Characteristics of nanosecond pulse needle-to-plane discharges at high pressure: a particle-in-cell Monte Carlo collision simulation

Chaofeng Sang, Jizhong Sun, Chunsheng Ren, and Dezhen Wang

School of Physics and Optoelectronic Technology and College of Advanced Science and Technology, Dalian University of Technology, Dalian 116024, China

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A model of one dimensional in position and three dimensional in velocity space self-consistent particle in cell with Monte Carlo collision technique was employed to simulate the argon discharge between the needle and plane electrodes at high pressure, in which a nanosecond rectangular pulse was applied to the needle electrode. The work focused on the investigation of the spatiotemporal evolution of the discharge versus the needle tip size and working gas pressure. The simulation results showed that the discharge occurred mainly in the region near the needle tip at atmospheric pressure, and that the small radius of the needle tip led to easy discharge. Reducing the gas pressure gave rise to a transition from a corona discharge to a glowlike discharge along the needle-to-plane direction. The microscopic mechanism for the transition can arguably be attributed to the peak of high-energy electrons occurring before the breakdown; the magnitude of the number of these electrons determined whether the breakdown can take place. © 2009 American Institute of Physics. [DOI: 10.1063/1.3082111]

I. INTRODUCTION

Corona discharge is a faint filamentary discharge, invariably generated by strong electric fields associated with small diameter wires, needles, or sharp edges on an electrode, and has a wide range of applications. The common electrode configuration of the corona discharge is needle-to-plane electrodes since such setup is simple and easy achieving discharge at atmospheric pressure. A small volume of nonthermal atmospheric discharge generated at the tip of a needle was first studied in 1930s by Trichel. Up to now a large number of experimental works have been conducted on the corona discharge with similar electrode configurations. These results showed that the discharge develops in the region around the needle tip where a high-electric field exists, and that the radius of the needle tip, which determines the nonuniformity of the electric field, has a big effect on the discharge characteristics. In the corona discharge, free electrons gain energy from the external electric field near the needle tip, and lose energy primarily by electron-neutral inelastic collisions (namely, excitation and ionization collisions). Each ionization process produces an electron-ion pair; the newly generated electron and the seed electron are accelerated by the electric field, and again ionize neutrals, and create electron-ion pairs. Thus, an avalanche happens. As time advances, electrons leave the cathode needle region and move toward the anode plane, and the electron density in the region away from the needle tip begins to increase gradually.

Although a number of experiments have been carried out to investigate the needle-to-plane discharge, discharge characteristics such as the evolutions of electron energy distribution, electron density, and electric field are not well understood. Most computational studies of atmospheric pressure discharges use fluid-based models. These models can give a reasonable description of discharge processes, and demand cheap computation resources. However, these models have a few intrinsic drawbacks; for example, they need unjustified parameters such as Townsend ionization coefficients, and transport and reaction rate coefficients. In particular, the application of inappropriate Townsend ionization coefficients would inevitably lead to a big error. These parameters are measured in equilibrium plasma but the corona discharge is a highly nonequilibrium plasma. Nonlocal effects are very important in the nonequilibrium plasma. As a result, the fluid models have difficulty in giving adequate predictions of local properties in the corona discharge; moreover, due to their macroscopic nature, the fluid models cannot give kinetic information of charged particles, such as the electron energy distribution.

To overcome the disadvantages of fluid models, especially, to remove the employment of Townsend ionization coefficients, a model that includes particle kinetics for analyzing the corona discharge is in demand. Settaoui et al. concluded that even a one-space-dimension and threedimensional velocity-dimension (1D3V) self-consistent Monte Carlo collision (MCC) simulation [literally, it is a particle-in-cell MCC (PIC-MCC)] can offer very detailed information of nitrogen corona discharges. Recently, Meige et al. and Sang et al. found that it is necessary to include the electron kinetics into the PIC simulation for a short-rise-time-pulse plasma immersion ion implantation. In this study we apply a 1D3V self-consistent PIC-MCC model to investigate the spatiotemporal evolution of the corona discharge between the needle and plane electrodes with an applied short rise time pulse. Instead of using unjustified macroscopic parameters, we make full use of particle-particle collision cross sections. In the following sections, we will focus on the evolutions of
the charged particle density, electric field, and electron energy distributions, and report a finding that a discharge mode transition happens when the operating pressure is in an appropriate range.

II. MODEL AND SIMULATION

The model in the present work is based on 1D3V PIC-MCC method. In the following, we briefly review the PIC-MCC method and physicochemical processes included in our model.

The argon is chosen as the working gas, and the species traced in the model are electrons (e\(^{-}\)) and argon ions (Ar\(^{+}\)). In the real simulation so-called e\(^{-}\) and Ar\(^{+}\) superparticles (SPs) are traced instead. Each SP represents W real particles (either electrons or ions), where W is known as weighting. Initially, these SPs are assumed to be homogeneous in space with velocities satisfying Maxwellian velocity distribution.

We are interested in only one dimension in this study, i.e., in the needle electrode pointing direction, and we define the dimension as the z axis. The needle electrode is located at z=0 mm and the plane electrode is located at z=d mm. A corresponding experimental setup is schematically illustrated in Fig. 1. Charged particles are driven by the electric field. The total field \(E\) along the z direction results from two sources: the applied voltage and space charge. The external field (often named as Laplacian field in literature) along the z axis can be described as a function of the axial distance z from the tip:\(^\text{21}\)

\[
E_L(z) = \frac{2V_0d}{\ln[(4d/r_c)][d(2z + r_c) - z^2]},
\]

where \(r_c\), \(d\), and \(V_0\) are, respectively, the radius of the needle tip, the spacing from the needle tip to the plane electrode, and the applied voltage. The external electric field \(E_L\) is a function of the applied voltage and the geometric configurations of electrodes, and does not vary with time. It needs to be calculated only once. The tricky part is to evaluate the electric field generated from the space charge. The space charge field \(E_C\) varies with time and position, and is calculated by solving Poisson’s equation at the end of each time step:

\[
\nabla^2 \phi_C = -\frac{e}{\varepsilon_0}(n_e - n_i),
\]

\[
E_C = -\nabla \phi_C,
\]

where \(\phi_C\), resulting from space charge, is the electric potential with Dirichlet boundary condition \(\phi_C=0\) at all boundary surfaces; symbols \(n_e\) and \(n_i\) represent the electron and ion SP densities, respectively, \(\varepsilon_0\) is the permittivity of vacuum, and \(e\) is the elementary charge. The movement of the SPs is governed by Newton’s equations of motion:

\[
E = E_L + E_C,
\]

\[
\frac{dv}{dt} = qE,
\]

where \(m\) is the mass of the corresponding SP, \(q\) is the charge of the SP, and \(v\) is the velocity of the SP in three-dimensional velocity space. The position of the SP is then obtained by integrating Eq. (5) with regard to time.

When these SPs move in space, they collide with neutrals, lose energy, and generate various species. Ultimately, the characteristics of discharges are determined by these random microscopic collisions. Accurately modeling these stochastic processes is very important to understand the corona discharge in depth. To achieve this aim, we employ Monte Carlo technique to treat these microscopic collisions. The technique can be illustrated briefly in the following text. The collision probability of particle \(i\) can be written as:\(^\text{22,23}\)

\[
P_i = 1 - \exp[-n_v(x)\sigma_T(e_i)v_t\Delta t].
\]

Here the total collision cross section \(\sigma_T(e_i)\) is the sum of the cross sections of various collision processes:

\[
\sigma_T(e_i) = \sum_{j=1}^{N} \sigma_j(e_i),
\]

where \(\sigma_j(e_i)\) is the cross section of the \(j\)th type of collision between the charged particle and the neutral. We consider in the simulation three types of collisions for electrons (elastic, excitation, and ionization collisions) and two types of collisions for ions (charge exchange and elastic collisions).\(^\text{22}\) The density of neutrals \(n_v(x)\) is assumed to be constant in space since the ionization rate is low, and can be easily calculated from the pressure. In present study, we do not include into the model the bulk recombination and other loss mechanisms of charged particles except for the electrons and ions that are absorbed by the anode and cathode, respectively. We think that this assumption is reasonable for a nanosecond discharge.

The ionization collisions may lead to a drastic increase in the simulated particles. If one traced all individual particles, the computation cost for the simulation would be unbearable. In order to keep the computation demanding under control, we set an upper limit for the number of each type of particles in our program. When the limit is reached, the number of each type of SPs is reduced by half (randomly sam-
pling 50 percent of the total number, and its weighting $W$ is doubled, that is, after the conversion each new SP represents twice as many actual particles as the old SP.24

III. RESULTS AND DISCUSSION

The simulation time parameters are chosen as follows: the time step, 0.1 ps, and the longest simulation time, 15 ns. Other initial state parameters are fixed to a constant: the initial densities of electrons and ions, $10^{14}$ m$^{-3}$; the initial energies of electrons and ions are 1 and 0.026 eV (i.e., room temperature), respectively. A rectangular waveform pulse of −5 kV is applied to the needle electrode.

A. Discharge characteristics

In this section, we present the characteristics of the needle-to-plane discharge at atmospheric pressure. The radius of the needle tip is chosen as $r_0=0.1$ mm.

The spatial distribution of the electric field versus time is shown in Fig. 2. At the beginning of the discharge, the Laplacian field $E_L$ dominates the field. There is a high-electric-field region near the needle electrode. As time progresses, the space charge field becomes significant, and leads to the variation of the total electric field. The electric field accelerates the electrons, and the electrons impact the neutrals and create electron-ion pairs. As a result, the electron and ion densities increase near the needle electrode (see Figs. 4 and 5). The difference (namely, the net space charge; see Fig. 3) between ions and electrons generates the space charge field $E_C$, which plus the Laplacian field $E_L$ constitutes the total electric field $E$. As can be seen in the inset graph of Fig. 2, the space charge field expands gradually toward the plane electrode as time advances. At the location of 0.1 mm away from the needle tip, the magnitude of the space charge field $E_C$ reaches the maximum value of $7.8 \times 10^6$ V m$^{-1}$ at 0.8 ns. Although the peak value varies with the time, the peak position of the space charge field changes little. From Figs. 2 and 3, we can see that the sheath edge is well defined along the $z$ axis.

Thus, a stable thin sheath establishes itself in the vicinity of the tip surface within an order of a nanosecond. However, it takes a much longer time for the space charge field to offset the Laplacian field $E_L$ outside the sheath edge. The electrons can respond swiftly to the electric field while the ions are more immobile than electrons since the ions are much heavier, which can be confirmed from the evolutions of electron and ion density distributions (see Figs. 4 and 5).

In companion with the evolution of electron density, the electron energy varies with time, which is shown in Fig. 6. Within 0.30 ns from the beginning of the discharge, the electron energy distribution expands toward the high energy [see Fig. 6(b)]; the velocity of the energy expansion drops as time
advances. This result implies that the energy that the electrons gain from the electric field is larger than that which the electrons lose through the inelastic collisions within 0.3 ns; but the energy loss gradually catches up with the energy gain since the inelastic collision cross sections become larger as the electron energy increases. After 0.3 ns, the physical picture is the other way around—the energy range shrinks as time progresses but its shrinking velocity falls with time. After 15 ns, few electrons have energy over the ionization threshold of 15.76 eV. The energy distribution of electrons then turns stable. In concert with the stable electron energy distribution, the distribution of the space charge density becomes stable, as well (see Fig. 3). The breakdown does not happen within 15 ns discharge time.

B. Tip size effect

In this section we briefly present the effect of the needle tip size upon the discharge. As aforementioned, the initial total electric field is equal to the Laplacian field $E_L$ since the net space charge does not exist. Evidently, as can be learned from Eq. (1), the thinner the needle tip, the stronger the electric field near the needle tip.

We now fix the tip radius $r_0=0.3$ mm, and keep other parameters the same as in Sec. III A to investigate the discharge properties. The spatial distribution of electron density is shown in Fig. 7. Compared with that in Fig. 4, we can see that the magnitude of the electron density is smaller at the same moment. In order to study the effect of the needle tip size, we have calculated the electron density distributions in the vicinity of the needle tips with different radius values ($r_0=0.1, 0.15, 0.2, 0.3, 0.5,$ and 1.0 mm). Figure 8 displays the electron density distributions for these needle tip radii at the discharge time of 15 ns. We can see that the smaller the value of $r_0$, the higher the electron density near the needle tip, and that the thickness of the sheath next to the needle tip becomes larger as the radius increases. All these results follow from one cause that the electric field is higher when the tip radius is smaller. From these results one could expect that a smaller radius of the needle electrode would lead to discharge more easily.

C. Discharge mode transition

Now we look at how the operating pressure influences upon the discharge characteristics. First we look at the spatial distribution of the electron density at different times, respectively, at the operating pressure of 50 and 100 Torr, as shown in Figs. 9(a) and 9(b). In the starting stage of the discharge, it is a typical corona discharge: a high electron density occurring only near the tip of the needle electrode. As the discharge time progresses, the electron density along the most part of $z$ axis in either case turns spatially uniform while near the tip of the needle electrode the electron density drops quickly, that is to say, the breakdown takes place. Comparing the two cases, we can see that in the lower pressure case the...
transition in the electron density happens sooner. Examining the spatial distribution of the electric field, we find that the electric field corresponding to the part of the constant-electron-density distribution in either case is actually zero. This result shows that there is no space charge in the constant-electron-density discharge channel. In most part of the z axis the channel looks like the positive column in the low pressure glow discharge between two parallel electrodes but the former does not have a distinctive transitional region between the sheath region and the positive column after the electron density becomes stable. The magnitudes of the stable electron density after breakdown at various operating pressures are summarized in Table I. As can be seen, the electron density falls approximately linearly as the pressure increases. Surprisingly, the electron density drops about 0.2 ×10^{19} \text{ m}^{-3} \text{ when the pressure increases by every 50 Torr. Based on the trend, we could speculate that the breakdown would not take place in a higher operating pressure with the present simulation parameters.}

To gain the insight into the breakdown process, we examine the energy distributions associated with these electron densities. The energy distributions are shown in Fig. 10. In the case of 50 Torr, we know that the breakdown starts in the period between 2 and 5 ns; in the case of 100 Torr, the breakdown starts in the period between 5 and 8 ns. Let us look carefully at the energy distributions at 2 and 5 ns in Fig. 10(a), and at 5 and 8 ns in Fig. 10(b). We can find that, before the breakdown, either energy distribution contains a higher percentage of electrons with energy over the ionization threshold (we call this part of electrons the OIT electrons for short in the following text). We expect that these OIT electrons might be necessary for the breakdown.

To further examine the correlation between the breakdown and the OIT electrons, we look at Fig. 11, in which the percentage of the OIT electrons accounting for the total electrons versus the discharge time is displayed. We can see that once the high voltage is applied to the electrode, the first peak of the OIT electron percentage occurs almost simultaneously. Although the percentage is high, the total electron density is much localized. In addition, the pulse-on time is short, not long enough for the breakdown to develop. Therefore, the first peak of the OIT electron percentage bears no direct relation to the breakdown for both cases. At the operating pressure of 50 Torr, the second peak of the OIT electron percentage appears between 2 and 3 ns; accompanying the peak, the breakdown is developing, as shown in Fig. 9(a). The statements are similar for the case at the operating pressure of 100 Torr. From Fig. 11, we can also see that the second peak of the OIT electron percentage at the operating pressure of 100 Torr is much lower than at the operating pressure of 50 Torr, and the occurrence of the peak takes a longer time. The peak values of the OIT electron percentage at different operating pressures are summarized in Table I. These values can be well fitted by a function form of exponential decay. Taking the magnitude of the electron density into account, we know that the magnitude of the OIT electron density drops even more drastically than the OIT electron percentage shows as the pressure increases. This result implies that it would be difficult for the breakdown to take place at high operating pressure. Our simulation shows that at the pressure of 200 Torr, even 300 Torr, the breakdown can take place but takes a much longer time than at the pressure of 50 Torr. It seems that the breakdown time is approximately in proportion to the pressure in the range from 50 to

<table>
<thead>
<tr>
<th>Pressure (Torr)</th>
<th>50</th>
<th>100</th>
<th>150</th>
<th>200</th>
<th>250</th>
<th>300</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron density (10^{19} \text{ m}^{-3})</td>
<td>1.3</td>
<td>1.1</td>
<td>0.75</td>
<td>0.52</td>
<td>0.36</td>
<td>0.15</td>
</tr>
<tr>
<td>Maximal OIT electron percentage</td>
<td>6.4</td>
<td>2.6</td>
<td>1.2</td>
<td>0.69</td>
<td>0.44</td>
<td>0.31</td>
</tr>
</tbody>
</table>

FIG. 11. The percentage of electrons with energy over the ionization threshold accounting for the total electrons versus the discharge time.
300 Torr. Qualitatively, it is easily understood since the electrons moving in a denser gas undergo more collisions. However, as the discharge time lengthens, the neglected loss mechanisms of charged particles, such as the bulk recombination and diffusional loss, will become significant. Therefore, we did not run simulations for the discharge mode transition at higher pressure in case our simple model fails.

Nevertheless, the breakdown also depends on other factors. As mentioned in Sec. III B, the radius of the needle electrode tip directly affects the electron density. Another factor, i.e., the needle-plate spacing, should be important for the breakdown; at atmospheric pressure, the breakdown may happen when the needle-plate spacing reduces. Diffusion and bulk recombination mechanisms should be considered if a longer scale of discharge simulation is carried out. These questions need to be studied further.

IV. CONCLUSIONS

The argon discharge between the needle-plane electrodes at high pressure has been investigated using PIC-MCC simulation. In the simulation, we fully took into account both ion and electron kinetics; we did not use any macroscopic coefficients, such as the first Townsend ionization coefficient, and treated the collision processes in an adequate way with MCC technique. At atmospheric pressure the discharge was a typical corona discharge. As the operating pressure was lowered, the corona discharge turned to a glowlike discharge in the needle electrode pointing direction. Along the direction, an equilibrium plasma channel came into existence. The transition of the discharge pattern depended on the occurrence of the second peak of fast electrons with energy over the ionization threshold; whether an equilibrium plasma could evolve from a corona discharge was determined by the magnitude of the fast electron peak.

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