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PIC Simulation of Microscale Breakdown in Gaps Filled with a Non-Uniform Background Neutral Gas Density

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An explicit, electrostatic particle-in-cell code with complex boundary conditions and direct simulation Monte Carlo particle collisions is utilized to investigate 1D direct current breakdown. Two electrodes are separated by a microscale gap with a non-uniform neutral gas distribution (e.g. a higher density near the anode as a result of vacuum seal failure near the anode). Breakdown was found to be sensitive to the neutral gas density distribution across the gap. If the gap is large enough that the cold field emission is negligible then gas concentrated near the cathode results in higher breakdown voltages since electrons leaving the cathode are not yet energetic enough to ionize the high density neutral gas near the cathode. Conversely, if the gap size is of order several mean free paths then gas concentrated near the anode results in lower breakdown voltages because electrons reaching the anode have energies near the peak of the ionization cross section.

1. Introduction

There is considerable interest in understanding the time evolution of non-equilibrium atmospheric pressure gas discharges in order to better design high-power switches, microelectronics, and other plasma devices. Even electrodes initially separated by vacuum can, if the seal is broken, fill non-uniformly with atmospheric air and thus potentially breakdown and fail. The desire to prevent potentially damaging breakdown has generated new interest in microscale discharges in air which can be rarefied and non-equilibrium due to the small scales involved, despite the atmospheric column density of gas between the electrodes.

Gas discharge in large (with respect to the electron ionization mean free path) scale gaps is understood to occur when an electron avalanche leads to the breakdown of the neutral gas in the gap. This is the so-called Townsend discharge and, assuming the background neutral gas is uniform, the breakdown voltage follows the Paschen curve and depends on electron impact ionization of the neutral gas and secondary emission from the cathode [1]. For small gaps, it has been found that cold field electron emission (CFE) can explain the measured breakdown voltage deviation from the Paschen curve [2, 3]. Furthermore, even in large gaps, as breakdown proceeds the cathode sheath becomes thin enough (due to increasing plasma density) that cold field emission dominates and super-exponential current growth results [4].

In the present work we simulate the dynamics of breakdown in microscale gaps with a total column of neutral gas in the gap equal to atmospheric pressure times the gap width. However, the background neutral gas density is not uniform across the gap in order to investigate what effect such non-uniform gas distributions might have on the breakdown voltage. This non-uniform background gas distribution could be due to a vacuum seal failure and the resultant flow of atmospheric gas into the vacuum gap. Specifically it is important to know whether gas concentrated near either the anode or cathode results in lower breakdown voltages than predicted by the Paschen curve. If lower breakdown voltages do result, they must be accounted for when designing failure tolerance for a vacuum gap.

2. Model

The temporal evolution of the collisional partially ionized gas is solved using the Particle-in-Cell (PIC) technique [5] along with a Direct Simulation Monte Carlo (DSMC) stochastic collision model [6] that includes electron-neutral elastic, excitation, and ionization collisions using available lab data [7-12]. Since the charged particle density increases 4–5 orders of magnitude during breakdown, the charged simulation particles are dynamically merged periodically so that there are ~60 electrons, ~60 ions, and ~30 neutrals per cell throughout breakdown. Selection of merger particles nearby in velocity space keeps energy errors small and any lost energy is added back as thermal energy for that element.

The current 3D finite element unstructured mesh PIC implementation utilizes an explicit Verlet time integration of the field solve and particle movement equations. In addition, the simulations include Auger neutralization of ions at the cathode resulting in a secondary electron yield given by:

$$\gamma_{se,s} \approx 0.016(E_{iz,s} - 2E_{\phi}), \qquad (1)$$

where $E_{iz,s}$ is the ionization energy of the incident ion and E_{ϕ} is the work function of the cathode in eV [13]. Finally, the electron flux due to Fowler-Nordheim cold field emission [14] has been included since for small gaps the electric field near the surface becomes sufficiently large that there is significant electron flux via CFE. For further details on the simulation model, see [4].

The present simulations of breakdown are of an iron cathode at ground separated by a variable distance from a silver anode held at a variable dc voltage. It is assumed that the gap is initially filled with air at 300 K consisting of 78.8% N_2 and 21.2% O_2 by number. Three background neutral gas distributions were used: a uniform background density at atmospheric pressure and two Gaussian density distributions with a standard deviation equal to $^1/_3$ of the gap width, one centered at the cathode and the other at the anode. In order to compare the breakdown voltages, the total mass of neutral gas in the gap was kept constant between each of the distributions.

Figure 1 shows a schematic of the Gaussian neutral gas density distribution used to simulate vacuum failure near the anode. It would be computationally expensive to model the neutral gas expansion while maintaining an appropriate timestep for the electron dynamics and therefore an initial Gaussian density distribution is used to simulate the neutral gas density sometime after a vacuum seal breaks. Other initial Gaussian distributions may yield more or less pronounced effects on the breakdown voltage and could be investigated in the future. In order to trigger breakdown, the gap is filled with an initial quasi-neutral plasma (78.8% N_2^+ and 21.2% O_2^+) with an electron density 4×10^{-9} times that of the background neutral density. This initial plasma might be thought of as being generated by solar ionization or cosmic rays since the equilibrium plasma fraction at 300 K is essentially zero.

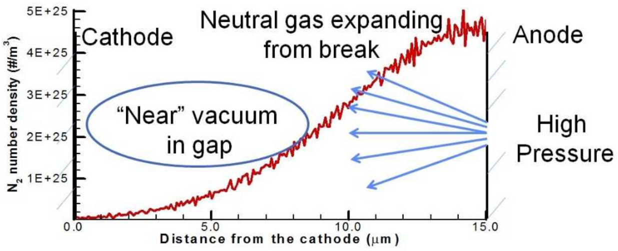

Figure 1: Schematic of the initial neutral gas density distribution (red curve) in the case that the vacuum seal broke near the anode.

The simulations used a timestep size from 2.5×10^{-15} s for the smallest gaps to 2×10^{-14} s for the largest gaps based on satisfying both the collision timescale and the requirement that (typical) particles not cross a cell in a single timestep. The simulated breakdown dynamics were found to be insensitive to at least 10-fold changes (reductions and increases) in the initial plasma density as well as 2-fold changes in the number of simulation particles per cell, the timestep, and the grid size (0.01–0.1 μm depending on gap size, typically 200–400 cells).

3. Results

Figure 2 shows the minimum voltage resulting in breakdown (the breakdown voltage) versus the size of the electrode gap. For the simulation data points the breakdown voltage is defined as a greater-than exponential rise in the anode current as the voltage collapses and a quasi-neutral plasma forms across the gap (see [4] for further discussion). Furthermore, the simulations were limited to 15 ns and thus the breakdown voltages are an upper limit within several percent of the actual simulation breakdown voltage. The green circles are data taken from [15], the dashed line is the theoretical Paschen curve assuming a secondary emission coefficient of 0.023, and the solid lines show the simulated breakdown voltages for three different neutral gas distributions.

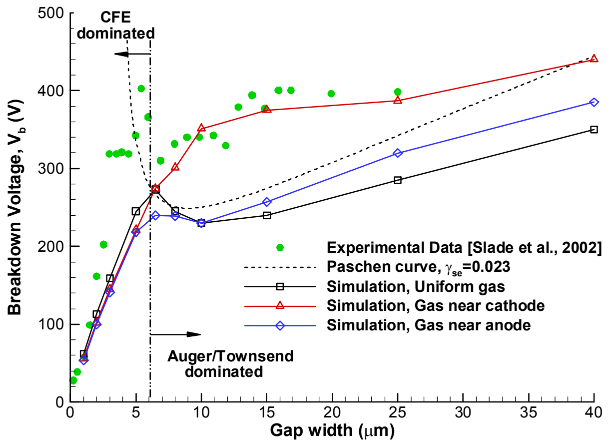

Figure 2: Comparison of breakdown voltage versus gap size for three different neutral gas distributions: Uniform (black), higher density near the cathode (red), and higher density near the anode (blue). Gaps smaller than ~6 μm are dominated by cold field emission (CFE).

Relatively good agreement between the simulated breakdown voltage for uniform neutral gas density and the Paschen curve is obtained for large gaps (electron production dominated by ionization and Auger neutralization). The simulated breakdown voltages are less than the theoretical Paschen curve values for the largest gaps because currently the model does not properly account for energy lost in double ionization or dissociative ionization collisions (a total ionization cross section is used and every ionization event is treated as single ionization in terms of energy loss). For small gaps the Paschen curve no longer holds as Fowler-Nordheim CFE becomes the dominate source of electrons. The simulation breakdown voltages agree well with the experimental results [15] given the uncertainty in the electric field enhancement due to surface roughness.

In Figure 2 it can clearly be seen that the neutral gas density distribution has a large effect on the breakdown voltage for large gaps in which the Townsend process dominates. It can be seen that higher gas density near the cathode results in increased breakdown voltages. This occurs because the secondary electrons created by Auger neutralization at the cathode surface do not have sufficient energy for ionization until they have moved further into the gap, passing the high neutral density region very near the cathode. Even once the electrons do have sufficient energy, the ionization cross sections peak at ~100 eV which for a typical breakdown voltage (~300V) occurs after the electron crosses at least 1/3 of the gap (assuming no energy loss due to excitation) where the neutral density has fallen by ~67% for the case with the gas density peaked near the cathode. Thus the ionization rate is much lower for an electron if gas is concentrated near the cathode versus uniformly distributed across the gap.

If the neutral gas density is higher near the anode (as shown in Figure 1), then more complicated behavior is observed. For gaps which are no more than several mean free paths wide (~10 μm), the breakdown voltage is seen to decrease relative to the uniform background gas case while for larger gaps many mean free paths wide the breakdown voltage actually increases.

When the gap is less than several mean free paths wide, the ionization rate is increased for the first couple of collisions since electrons from the cathode have been able to accelerate to energies near the peak ionization cross section before reaching the dense neutral gas closer to the anode. In the uniform gas, the electrons undergo energy-losing excitation collisions while accelerating which prevent the average electron from reaching the higher energies at which the ionization cross section peaks. Therefore an electron, on average, produces more secondary electrons (and ions) across the gap when the neutral background gas is concentrated near the anode as compared to when the background gas is uniform.

However, for very large gaps with gas concentrated near the anode, after the first couple of collisions the ionization rate becomes much less than if the gas were uniform. This is because the collision rate in the high density region near the anode is much higher and thus the electrons do not gain as much energy between collisions by accelerating along the field as they do when the gas is uniform and the collision rate is lower. In other words, the electrons, after the first couple collisions, now lose more energy to excitation collisions which lowers the ionization rate as fewer electrons have sufficient energy to ionize the gas. For sufficiently large gaps this reduction in ionization rate dominates the initial increased ionization rate and thus an electron, on average, produces fewer secondary electrons when traversing the gap.

4. Conclusions

An explicit, electrostatic PIC code with complex boundary conditions and DSMC particle collisions is utilized to investigate one dimensional direct current breakdown between two electrodes separated by a non-uniform neutral gas distribution. The simulation model includes Auger neutralization and cold field electron emission from the cathode as well as electron-neutral elastic, ionization, and excitation interactions. The simulated breakdown voltages at various electrode gap sizes are compared to experimental data and the Paschen curve. Breakdown was found to be sensitive to the neutral gas density distribution across the gap. Specifically, if the gap is large enough that cold field emission is negligible then gas concentrated near the cathode results in higher breakdown voltages since electrons leaving the cathode due to Auger neutralization are not yet energetic enough to ionize the high density neutral gas at the cathode. Conversely, if the gap size is of order the mean free path then gas concentrated near the anode results in smaller breakdown voltages because the electrons reaching the higher density region near the anode have energies near the peak of the ionization cross section. These lower breakdown voltages should be taken into account when designing vacuum electronics for failure tolerance.

5. References

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