Particle-in-cell/Monte Carlo simulation of filamentary barrier discharges

Weili FAN (范伟丽)1,2,3, Zhengming SHENG (盛政明)1,2,4 and Fucheng LIU (刘富成)3

1 Key Laboratory for Laser Plasmas (MoE) and Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, People’s Republic of China
2 Collaborative Innovation Center of IFSA (CICIFSA), Shanghai Jiao Tong University, Shanghai 200240, People’s Republic of China
3 College of Physics Science and Technology, Hebei University, Baoding 071002, People’s Republic of China
4 SUPA, Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom

E-mail: fanweili@sjtu.edu.cn

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Abstract
The plasma behavior of filamentary barrier discharges in helium is simulated using a two-dimensional (2D) particle-in-cell/Monte Carlo model. Four different phases have been suggested in terms of the development of the discharge: the Townsend phase; the space-charge dominated phase; the formation of the cathode layer, and the extinguishing phase. The spatial-temporal evolution of the particle densities, velocities of the charged particles, electric fields, and surface charges has been demonstrated. Our simulation provides insights into the underlying mechanism of the discharge and explains many dynamical behaviors of dielectric barrier discharge (DBD) filaments.

Keywords: dielectric barrier discharge, filamentary discharge, particle-in-cell/Monte Carlo simulation

(Some figures may appear in colour only in the online journal)

1. Introduction

Dielectric barrier discharge (DBD) has been the subject of active research due to its wide applications [1–6]. Depending on the external conditions, the discharge can be sustained in different modes: Townsend, filamentary or glow [5–7]. Generally, it is believed that a uniform discharge can be produced under the Townsend or glow regime. Recently, it has been shown that the glow DBD is not always uniform but possibly exhibits isolated filaments or filamentary structures. A rich variety of well-ordered, stable or dynamic, filamentary structures have been observed in the glow discharge regime [7–10]. These intriguing phenomena drive fascination and meanwhile pose deep questions about the underlying physics of DBD.

To date, great efforts have been made in experimental studies on filamentary barrier discharges [1–4]. However, the underlying mechanism is still not fully clear, given the fact that many space- and time-resolved diagnostics are not available due to the high collisionality, rapid dynamical behavior, and small scale and large space gradients of the discharge. As a significant tool, the numerical simulation has attracted increasing attention in recent years. Substantial efforts have been made for fluid-based simulations, which successfully explain the elementary properties of the discharge [7–13]. These models are generally based on a macroscopic description of electron and ion kinetics, in which a Maxwellian distribution of the velocities of the charged particles is assumed. Since the discharge is inherently complex and has nonequilibrium, in which the velocities of the particles could stray from the Maxwellian distribution, a full kinetic simulation is required [14–23], which could provide further kinetic and statistical information.

In this contribution, the plasma behavior in filamentary barrier discharges operating in a glow regime is investigated using a two-dimensional (2D) particle-in-cell/Monte Carlo
Consequently, the value $p$ is sustained in a glow mode. The right electrode at $200$ kHz, $V_{p,p} = 870$ V is applied to the left electrode.

We use the 2d3v PIC-MCC code XOOPIC for simulation [21]. Here a $(x, y)$ bounded electrostatic model is specified. At the left boundary $x = 0$, an equipotential boundary is defined, whose potential is given by the applied voltage. The right boundary is defined to be a perfect conductor that is grounded. These two boundaries are given as the Dirichlet boundary conditions. For the top and bottom sides of the system, as the particle boundary condition, the charged particles which strike on the boundaries will be deleted. Meanwhile, as the field boundary condition, the Neumann boundary condition is used with $E_y = 0$. On the other hand, at the interface between the plasma and dielectric layers, the charged particles can accumulate on the surface of the dielectric layer when they reach the layers. It is assumed that the positions of surface charges are fixed once they deposit on the layer, which can neither move along the dielectric surface nor draw back into the gas gap. In the simulation, the behaviors of the electrons and He\textsuperscript{+} ions are tracked and the neutrals are considered to distribute uniformly. In the procedure of Monte Carlo collisions, elastic, ionization, and excitation collisions between electrons and neutrals are accounted for. On the other hand, the elastic scattering and charge exchange collisions between ions and neutrals are taken into account [19, 20, 25, 26]. We assume that the initial electrons and ions are distributed uniformly, with the density $10^{15}$ m\textsuperscript{-3}. The time step in the simulation is set as $10^{-13}$ s. The computational grid is defined to be $300 \times 300$ cells, with a spatial step $\Delta x = 5 \times 10^{-6}$ m, $\Delta y = 1 \times 10^{-4}$ m. Despite the fact that $\Delta y$ is somewhat coarse, this has little influence on the basic physics that we have discussed since the main plasma processes do not occur in this direction. This is a basic model to give a qualitative explanation of the dynamical aspects of the DBD filaments.

3. Results and discussion

Figure 2 presents the evolution of filamentary discharges operating in the glow regime. We can subdivide it into four distinct phases, which are: the Townsend phase (figure 2(a)), the space-charge dominated phase (figure 2(b)), the formation of the cathode layer phase (figure 2(c)), and the extinguishing phase (figure 2(d)).

3.1. Townsend phase

The discharge in this phase is featured by impact-ionization avalanches. When the simulation starts, all of the initial electrons move quickly to the anode and deposit on the left dielectric layer within 0.03 $\mu$s. In contrast, the initial ions that are much heavier move slowly and most of them are left in the gas gap. These ions obtain sufficient energy with the increase of the applied voltage swing, and some energetic ones lead to secondary electron emission when striking occurs on the surface of the right layer. The secondary electrons are greatly accelerated to the anode and impact-ionization collisions occur, giving rise to the formation of distinct filaments, as shown in figure 2(a). At this stage, all the electrons produced in avalanches will accumulate immediately on the left dielectric layer to form surface charges, while the majority of ions are left in the gas gap, inducing secondary electrons as the seed charges to sustain the discharge. Therefore the plasma channels are positively charged by He\textsuperscript{+}, with the ion density significantly larger than that of electrons. Moreover, the profile of the total electric field in the $x$ direction ($E_x$) is approximately flat along the gas gap $x \in [0.5 \text{ mm}, 1 \text{ mm}]$, as shown in figure 2(a1) and (a2). Only small distortions can be observed. The influence of the space charges on the total electric field is nearly negligible.
3.2. Space-charge dominated phase

During this discharge phase, the space charge will establish a remarkable electric field, leading to full development of the discharge. As shown in figure 2(b), a great deal of electrons have accumulated on the left layer with the development of the Townsend discharge. They will produce an opposite electric field in the vicinity of the left dielectric layer to prevent further deposition of the subsequent electrons generated in discharges (figures 2(b1) and (b4)). Consequently, the electrons start to accumulate in the discharge gas gap; we call these the space electrons. As shown in figure 2(b2), the left part corresponds to the bulk plasma region where the space ions and electrons coexist, while in the right part the distribution of ions and electrons separates. We define the boundary where the electrons and ions separates as the edge of the plasma sheath. It is evident that in the regions of bulk plasma, the profiles of the electric field always exhibit as platforms with $E_x = 0$ (figures 2(b3) and (b4)). Remarkable distortions of the electric field are produced in regions of the plasma sheaths, due to spatial separation of He$^+$ and electrons. These $E_x$ peaks have two functions: (1) driving He$^+$ towards the right dielectric to generate the secondary electrons and (2) accelerating the secondary electrons to the left layer for electron avalanches. They lead to the full development of the discharge and proliferation of the charged particles.

Figure 2. The evolution of filamentary barrier discharges. The electric field along the $+x$ direction is defined to be positive. The 2D $E_x$ profiles in the gas gap are displayed in the third column, while the fourth column denotes the corresponding three-dimensional $E_x$ distributions. (a) Townsend discharge at $t = 0.57 \mu s$. The white arrow in (a2) shows the moving direction of the electrons. The $E_x$ shown in (a1) has been multiplied two times. (b) Space-charge dominated discharge phase, $t = 0.78 \mu s$. The $E_x$ peak marked by the black arrow has been magnified in the nearby inset ($y = 3.9$ mm). (c) Formation of the cathode fall layer, $t = 0.87 \mu s$. At this instant, the total number of space charges in the gas gap has been attained to the maximum. (d) The discharges have decayed, $t = 1.27 \mu s$. The edges of the plasma sheaths are indicated by the dashed lines, as shown in (b2) and (c2). Note that each filament has its own plasma sheath corresponding to its developing level. Here, in a simple way, we approximately utilize one line to indicate the boundaries of the plasma sheaths for all the filaments.
3.3. Formation of cathode layer

With the increase of the number of plasma particles, the regions of bulk plasma expand gradually. This exhibits as a shifting of the plasma sheath towards the right dielectric layer, as shown in figure 2 and later in figure 4. A stable cathode fall layer is generated when the total number of charged particles has attained to the maximum. At this instant, the electrons generation due to ionization collisions just compensates the loss of electrons owing to deposition on the left dielectric layer. From figure 2(c), it can be seen that the cathode layer has been established for the discharges at the bottom part of the gas gap $y \in [0, 18 \text{ mm}]$. However, the filaments located at the top part remain in the space-charge dominated phase. These discharge stages can be identified by profiles of $E_x$, as shown in figures 2(c3) and 2(c4). Here we can see that the $E_x$ peaks in the lower part have significantly deceased, suggesting that these filaments tend to decay. In contrast, the $E_x$ peaks in the top part are still very strong, which indicates that these filaments are developing intensely. The position of the cathode fall layer is nearly invariant with further development of the discharge.

3.4. Extinguishing phase

With more surface charges accumulated on the two dielectric layers (as shown later in figure 6), the electric fields in the gas gap start to decrease. The $E_x$ peaks in the plasma sheaths gradually disappear. Correspondingly, the discharge decays and the density of the charged particles declines (figure 2(d)).

All these stages can be distinguished by time evolution of the number of simulated particles, as shown in figure 3. It is evident that there are nearly no space electrons during the Townsend phase, but that they move quickly and accumulate on the left dielectric layer. The rise time is mainly determined by the space-charge dominated phase. Here the discharge develops intensely and appreciably charged particles have been generated. The cathode fall layer is established when the total number of charged particles has reached the maximum. After this kink, the discharge starts to decay. We can see that the discharge has been extinguished before the applied voltage reaches the peak. This is well consistent with the experimental observations [3, 9]. These discharges will be ignited again; they are prone to forming at the old positions due to the ‘memory effect’, in the following half period when the applied voltage reverses.

To demonstrate the kinetic properties of the discharge, the velocities of different charged particles have been studied, as shown in figures 4 to 5. Here the velocity along the $x$ direction ($v_x$) is focused on, and we define the $v_x$ along the $+x$ direction as positive. We can see clearly that both of the ions and electrons exhibit complex kinetic behaviors with the development of the discharge. It is shown that (1) the velocities of He$^+$ and electrons are in the order of $10^4 \text{ m s}^{-1}$ and $10^5 \text{ m s}^{-1}$, respectively. Both of these velocities are significantly increased when the discharge transits from the Townsend discharge to the space-charge dominated phase (figure 4). Then, they decline as the discharge expires. (2) The energetic He$^+$ ions (with high kinetic energy) are generally produced in the regions of plasma sheaths (figures 4(a2) and (a3)), which are greatly accelerated by the strong electric field. In contrast, the energetic electrons can be found all over the discharge channels, no matter in the bulk plasma region, or...
the plasma sheaths (figures 4(b2) and (b3)). These electrons, which originate from the secondary electrons and their progeny from subsequent avalanches, are accelerated to the anode and integrate into the bulk plasma eventually. (3) The velocity distributions of the charged particles are complex and dynamic. As shown in figure 5(a2), the velocities of He⁺ in the lower part $y \in [0, 18 \text{ mm}]$, where the discharge has transited into the space-charge dominated phase, is obviously larger than that of the upper part. Then, these filaments start to decay, while the velocities of the particles in the upper part are significantly increased (figures 5(a3) and (b3)).

Next we examine the evolution of surface charges with the development of the discharge. As illustrated in figure 6, we can see that (1) the distribution of electrons is more uniform, which generally takes up a wider area than that of the ions. This is attributed to the difference in electron and ion velocities in the gas gap. (2) The accumulation of surface charges is synchronized with the discharge evolution. A large quantity of surface charges first deposits on the lower part of the gas gap and then transfers to the upper part, where the filaments are ignited later. (3) The density of surface charges is in the order of $10^{-5} \text{ C m}^{-2}$. They will establish a field with an order of $10^6 \text{ V m}^{-1}$, which is comparable with the fields of applied voltage and space charges as shown in figure 2. It plays a primary role in extinguishing this discharge, while assisting the next discharge when the applied voltage has been reversed.

4. Conclusion

The filamentary barrier discharges operating in the glow regime in helium are studied using a 2D particle-in-cell/Monte Carlo simulation. The discharge evolution as well as the kinetic behaviors of the plasma particles have been demonstrated. It is shown that the discharge undergoes four different phases: the Townsend phase; the space-charge dominated phase; the formation of the cathode layer, and the
extinguishing phase. The velocities of different plasma particles are presented, which are $10^4 \text{ m s}^{-1}$ and $10^6 \text{ m s}^{-1}$ for He$^+$ and electrons, respectively. The evolution of surface-charge distribution has also been studied. These results unveil the deep physics of filamentary barrier discharge and provide important kinetic information to aid understanding of the dynamical behaviors of the discharge.

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References