenomena and the transition to the next stage of high-current breakdown cannot be based on ideas about classical electron avalanches. Here only a part of the electrons crossing the gas-discharge gap take part in ionization processes. Then, as shown in [6, 7], in the prebreakdown stage the increase of current is associated with a distortion of the electric field by the spatial charge of ions and ionization of the gas due to the oscillating motion of electrons in the region with nonmonotonic distribution of potential.

However, with a slight increase in pressure or with increasing the length of the discharge gap, one can already speak of electronic avalanches. Although as will be seen from the present work the some corrections should be introduced into the generally accepted interpretation and terminology.

When describing the ionization process in the prebreakdown stage the impact ionization coefficient is usually used. Impact ionization coefficient is the number of ionizations produced by one electron.
per unit path length in the direction of drift motion. If we are talking about the low pressure range then there is a situation when the normalized electric field strength, i.e. the ratio of electric field to pressure $E/p$ reaches extremely high values. This is typical condition for the range of minimum and left branch of the Paschen curve. To emphasize the specific features of ionization under such conditions, one usually indicates to “electron avalanches at high $E/p$” [8].

2. Experimental results and theory of electron avalanche

The classical method to obtain the data on the impact ionization coefficient $\alpha$ is the measurement of weak currents of a non-self-sustaining discharge with amplification by ionization. For these experiments the special gas-discharge chambers with a large diameter of electrodes were created. In this diodes the electric field is uniform in the interelectrode gap length up to a several centimeters [9, 10].

Under initial conditions a voltage lower than breakdown voltage $V_{br}$ is applied to the interelectrode gap. The surface of the cathode is illuminated by a stationary source of UV radiation and the electron emission current $I_{em}$ generated at the cathode is amplified in accordance with the expression:

$$I = I_{em} e^{ad},$$

where $I$ is the current in the external electric circuit equals to the electron current at the anode.

To determine the coefficient $\alpha$ the dependence of current $I$ on the length of the interelectrode gap $I(d)$ is measured under conditions when the ratio $E/p$ is kept constant. This dependence as follows:

$$\ln \left( \frac{I(d)}{I_{em}} \right) = ad.$$

Thus in the experiment a set of lines corresponding to different values of $E/p$ are obtained and the coefficients $\alpha$ are determined from the slope of these lines.

Some features of the technique of the discussed measurements are as follows. In each series of measurements the maximum gap length should not be too large so that the gain of the emission current $e^{ad}$ does not exceed 100. Otherwise the secondary electrons arising at the cathode due to the $\gamma$-processes contribute to the current and there is a deviation from current lines (2).

For measurements in the region of high $E/p$ experiments are carried out at low gas pressures down to $p = 0.075$ Torr at $E/p = 1000$ V-cm$^{-1}$Torr$^{-1}$ [9]. These conditions correspond to the left branch of the Paschen curve where the ionization can occur over long distances. In order for ionization to occur in the central part of the gap in the region of a uniform electric field the voltage range in the gap is chosen obviously below the minimum of the Paschen curve.

Using the described method a large amount of data on impact ionization coefficients was obtained. The data obtained are summarized in number of monographs, for example [11–13]. For the convenience of data use various approximation formulas are proposed that correspond to different $E/p$ ranges. Several commonly used approximations are given in table 1.

The approximations from table 1 and impact ionization coefficients from the experiments [9, 10] are shown in figure 1. It should be noted that in the entire range of normalized electric field $E/p$ there is a significant spread in the impact ionization coefficient. It leads to a significant discrepancies and errors, for example, in the estimations of the number of electrons in avalanches.

The measurement method presented above is often interpreted as measurements of the impact ionization coefficient in electron avalanches developing in the gap. However as applied to the described experiments it is more correct to speak of a certain averaged ionization coefficient $\alpha$, on the basis of which the data on measurements of the emission current gain are interpreted.

In the framework of modern concepts an electron avalanche is a well-defined object that can be distinguished in the space of the interelectrode gap and photographed, for example, using a Wilson camera or using light amplifiers [14]. The electron cloud is concentrated in the avalanche head which
size is determined by the diffusion of electrons during the movement of the avalanche front. The core of the avalanche is composed of ions which remain practically motionless during the propagation time of the avalanche front from the cathode to the anode.

### Table 1. Approximation for the impact ionization coefficient $\alpha$.

| №   | Approx. | Equation                                                                 | Range of $E/p$ $(\text{V cm}^{-1}\text{ Torr}^{-1})$ | №   | Approx. | Equation                                                                 | Range of $E/p$ $(\text{V cm}^{-1}\text{ Torr}^{-1})$ |
|-----|---------|---------------------------------------------------------------------------|-------------------------------------|-----|---------|---------------------------------------------------------------------------|-------------------------------------|
| (A) | $\frac{\alpha}{p} = 3.3 \cdot 10^{-7} e^{0.26 \frac{E}{p}}$            | 20–36                             | (D) | $\frac{\alpha}{p} = 12 \cdot e^{- \frac{342}{E/p}}$              | 100–600                         |
| (B) | $\frac{\alpha}{p} = 1.2 \cdot 10^{-4} \left( \frac{E}{p} - 30 \right)^2$ | 45–150                           | (E) | $\frac{\alpha}{p} = \left( 0.54 \frac{E}{p} \right)^{1/2} - 5$ | 120–350                         |
| (C) | $\frac{\alpha}{p} = 8.8 \cdot e^{\frac{275}{E/p}}$                      | 27–200                           | (F) | $\frac{\alpha}{p} = \left( 0.21 \frac{E}{p} \right)^{1/2} - 3.65$ | 200–1000                         |

At present there are results of measurements of the impact ionization coefficient and other parameters in studies of a single avalanche [8, 14]. One of the methods is based on oscillography of a current pulse created by the movement of charged particles in the gap. In the stage of electron drift from the cathode to the anode this current is mainly due to electrons. The shape of the oscillogram of the current in the external circuit is largely determined by the diffusion of the electron cloud in the avalanche head and by the electron drift velocity. Accordingly from a comparison of the measured waveforms with the calculated ones it is possible to determine the impact ionization coefficient, also the electron drift velocity $v_{dr}$ as well as the diffusion coefficient $D$.

![Figure 1](image1.png)  
**Figure 1.** Impact ionization coefficient $\alpha$ from experiments and approximations from table 1. Red and black squares – Posin’s and Bowls’ experiment, respectively.

![Figure 2](image2.png)  
**Figure 2.** Oscillogram of the electron avalanche current and its comparison with the calculation. Blue curve – exponential law, red curve – Schlumbohm’s model, black curve – xoopic simulation.

In experiments the voltage $V < V_{br}$ is applied to the gap. At some moment in time $t = 0$ due to a short flash of UV radiation focused on a small area of the cathode $N_0$ electrons are created on the cathode. The duration of a burst of radiation is usually about 10 ns and the initial number of electrons $N_0$ can be between 10 and 100 [14]. To obtain the shape of the current oscillogram it is necessary to
know the distribution of electron concentration in interelectrode gap at each time \( n(x, y, z, t) \). For this the electron balance equation is solved taking into account impact ionization, drift and diffusion. In the case when the directed motion of the electrons along the \( x \) axis is determined mainly by the drift velocity the solution is well known:

\[
\begin{align*}
n(x,y,z,t) &= \frac{N_0}{(4\pi Dt)^{3/2}} e^{\alphavt} \exp\left(-\frac{(x-vt)^2 + y^2 + z^2}{4Dt}\right) \\
&= \frac{N_0}{(4\pi Dt)^{3/2}} e^{\alphavt} \exp\left(-\frac{x^2 + y^2 + z^2}{4Dt}\right) \\
\end{align*}
\]

(3)

It can be seen from the presented solution that the electron cloud has a spherical shape and it is convenient to determine the characteristic diffusion radius of the cloud at each moment of time as \( r_D = (4Dt)^{1/2} \).

For high ratios of the reduced electric field \( E/p \) the electron cloud is elongated in the longitudinal direction. The electron balance equation for this case in one-dimensional geometry was written in [15] then improved in [16–18]. In these papers the solution was given to the equation and the method for obtaining the oscillograms of current in an external circuit was presented. The shapes of the current oscillograms calculated by this method are compared with the experimental oscillograms. As the result the data on the \( \alpha \) coefficient, on the drift velocities \( v_{dr} \) of the electrons and on the average electron energy in the avalanche are extracted.

The peculiarity of the electron balance equation in a layer of thickness \( dx \) located at a distance \( x \) from the cathode was that the total speed of the directed motion of the electrons \( v_{tot} \) was written as the sum of the drift velocity \( v \) and velocity due to diffusion:

\[
v_{tot} = v - \frac{1}{n} D \frac{\partial n}{\partial x}.
\]

(4)

Taking into account the fact that in a constant electric field the drift velocity \( v = \text{const} \) the electron balance equation is written as:

\[
\frac{\partial n(x,t)}{\partial x} = \alpha n \left( v - \frac{1}{n} D \frac{\partial n}{\partial x} \right) - \frac{\partial n}{\partial x} + D \frac{\partial^2 n}{\partial x^2}.
\]

(5)

In [16] an analytical expression is given for solving this equation in the case of a single electron avalanche. This solution gives the distribution of electron concentration along the \( x \)-axis at a given moment of time \( n(x,t) \).

\[
n(x,t) = \frac{n_0}{(4\pi D t)^{3/2}} e^{\alpha vt} \left[ e^{-\frac{(x-vt-aD)^2}{4Dt}} - e^{-\frac{(x-vt-aD)^2 + (x-2d-vt-aD)^2}{4Dt}} \right].
\]

(6)

The conduction current density in each section are determined as:

\[
j(x,t) = env - eD \frac{\partial n}{\partial x}.
\]

(7)

Then taking into account the conduction current in each section the shape of the current in the external circuit is written as:

\[
J(t) = \frac{1}{d} \int_0^d j(x,t) dx.
\]

(8)

An example of the current oscillogram calculated by this model with the appropriate selection of the impact ionization coefficient, drift velocity and diffusion coefficient is shown in figure 2 for conditions: \( E/p = 59 \text{ V}\cdot\text{cm}^{-1}\cdot\text{Torr}^{-1} \), \( V_{dr} = 2.38\cdot10^8 \text{ cm}\cdot\text{s}^{-1} \), \( D = 6\cdot10^4 \text{ cm}^2\cdot\text{s}^{-1} \), \( \alpha/p = 0.12 \text{ (cm\cdottorr)}^{-1} \),
$p = 1.0$ Torr (nitrogen), $d = 4.0$ cm. The figure shows a good agreement between this simple model and the simulation which will be discussed further.

Since the coincidence of the current oscillogram calculated by formula (8) with the experimental one was carried out by fitting the diffusion coefficient, average electron drift time in the interelectrode gap and the electron drift velocity, we can calculate coefficient $D$ for any conditions. Thus it is possible to estimate the average electron energy in the avalanche $\varepsilon_T$ or the electron temperature $kT$ which are determined from the well-known relation:

$$\frac{eD}{\mu} = kT = \frac{2}{3} \varepsilon_T,$$

where $\mu = v/E$ – electron mobility.

Figure 3 shows the measured electron temperatures in the head of an avalanche propagating in nitrogen for a wide range of $E/p$ values.

![Figure 3](image)

**Figure 3.** Electron temperature depending on the normalized electric field $E/p$ for an avalanche in nitrogen. Experimental results from: circles – [19], crosses – [20], rectangles – [21].

The points on the left side of the figure 3 are located on the right branch of the Paschen curve. The measured electron temperatures of 4 eV and less seem quite reasonable. However in the region of the minimum of the curve and in the left branch (right side of the picture) the electron temperatures measured by the above method are incredibly high. For example, for $E/p = 800$ V·cm$^{-1}$·Torr$^{-1}$ the temperature $kT$ obtained from the processing of waveforms is 20 eV and higher which exceeds the ionization potential of nitrogen. As will be shown below the reason is that in the condition of high $E/p$, the description of the spatial distribution of electrons in the avalanche head on the basis of generally accepted concepts of electron mobility during their drift motion and diffusion coefficient is not quite correct.

3. PIC+MC simulations

To study the formation of electron avalanches under the conditions indicated above the two-dimensional electromagnetic PIC code *xoopic* was used [22]. The xoopic code is a well-known tool for modeling plasma and processes in a gas discharge. In the code takes into account elastic scattering of electrons by gas molecules, excitation and a single ionization by electron impact in a wide range of
energies. We upgraded the code to solve the problems of breakdown and gas discharge in the electromagnetic formulation for nitrogen. The excitation cross sections (24 levels) of nitrogen molecules and single ionization for the energy range from 0.1 to 300 keV were taken into account [23].

The computational domain consisted of a cylindrical diode with cathode outer radius of 25 cm and anode radius of 30 cm, the length of the entire diode was 50 cm (figure 4). The gap between the edge of the flat cathode and the anode wall in the simulation could reach up to 12 cm. The geometry parameters were set in such a way that the range corresponding to the experimental conditions [9, 10] was covered.

Figure 4. Schematic of diode in PIC+MC simulation.

The constant electric field strength was set on the diode. A coaxial homogeneous part of the cylindrical cathode was used as an element of the external circuit for oscillography the electron avalanche current. Depending on the required value of the normalized electric field $E/p$ the gas pressure in the calculations varied in range $10^{-3}$–$10^3$ Torr. The computational grid for solving field equations consisted of 500×200 cells (along the axes $0x$ and $0r$, respectively). Time step was $\Delta t = 10^{-15}$ s, number of macroparticles up to $10^6$ psc. The selected parameters ensured the stability of calculations under any initial conditions.

We focused on modeling electron avalanches and interpreting the results at high $E/p$, but at the first stage we conducted a special series of calculations in low and moderate $E/p$. These test calculations were necessary to verify the selected computer code and simulation algorithm. The result of one of the checks is shown in figure 5.

Figure 5 shows a set of lines (which correspond eq. (2)) for experimental data [9] and [10]. The reduced electric field $E/p$ equals 59 V·cm$^{-1}$·Torr$^{-1}$. These experiments were carried out under different conditions in terms of gas pressures and interelectrode gaps. In Posin's experiments the interelectrode gaps of more than 5 cm were used at a nitrogen pressure of 0.985 Torr, in Bowles experiments the pressure was ~10 Torr and the gaps were 1.6–2.2 cm. The figure also shows the calculated dependence for 30 Torr which was used for comparison. The conclusions from this simulation are as follows.

Firstly, the figure shows that the slope of the straight line $\alpha d$ for conditions [9] and [10] differ by more than 25%. Secondly, the impact ionization coefficients which are calculated from the current oscillograms in the external circuit in the simulation coincide with the experimentally measured coefficients with high accuracy in both cases. The reason is that because of the difference in the gas pressures and different diffusion coefficients in the external circuit the different shape of current oscillograms have been obtained. Accordingly, the maximum current value occurs at different moment in time. Because of this we get a different slope of the curve and different impact ionization coefficients.
Figure 5. Normalized current $p^{-1}\ln(j_0^{-1})$ for different gaps and pressures. Rectangles – Bowls’ experiments (10 Torr), red triangles – Posin’s experiments (0.985 torr), black line – xoopic (30 Torr). $E/p = 59$ V·cm⁻¹·Torr⁻¹.

And this despite the fact that in both cases the electron cloud has a spherical shape and are described from the point of view of classical electron avalanche (figure 6). If we determine the impact ionization coefficient not from the current oscillogram, but by directly counting the number of particles in the avalanche we will obtain values that are directly realized in the interelectrode gap in the experiment during the formation of the avalanche.

From the above simulation results we can conclude that for the same value of the reduced electric field $E/p$ the impact ionization coefficient (determining by this method) strongly depends on the diffusion coefficient $D$. Moreover, the higher the pressure used and the more compact the electron avalanche the more accurate the method of determining the impact ionization coefficient from the current in the external circuit. Figure 5 shows the $ad$ curve for 30 Torr for comparison. It can be seen that it is close enough to experiments [10] in which the gas pressure is higher.

The obtained result can explain the wide scatter experimental data on the measurement of the impact ionization coefficient for the identical values of the reduced electric field $E/p$. Modern methods of numerical modeling already allow such calculations to be carried out directly. With their help this spread can be significantly reduce.

Similar calculations were performed for conditions of high $E/p$. Figure 7 shows the electron distribution in the avalanche at different moment of time in conditions that correspond to experiments [10] for the reduced electric field $E/p = 750$ V·cm⁻¹·Torr⁻¹. Under these conditions the electron cloud is not only elongated in the longitudinal direction, but also in the head of the avalanche the part of the electrons crosses through the interelectrode gap without collision with gas molecules. This part of the electrons goes into "run-away" mode. The avalanche does not break away from the cathode by the time when the first fast electrons already reach the anode. Here the electron cloud does not have space and time to take shape in the gap. In our calculations which are as close as possible to the experimental conditions, there can be a significant number of such electrons. That is why with an increase in normalized electrical field $E/p$ the impact ionization coefficient can decrease [24, 25]. In this case the behavior of decreasing the impact ionization coefficient will depend on the specific conditions in the interelectrode gap and will be unique for each diode geometry.

Figure 8 shows the coefficients of impact ionization $\alpha$ calculated in simulation in the entire range of $E/p$ in identical conditions at a nitrogen pressure of 20 Torr. The results show good agreement with various experiments at low and moderate $E/p$ and a significant discrepancy at high $E/p$. In this regard the question arises as to the validity of describing processes in an avalanche at high $E/p$ using the
impact ionization coefficient, drift velocity and diffusion coefficient. Obviously, under these conditions the impact ionization coefficient is unsteady in space [8].

**Figure 6.** The spatial distribution of electrons in avalanche in different moments of time. Number of injection particles – $10^3$ pcs, $dx = 10^{-4}$ m. Nitrogen, 1.0 Torr, $d = 2.0$ cm, $E/p = 59$ V·cm$^{-1}$·Torr$^{-1}$. Red curve – theory model, black curve – xoopic simulation. $V_{dr} = 2.38 \times 10^8$ cm·s$^{-1}$, $D = 6 \times 10^4$ cm$^2$·s$^{-1}$.

**Figure 7.** The spatial distribution of electrons in avalanche in different moments of time. Number of injection particles – $10^4$ pcs, $dx = 10^{-4}$ m. Nitrogen, 0.075 Torr, $d = 4.0$ cm, $E/p = 750$ V·cm$^{-1}$·Torr$^{-1}$. Red curve – theory model, black and blue curves – xoopic simulation, $V_{dr} = 1.8 \times 10^8$ cm·s$^{-1}$, $D = 2 \times 10^7$ cm$^2$·s$^{-1}$.

**Figure 8.** Impact ionization coefficient $\alpha$ from simulation (nitrogen, 20 Torr) and experiments [9] and [10].
Therefore, at present the results of experiments on measuring the impact ionization coefficient, drift velocities and diffusion coefficients should be considered taking into account the circumstances described above. At the moment in the conditions of a real experiment only direct simulation must be used. There is an urgent need to build a convenient model for describing ionization processes under conditions of high and ultrahigh $E/p$ which will be the goal of further work.

4. Conclusion
The direct simulation by PIC+MC code showed that in the condition of high $E/p$ the spatial distribution of electrons in the avalanche head based on the concepts of electron mobility during their drift motion and diffusion coefficient is not quite correct. From this we can conclude that at the very low pressures pre-breakdown phenomena and the transition to the next stage of high-current breakdown cannot be based on ideas about classical electron avalanches. Here only a part of the electrons crossing the gas-discharge gap take part in ionization processes. There is an urgent need to build a model for describing ionization processes under conditions of high and ultrahigh $E/p$.

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