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Two-dimensional particle-in-cell simulations of standing waves and wave-induced hysteresis in asymmetric capacitive discharges

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Abstract
Asymmetrically excited, high frequency cylindrical capacitive discharges are widely used for materials etching and thin film deposition. Two-dimensional (2D) electrostatic particle-in-cell (PIC) simulations show the existence of standing waves and wave-induced hysteresis of the plasma density, i.e. two different steady states for the same driving rf voltage amplitude, when the voltage is increased from a low value or decreased from a high value. The phenomenon is explored over a range of pressures (10–30 mTorr) and frequencies (60–80 MHz). Examined at 73 MHz, with increasing gas pressure, the hysteresis loop gradually shrinks and vanishes. To understand the hysteresis induced by \( z \)-symmetric and \( z \)-antisymmetric radial wave propagation modes, the PIC results are compared with a nonlinear transmission line model assuming uniform bulk plasma density, to determine the symmetric and antisymmetric voltage amplitudes. The model results are in good agreement with the PIC observations, showing central-low and central-high profiles of the antisymmetric mode voltage at low density and high density, respectively. The results are then used to determine the parameters of a lumped circuit model of the two modes, from which the hysteresis is induced by the density dependence of the symmetric and anti-symmetric wave mode absorbed electron powers. For the low density state, the discharge is sustained mainly by the symmetric mode excitation. At high density, the discharge is sustained by both symmetric and anti-symmetric modes, with the latter partly showing a spatial resonance. The results are also shown to be frequency dependent, with an onset of the hysteresis at about 66 MHz.

Keywords: asymmetric capacitive discharge, standing waves and wave-induced hysteresis, two-dimensional particle-in-cell simulations, lumped circuit model

(Some figures may appear in colour only in the online journal)
and large areas, such as standing waves and skin effects, come into play and can negatively affect the plasma uniformity [4, 5]. To understand these effects, discharge models and simulations, treating the electromagnetic field both in the linearized frequency domain [6–12] and in the time domain [13–18], have been developed. The linear models initially considered uniform electron density in the bulk plasma and fixed sheath size, but linear (in frequency domain) transmission line models were later coupled to Child law sheaths and to particle and energy balance to obtain more self-consistent radial variations of the wave properties, sheath size, and electron density [7, 19–23]. Two-dimensional numerical simulations in the frequency domain, which considered plasma transport, were also used to self-consistently study the electromagnetic effects [9–12, 24]. In asymmetrically excited capacitive discharge, harmonics can be nonlinearly excited near the series resonance frequency [25–27], and the resulting enhancement of electron heating has been investigated by electrostatic and electromagnetic calculations [28–36]. Experiments indicate that the discharge nonlinearities can significantly affect the plasma uniformity [37–39], with the shortened wavelengths of the surface waves of the harmonics giving rise to radially central-high plasmas, related to the generation of harmonics, with the central peaks increasingly enhanced with increasing voltage, along with the increasing harmonic content [40–42].

Both a \( z \)-symmetric [5–7, 19, 43–47] and a \( z \)-antisymmetric mode [8, 23, 45, 48–53] can exist in an asymmetrically excited capacitive discharge. In previous work, considering only the symmetric mode within the central region over the powered electrode, we constructed a nonlinear (in time domain) radial transmission line model for single frequency [54] and dual frequency [55] driven discharges. The model is fully electromagnetic with a single nonlinear homogeneous or Child law sheath including the nonlinear coupling of the series resonances and spatial resonance effects. The model was later extended to investigate a more realistic asymmetrically-excited discharge with a powered-electrode/plasma/grounded-electrode sandwich structure, incorporating both symmetric and antisymmetric wave modes [56], and waves generated in the electrostatic limit, with uniform bulk plasma density assumed. The role of discharge asymmetry in determining the spatial resonances was analytically examined by scanning the rf driving frequency from 30 MHz to 120 MHz [23]. With increasing frequency, a series of system resonances showing symmetric and antisymmetric character was found. It was also found that adding a dielectric layer, which increases the effective sheath width over the powered electrode, can somewhat suppress wave effects [57]. Using an electrostatic implicit particle-in-cell (PIC) code, Eremin et al found that a high frequency driven large-area capacitively coupled plasma (CCP) discharge can exhibit strong wave effects [52]. They also demonstrated that the two types of wave modes lead to non-uniformities of the plasma density profile [58], and that large collisionality gives rise to a strong damping of the waves as they propagate [53].

In the present work, to capture the underlying physics of asymmetrically-excited cylindrical capacitive discharges, self-consistently considering the wave effects, electron heating and plasma transport, a 2D electrostatic PIC simulation driven by a voltage source is employed. The simulated discharge is somewhat smaller than that used in most commercial applications, and argon gas cross sections with reduced (helium) ion mass are used to reduce the computation time, but the important physics processes are preserved. We observe a plasma density hysteresis, similar to the hysteresis in inductively coupled plasma at a transition between E-mode (capacitive discharge) and H-mode (inductive discharge) [59]. In section 2, we describe the 2D electrostatic PIC simulation and clarify the application of electrostatic simulations to our system, where both \( z \)-symmetric and \( z \)-antisymmetric propagating waves can exist. In section 3, the observed driving voltage hysteresis of the plasma density at different pressures is presented. A nonlinear electromagnetic transmission line model [56] is used to calculate the symmetric and antisymmetric mode voltages at low and high density, and these are compared with the PIC simulations. The corresponding radial voltage amplitude profiles are interpreted using a simple lossy dispersion relationship. Section 4 gives a lumped circuit model to analyze the hysteresis and compares the corresponding model results with the 2D PIC simulations. Conclusions and further discussion are presented in section 5.

2. 2D electrostatic PIC simulation

As shown in figure 1, the 2D PIC simulation has an asymmetric cylindrical (axisymmetric) geometry with center of symmetry at \( r = 0 \). The reactor is \( 2l = 0.02 \) m in height and \( R_0 = 0.1 \) m in radius. The bottom electrode is \( R_{x-} = 0.06 \) m in radius and driven by a voltage source. An 0.01 m insulator with relative dielectric constant of unity (light gray line) separates the driven electrode from the grounded side and top chamber surface. The values of the mean insulator ring radius \( R_x \) and \( R_{x+} \) are 0.065 m and 0.07 m, respectively.

![Figure 1. Schematic of the 2D electrostatic PIC simulation asymmetrically driven by an rf voltage source. The driven electrode radius is \( R_{x-} = 0.06 \) m and the chamber radius is \( R_0 = 0.1 \) m with the electrode gap \( 2l = 0.02 \) m. The values of \( R_x \) and \( R_{x+} \) are 0.065 m and 0.07 m, respectively.](image-url)
both $z$-symmetric and $z$-antisymmetric radial wave modes. The axially-varying field symmetries of the two modes are shown in figure 2. The electromagnetic (EM) wave dispersion relation for a bulk plasma width $2d$ and two equal sheath widths $s$ over the driven and grounded electrodes is [23, 52, 53, 60]

$$\kappa_p \beta \tanh \beta s + \alpha \tanh \alpha d = 0, \tag{1}$$

for the symmetric mode, and

$$\kappa_p \beta \tanh \beta s + \alpha \coth \alpha d = 0, \tag{2}$$

for the antisymmetric mode, where $\alpha^2 = k^2 - \kappa_p \omega^2/c^2$ and $\beta^2 = k^2 - \omega^2/c^2$ are the squared axial wave propagation constants in the plasma and in the sheath, respectively, with

$$\kappa_p = 1 - \frac{\omega_p^2}{\omega(\omega - j\nu)} \tag{3}$$

the relative plasma permittivity, $\omega_p$ the electron plasma frequency in the bulk, $\omega$ the wave frequency, and $c$ the speed of light.

Taking the limit $c \to \infty$ gives the electrostatic (ES) limit, where $\alpha$ and $\beta \to k$. For low effective collisionality, we can set $\nu = 0$, so that (1) and (2) give [52, 53, 60]

$$\omega = \omega_p \sqrt{\frac{\coth kd}{\coth ks + \coth kd}} \tag{4}$$

for the symmetric mode, and

$$\omega = \omega_p \sqrt{\frac{\tanh kd}{\coth ks + \coth kd}} \tag{5}$$

for the anti-symmetric mode.

As an example, solving (1)–(5) at $n_e = 5 \times 10^{15} \, \text{m}^{-3}$, $d = 0.01 \, \text{m}$, $s = 0.002 \, \text{m}$, driven electrode radius $R_x = 0.065 \, \text{m}$, driving frequency $f = \omega/2\pi = 73 \, \text{MHz}$, gives the dispersion curves for the EM mode and the corresponding ES limit shown in figure 3. For the anti-symmetric mode, the EM mode and its ES limit give practically the same dispersion relation for all $k$. For the symmetric mode, the EM dispersion curve and its ES limit differ for small $k$ value (long wavelength), but in the frequency range of interest, $\omega \ll \omega_p$, the EM dispersion relation gives $k \approx 0$ (an infinite wavelength), corresponding to the ES limit. This justifies the use of an electrostatic 2D PIC code to capture both the symmetric and antisymmetric mode wave propagation properties in this frequency range of capacitive discharges. A similar justification for using an electrostatic 2D PIC code to simulate a larger, symmetrically-excited capacitive discharge was given by Eremin [52, 53].

The particle-in-cell Monte Carlo collision (PIC-MCC) code XOOPIC used here was originally developed by Verboncoeur et al [61]. The details are described in references [61–63]. The neutrals are assumed to form a uniform background at constant pressure and temperature. The charged particles (super-particles) are advanced in phase space using an explicit leap-frog algorithm. A super-particle represents a cluster of $10^8$–$10^9$ actual electrons (or ions). The reactions considered are elastic, excitation and ionization collisions for electrons, and elastic and charge transfer collisions for Ar$^x$ ions, using the null collision Monte Carlo model [63]. The ion mass is set to be 10 percent of the actual argon ion mass, $m_i = 0.1 M_{Ar}$, to decrease the computation time, while preserving the important physics processes, particularly the electron power deposited. To further speed up the code, the ion time step is five times the electron time step $\Delta t_i = 5\Delta t_e$ with $\Delta t_e = 10^{-11} \, \text{s}$.

Both electromagnetic and electrostatic fields could be solved in XOOPIC [61]. Here we solve Poisson’s equation by...
a multi-grid method to obtain the voltage distribution and then the electrostatic field by finite differences. The grid spacings are fixed for the simulations with $\Delta r = 0.1/256$ m and $\Delta z = 0.02/64$ m. The chosen time step, number of super particles, and grid spacings ensure practical convergence of the PIC simulations. We also ran a case with increased spatial resolution ($\Delta r = 0.1/512$ m and $\Delta z = 0.02/128$ m) at higher plasma density and the results are very similar to the lower resolution. The bottom electrode has an equipotential boundary condition, $V = V_{rf \cos \omega t} + V_{dc}$ with $V_{rf}$ the rf voltage amplitude and $V_{dc}$ the dc component. A self-consistent dc voltage can be obtained by setting the dc current to zero at each electrode. Instead for simplicity, we take $V_{dc} = -0.83V_{rf}$, as obtained in Child law sheath theory. The small difference between the $V_{dc}$ used here and the self-consistent value would induce a flowing DC current in the circuit. To address this issue, we therefore varied $|V_{dc}/V_{rf}|$ from 0.65 to 1.0, a range where the self-consistent value $V_{dc}$ should exist to make the DC current zero. We observed only small difference (a 14% change in the hysteresis density gap at 73 MHz). The upper electrode and sidewalls are grounded by setting the voltage to zero. Electrons and ions flowing to the dielectric are accumulated, and the resulting field is self-consistently determined in the XOPPIC field solver. At high frequencies, the secondary electron emission from surfaces, induced by ions or electrons, is small and is set to zero. After the system evolves to a steady state, approximately $1 \times 10^6$ super particles for electrons (and ions) are present in the simulation. For most cases shown in this work, the convergence time to steady state is about one day.

### 3. 2D electrostatic PIC/MCC simulation results

#### 3.1. Driving voltage hysteresis of plasma density

A series of 2D PIC/MCC runs were conducted at frequencies of 60–80 MHz. Two initial densities are used, a low density of $7 \times 10^{14}$ m$^{-3}$ and a high density of $1.5 \times 10^{15}$ m$^{-3}$, which give different results when scanning the rf voltage from a small value to a large value, and in the opposite direction. The initial electron and ion temperatures are 3.5 V and 0.026 V, respectively. Sweeping the driving voltage up and down (indicated by arrows) at three different pressures (10, 30 and 60 mTorr), the corresponding peak plasma densities at 73 MHz are shown in figures 4(a)–(c). We see in figure 4(a) at 10 mTorr, that the density approximately linearly increases as the driving voltage increases (□) with a density jump at $V_{rf} \approx 75$ V. Decreasing the driving voltage (∗), the density linearly decreases, with a density jump occurring at $V_{rf} \approx 52.5$ V. The two driving voltage scans give two different density jumps, defining a hysteresis, i.e. two different steady state densities for the same rf driving voltage amplitude. The small differences of the densities in the driving voltage ranges of 40–50 V and 80–90 V are statistical deviations. The voltages of the hysteresis loop are within the range of 30–70 V, i.e. the hysteresis vanishes (figure 4(c)). The hysteresis phenomenon is not seen at a lower driving frequency of 60 MHz and starts to be observed near 66 MHz. The hysteresis will be analyzed in section 4.

Figures 5(a) and (b) show the ion plasma density contours of the low and high density states at 10 mTorr, 60 V, respectively. We can see, in the low density state, that the plasma is maintained mainly within the region $0 < r < R_x$, with a peak ion density $n_i \approx 1.5 \times 10^{15}$ m$^{-3}$ at the discharge center. There is a low plasma density in the outer region $R_x < r < R_0$. At high density, the plasma fills the entire chamber with a relatively flat profile but with a thicker sheath over the driven electrode.
3.2. Symmetric and anti-symmetric mode wave propagation

As is well known, for low pressure discharges, the wave propagation is nearly lossless, and at high frequencies the standing wave effect can be significant [6, 8]. At high pressures, the wave propagation is lossy and the standing wave effect is reduced [53]. Also, both \( z \)-symmetric and \( z \)-antisymmetric waves can exist in an asymmetric system, which could be responsible for the observed hysteresis. Integrating the electric fields in the \( z \) direction (see figure 2) to obtain the voltages gives a voltage description of the wave propagation modes [54–56].

The symmetric mode voltage is

\[
V_s(r, t) = V_t(r, t) + V_b(r, t)
\]

where \( V_t(r, t) \) is the upper electrode potential with respect to the plasma potential, and \( V_b(r, t) \) is the plasma potential with respect to the lower electrode. Similarly, the anti-symmetric mode voltage is

\[
V_a(r, t) = V_t(r, t) - V_b(r, t)
\]

To explore the wave propagation at 73 MHz, we analyzed from the PIC simulations the symmetric and anti-symmetric mode voltage magnitudes of the Fourier transforms at the fundamental frequency (73 MHz), normalized to the driving voltage, while sweeping the driving voltage up and down. The results at pressure 10 mTorr and driving voltage 60 V are shown in figure 6. Figures 6(a) and (b) give the symmetric and anti-symmetric mode voltage versus radius, respectively corresponding to peak densities \( n_e \approx 1.5 \times 10^{15} \text{ m}^{-3} \) and \( n_e \approx 6 \times 10^{15} \text{ m}^{-3} \). The symmetric mode voltage amplitudes are independent of radius due to the infinite wavelength as discussed in section 2. For the low density state, the antisymmetric mode voltage has a center-low profile, meaning the wave radially decays from the driven electrode edge into the center. However, at high densities, the antisymmetric mode voltage shows a center-high profile, i.e. a standing wave effect.

We compare the results to the nonlinear electromagnetic transmission line model developed previously [56] to determine the mode voltages at the same external discharge parameters. We use \( c \rightarrow 10c \) to approximate the electrostatic limit. The uniform bulk plasma densities \( n_e = 8 \times 10^{14} \text{ m}^{-3} \) and \( n_e = 4 \times 10^{15} \text{ m}^{-3} \) in the model are approximately estimated by spatially averaging the plasma density in the 2D PIC simulations. Despite simplifying the radially varying plasma density by a constant value in the transmission line model, we find that the voltage amplitude profiles within the driven electrode region \( r < R_x \) agree reasonably well with the results of the 2D PIC/MCC simulation (see figure 7, described below). The outer cylindrical region \( R_x < r < R_0 \) shows a deviation due to the existence of the insulator (on the lower electrode) and the sidewall in the 2D PIC simulation. Another reason for a difference is that there is a low plasma density in the region \( R_x < r < R_0 \) at the low density state as shown in figure 5(a), significantly different from the assumption of a uniform bulk plasma in the transmission line model. Radially excited nonlinear harmonics exist in both the 2D PIC simulations and the transmission line model, but these are small for our discharge simulation parameters.

To explicitly show the source of the center-low and center-high profiles of the anti-symmetric mode voltage, the lossy wave dispersion (2) is solved in the electrostatic limit for a

![Figure 5. The contour plots of the ion density from the 2D PIC/MCC simulation for two different states of the hysteresis: (a) the low density state; (b) the high density state. The driving frequency is 73 MHz, the rf voltage is 60 V and the pressure is 10 mTorr.](image-url)
uniform bulk plasma density. The effective collision frequency is \( \nu = 0.35 \omega \) at 10 mTorr. The wave dispersion at low density \( 8 \times 10^{14} \) m\(^{-3} \) and high density \( 4 \times 10^{15} \) m\(^{-3} \) are given in figures 7(a) and (b), respectively. The electrostatic potential has the form

\[
\Phi = V_{rf} J_0(Re(kr)) e^{-Im(kr)f(z)}
\]

with function \( f(z) \) describing the \( z \)-directional variation, the imaginary part of \( kr \) giving the radial decay during the wave propagation, by the factor \( e^{-Im(kr)} \), and the real part of \( kr \) giving the radially-varying amplitude (standing wave effect). For the low density state, a typical sheath width \( s = 0.0035 \) m and a half-bulk plasma width \( d = 0.01 \) m were used. As shown in figure 7(a), the imaginary part gives a value \( \text{Im}(kr_x) \approx 0.8 \), which indicates that the voltage amplitude decays at the center with respect to the edge by a factor of \( e^{-0.8} \approx 0.45 \), even as the real part \( \text{Re}(kr_x) \) gives a radially-varying amplitude. For the high density case, the sheath width decreases to 0.002 m and figure 7(b) shows an imaginary part value \( \text{Im}(kr_x) \approx 0.3 \), indicating a weak decay. The real part has a value of \( \text{Re}(kr_x) \approx 2.0 \) somewhat smaller than 2.405, the zero of the zero-order Bessel function, and induces a significant standing wave effect (or partial spatial resonance), as shown in figures 6(b) and (d).
4. Lumped circuit model of hysteresis

We develop a lumped circuit model to explain the driving voltage hysteresis seen in section 3. The discharge chamber shown in figure 1 is simplified to consist of two circular conducting electrodes of radius $R_0$, separated by a gap of width $2l$, driven by a voltage source across a small opening at radial position $R_e$ in the lower electrode. The driven electrode radius is chosen to be $R_e = 0.065 \text{ m}$ with the insulator neglected. The discharge voltage has a maximum at $r = R_e$ due to the boundary condition $\partial V_{rf}/\partial r|_{r=R_e} = 0$ [56]. The region $0 < r < \chi_0 R_0/\chi_{11}$ is considered to be capacitive with a radius $R_0/\chi_{11}$. Thus for the capacitive area we use $A_a = \pi(\chi_0 R_0/\chi_{11})^2$, with $\chi_0 \approx 2.405$ the first zero of $J_0$, obtaining $A_a \approx 0.39 \pi R_e^2$. For the symmetric mode, the antisymmetric capacitance is then

$$C_a = \frac{\varepsilon_0 A_a}{s},$$

(11)

where $\eta$ is an antisymmetric/symmetric voltage asymmetry ratio (see figure 8); typically, $\eta \lesssim \frac{1}{2}$. To determine $L_a$, we note that the wavenumber $k_a$ for the antisymmetric mode at resonance is given by [23, equation (B12)]

$$k_a^2 = \frac{\omega_{res}^2}{\omega_p^2 \varepsilon_0} = \frac{\chi_{11}^2}{R_e^2}.$$

(12)

Solving for the resonance frequency yields

$$\omega_{res}^2 = \frac{\chi_{11}^2}{R_e^2} \frac{e^2 n_s}{\epsilon_0 m} s d,$$

(13)

and substituting (7) into (13), we obtain

$$\omega_{res}^2 = \frac{\chi_{11}^2}{R_e^2} \frac{e^2 K_{CL} d}{\epsilon_0 m} \eta \frac{V_{rf}^{3/4}}{n_e^{1/4}}.$$

(14)

Letting the lumped element antisymmetric inductance be

$$L_a = \frac{1}{\omega_{res}^2 C_a},$$

(15)

we substitute (11) and (14) into (15) to obtain

$$L_a = \frac{m}{e^2 n_s d} \frac{R_e^2}{\chi_{11} A_a}.$$

(16)

The antisymmetric resistance is then

$$R_a = \nu L_a,$$

(17)
The current flowing in the symmetric leg of the circuit is (neglecting the small resistance $R_s$)

$$I_s = j\omega C_\| V_\| = j\omega \frac{\epsilon_0 A}{K_{CL}} n_e^{1/2} \sqrt{\omega_\|}.$$  \hspace{1cm} (18)

The symmetric electron power absorbed is then $P_s = \frac{1}{2} |I_s|^2 R_s$ or

$$P_s = \frac{1}{2} \omega^2 \epsilon_0^2 \frac{m_e}{\epsilon^2} 2d A V_\|^{1/2}.$$  \hspace{1cm} (19)

We see that $P_s$ increases slowly with $V_\|$ and is independent of $n_e$.

The antisymmetric mode displays a series resonance behavior. The current in the anti-symmetric leg of the circuit is

$$I_a = \frac{\eta V_\|}{R_a + j\omega L_a + \frac{1}{j\omega C_a}}.$$  \hspace{1cm} (20)

Similar to the calculation of $P_s$, the anti-symmetric electron power absorbed is

$$P_a = \frac{1}{2} |I_a|^2 R_a,$$  \hspace{1cm} (21)

as a function of $n_e$ and $V_\|$. The maximum absorbed electron power is at the resonance frequency, $\omega_{res} = \omega$, the driving frequency,

$$P_{a,max} = \frac{1}{2} \frac{\eta^2 V_\|^2}{R_a} = \frac{1}{2} \frac{\epsilon_0^2 \epsilon^2 A_d}{m_e R^2} \eta^2 V_\|^{1/2} n_e.$$  \hspace{1cm} (22)

The resonant density for a given voltage $V_\|$ is found from (14) to be

$$n_{e,res} = \frac{R^4}{\chi_1^2} \left( \frac{\omega^2 \epsilon_0 m_e}{\epsilon^2 K_{CL} \lambda} \right)^2 \frac{1}{\eta^{3/2} V_\|^{1/2}}.$$  \hspace{1cm} (23)

We see that the resonant density decreases as the 3/2 power of the driving voltage.

At low density, the antisymmetric mode current $I_a$ is limited by the inductance $L_a$ and $I_a = \eta V_\|/j\omega L_a \propto \eta V_\| n_e$. Then at low densities $P_a \propto |I_a|^2 R_a \propto \eta^3 V_\|^2 n_e$. Hence $P_a \to 0$ as $n_e \to 0$. At high density, $I_a$ is limited by the capacitance $C_a$, and we have a similar expression for the absorbed power as in (19); i.e. $P_a \to (\eta/2 A_d/A_s) P_s$ as $n_e \to \infty$.

The total electron power lost, which is a linear function of $n_e$, independent of $V_\|$, is

$$P_{loss} = 2\pi R^2 h\epsilon_n u_B \cdot (e(\epsilon_c + \epsilon_e)).$$  \hspace{1cm} (24)

where $\epsilon_c + \epsilon_e$ is the total electron energy lost (in voltage units) per electron-ion pair lost from the discharge. $\epsilon_e$ gives the collisional electron energy lost per electron-ion pair created and $\epsilon_c = 7.2 T_e$ is the electron energy carried across the sheath to the surface. For an argon discharge, we have $\epsilon_e = 15.79 + 12.14 K_{exc}/K_{ir} + 4.08 \times 10^{-5} T_e K_{el} / K_{ir}$, where $K_{ir} = 2.34 \times 10^{-14} T_e^{-0.1047} \ln T_e$ m$^3$ s$^{-1}$, and $K_{el} = 1.619 \times 10^{-14} T_e^{1.566} e^{-0.0207(\ln T_e)^3}$. $\epsilon_c$, the collisional loss per electron-ion pair is chosen to be $\epsilon_c = 0.3$, which is a reasonable assumption from the calculation of the 2D PIC simulation and the nonlinear transmission line model as shown in figures 6(a) and (c). We can see that, for the driving frequency at 30 MHz, the curve

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**Figure 9.** Electron power absorbed, $P_{abs}$, by the symmetric and antisymmetric modes and the power dissipated by the discharge electrons, $P_{loss}$, versus density $n_e$ for (a) a driving voltage range 30—75 V at an rf frequency 30 MHz; (b) three different values of the driving voltage, 35 V, 50 V and 70 V, at an rf frequency 73 MHz. For both cases, the ratio $V_a/V_s = 0.3$, the pressure is 10 mTorr, and electron temperature is $T_e = 3$ V. 

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4.2. Analysis of hysteresis and results of lumped circuit model

The total absorbed electron power $P_{abs}$ at a given $V_\|$ can be obtained as a function of $n_e$ as follows: as given by (10), (17), (18) and (20), the pressure (described by $\nu$) and the angular frequency ($\omega = 2\pi f$) determine the current and resistance in the symmetric and anti-symmetric legs of the circuit, and hence the $P_s$ and $P_a$ versus $n_e$ curves. While $P_s$ varies slowly (non-resonantly) with $n_e$, $P_a$ versus $n_e$ exhibits a resonance that can be broad or sharp, depending on the discharge parameters. Letting the total absorbed electron power be $P_{abs} = P_s + P_a$ and plotting $P_{abs}$ versus $n_e$ for $T_e = 3$ V for different values of the driving voltage (30—75 V) at 30 MHz and 10 mTorr gives the total absorbed power versus density curves shown in figure 9(a). Also shown in the figure is the electron power lost given by (24), which is a linear function of $n_e$. Here the ratio of the anti-symmetric voltage and symmetric voltage is chosen to be $\eta = 0.3$, which is a reasonable assumption from the calculation of the 2D PIC simulation and the nonlinear transmission line model as shown in figures 6(a) and (c). We can see that, for the driving frequency at 30 MHz, the curve...
of $P_{\text{abs}}$ is relatively flat and there is only one equilibrium point for every voltage value. This explains why no hysteresis was found in the discharges driven at low frequencies. Increasing the driving frequency to 73 MHz and keeping the other parameters unchanged, as shown in figure 9(b), for three different values of voltage (35, 50 and 70 V), we can see a fairly sharp anti-symmetric resonance, and three kinds of equilibrium situations arise: (a) For a low voltage, e.g. 35 V, a low density equilibrium point at about $4 \times 10^{14}$ m$^{-3}$ is found, where the total absorbed electron power is mainly from the symmetric mode excitation. (b) Increasing the voltage to 50 V, three equilibrium points are found, with the middle point unstable. Again the low density stable point at about $6 \times 10^{14}$ m$^{-3}$ is mainly sustained by the symmetric mode power. At the high density ($7 \times 10^{15}$ m$^{-3}$) stable point, the total absorbed power is a mixture of symmetric and antisymmetric mode powers indicating the presence of hysteresis. (c) Further increasing the voltage to 70 V, again there is only a single equilibrium point at high density $5.5 \times 10^{15}$ m$^{-3}$, which is sustained by both the symmetric and antisymmetric mode powers.

Sweeping the driving voltage from 30 V to 80 V and calculating the equilibrium points in figure 9(b), the densities versus driving voltage are plotted in figures 10(a)–(c), separately corresponding to 10, 30 and 60 mTorr. The rf frequency is fixed again at 73 MHz. A significant hysteresis loop occurs at low pressure 10 mTorr (approximate 20 V width) and shrinks at 30 mTorr (approximate 10 V width) and ultimately vanishes with the pressure further increasing to 60 mTorr. The driving voltages and the corresponding density ranges, within which the hysteresis occurs in the lumped circuit model, agree well with the observations in the 2D PIC/MCC simulations for these three different pressures (see figure 4).

By sweeping the driving frequencies, the hysteresis is found to start at about 50 MHz within a fairly narrow range of voltage (about 4 V). Even up to 60 MHz, the voltage width of the hysteresis is narrow (8 V), which might be responsible for the absence of the hysteresis at 60 MHz in the 2D PIC simulation, where the hysteresis starts to be observed at 66 MHz. We note that the variation of the total power $P_{\text{abs}}$ with driving frequency is complicated, and it is not a simple scaling relationship. With increasing driving voltage, the densities at the upper branch of the hysteresis slightly decrease in the lumped circuit model, which is different from the observations in 2D PIC simulations (figure 4). This may be understood from the simplifying assumptions made in the model, such as a fixed ratio $\eta$ of anti-symmetric and symmetric mode voltages which in fact is a function of radius, the assumption of two equal sheaths at the powered and grounded electrodes, etc.

5. Conclusions and discussion

Both $z$-symmetric and $z$-antisymmetric wave modes exist in asymmetrically excited cylindrical capacitive discharges. From the lossless wave dispersion for these two modes for both the EM case and the corresponding ES limit, we justified the application of a 2D electrostatic PIC code to our relatively high-frequency driven system. 2D electrostatic PIC simulations conducted at high frequencies (60–80 MHz) and low pressures (10, 30 and 60 mTorr) were used to capture the underlying physics of the discharge over a range of densities, self-consistently considering the wave effects, electron heating and plasma transport.

Sweeping the driving voltage up and down, a plasma density hysteresis was observed for driving frequencies higher than 60 MHz. We presented results at 73 MHz for three different pressures (10, 30 and 60 mTorr). The hysteresis loop voltage width, approximately 20V at 10 mTorr, shrinks with increasing pressure to approximate 10 V at 30 mTorr and vanishes at 60 mTorr. To understand this hysteresis, the symmetric and anti-symmetric mode wave voltages were determined separately at the low and high density states at 10 mTorr. The symmetric mode voltage amplitudes were found to be independent of electrode radius due to the long wavelength...
(infinite wavelength in the ES limit). The anti-symmetric mode voltages had a central-low and central-high profile for the low and high density states, respectively. These 2D PIC results were also found in a nonlinear electromagnetic transmission line model [56], with a radially uniform bulk plasma density. The anti-symmetric mode voltage profiles were determined using a lossy wave dispersion relationship, giving a strongly decaying voltage amplitude at the center with respect to the edge at low density. At high density, the solution gave a significant standing wave from a spatial resonance effect.

A lumped circuit model was developed to explain the driving voltage hysteresis observed in the 2D PIC simulation. This model consists of two circuit branches for symmetric and antisymmetric mode excitation. The symmetric mode branch is non-resonant and modelled by the series combination of a resistance $R_s$ and capacitance $C_s$. The antisymmetric mode branch has a spatial-resonance and was modelled by a series combination of inductance $L_s$, resistance $R_s$, and capacitance $C_s$. The absorbed electron powers of these two branches were calculated as a function of driving voltage, driving frequency, and gas pressure. Compared with the more realistic 2D PIC simulation, the lumped circuit model is relatively simplified, and based on a uniform slab model for symmetric mode wave propagation, assuming two equal sheath widths near the driven and grounded electrode. For the antisymmetric mode, the impedance elements are phenomenologically modelled. Even with a variety of assumptions, from the electron power balance, a hysteresis was still obtained for the lumped circuit, similar to that found in the PIC simulations. Varying the driving frequency, the onset of the hysteresis, in the lumped circuit model, was obtained to be around 60 MHz, also in reasonable agreement with the 2D PIC simulations.

For further studies, the driving point impedance of the discharge can be expanded into a parallel combination of infinitely many series resonance circuits (the second Foster form [64]), and thus higher frequency harmonics of the anti-symmetric and symmetric mode voltages could be accounted for. From the solutions for the fields given in reference [23], more accurate expressions for the lumped circuit elements, accounting for the differing sheath widths at the powered and grounded electrodes, could also be determined. It would also be valuable to obtain more detailed plasma characteristics of the hysteresis in the 2D PIC simulation, such as the electron energy distribution, the current distribution in the bulk plasma, and the effects of nonlinear-excited harmonics. These improvements could be explored in future work.

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