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Model and particle-in-cell simulation of ion energy distribution in collisionless sheath

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In this paper, we propose a self-consistent theoretical model, which is described by the ion energy distributions (IEDs) in collisionless sheaths, and the analytical results for different combined dc/radio frequency (rf) capacitive coupled plasma discharge cases, including sheath voltage errors analysis, are compared with the results of numerical simulations using a one-dimensional plane-parallel particle-in-cell (PIC) simulation. The IEDs in collisionless sheaths are performed on combination of dc/rf voltage sources electrodes discharge using argon as the process gas. The incident ions on the grounded electrode are separated, according to their different radio frequencies, and dc voltages on a separated electrode, the IEDs, and widths of energy in sheath and the plasma sheath thickness are discussed. The IEDs, the IED widths, and sheath voltages by the theoretical model are investigated and show good agreement with PIC simulations.

I. INTRODUCTION

Capacitive discharges are widely used in a number of applications such as surface treatment. These discharges are well-studied both experimentally and theoretically. Different approaches such as applying more power source to the reactor electrode are used to modify and improve the performance of radio frequency (rf)-capacitive coupled plasma (CCP) discharges.1,3 A number of theoretic modeling studies have been published recently, which indicate the analytic results in Ref. 3 of the effect of secondaries on the operation of plane-parallel rf discharges and the analysis to the dc/rf-driven case.4 Moreover, in some approaches, a hybrid RF/dc CCP in hydrogen was simulated.5 A particle-in-cell (PIC) Monte Carlo simulation of an rf discharge in methane: frequency and pressure features of the ion energy distribution function (IEDF).6 A global model for high voltage rf argon capacitive discharges in the collisionless sheath regime was verified by particle-in-cell simulations, for both current- and voltage-driven sources. The IEDs and the IED widths are investigated.7 A review and analysis of IED for a rf discharge on the collisionless regime were discussed.8 However, although most fundamental processes for such discharges have been well understood, there are no reports on the altering sheath voltages error between IEDs theory and simulation on combination of dc/rf voltage sources electrodes.

A dc bias can be externally imposed on the electrode opposite to the wafer connected rf power source, thereby producing a dc-augmented and rf CCP (dc/rf-CCP), as shown in Fig. 1. In this paper, the characteristics of dc/rf-CCPs will be discussed using the results from a new modifying model, where attempts have been made to investigate how key discharge parameters depend on both rf voltage $V_{rf}$ and dc bias voltage $V_{dc}$ connected reactor electrodes. We found that for a given rf power and an augmented dc bias power, the sheath thickness and average voltage amplitude across a single sheath are larger than that for only rf power, and we obtain a new self-consistent model for computing IEDs and widths of energy in collisionless sheath by applying Child law and new proposed a sheath voltage scaling parameters.

**FIG. 1.** Schematic diagram of a symmetric plasma reactor by a different dc-augmented bias voltage and a rf capacitive coupled plasma (dc/rf-CCP) power source, with the dc/rf sheath at electrode.

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II. NEW RESULTS FOR CHILD LAW OF THE COLLISIONLESS REGIME ON DC/RF VOLTAGE SOURCES ELECTRODES

A. Sheath for rf/dc

First, consider the case of collisionless ion motion in the sheath. The sheath structure has been determined previously for a step-function model of the time-varying electron dynamics.\(^9\) The result for the Child law in the high voltage limit is

\[
J_i = \frac{4}{9} \alpha_i \left( \frac{2e}{M} \right)^{1/2} \left( V_s^{1/2} - 1/3 V_i^{1/2} \right) \left( V_s^{1/2} + 2/3 V_i^{1/2} \right)^2, \tag{1}
\]

where \(J_i\) is the ion current density flowing across the sheath, \(V_s = V_0 + V_1\) is the DC voltage, \(V_i = V_0 + V_1\) is the RF voltage, a sum of dc sheath and rf sheath is \(S_m = S_0 + S_1\). For a rf sheath without an extra dc voltage \(V_0 = 0\), ion sheath thickness is

\[
s_{m0} = \frac{10\sqrt{2}}{9\sqrt{3}} \left( \frac{\alpha_0}{J_i} \right)^{1/2} \left( \frac{2e}{M} \right)^{1/4} V_1^{3/4}. \tag{2}
\]

The result is the same as that shown in Sec. 11.2 of Ref. 10. For a rf sheath with an extra dc voltage \(V_0 \neq 0\), as \(V_s > V_0\),

\[
S_m = \frac{2}{3} \left( \frac{\alpha_0}{J_i} \right)^{1/2} \left( \frac{2e}{M} \right)^{1/4} \times \left( V_s^{1/2} - \frac{1}{3} V_i^{1/2} \right) \left( V_s^{1/2} + \frac{2}{3} V_i^{1/2} \right)^2 \right)^{1/2}, \quad S_m > S_{m0}. \tag{3}
\]

B. Sheath voltage for rf and rf/dc

The ion sheath voltage \(\tilde{V}_s\) is obtained by the Child law for collisionless only if rf sheath is without the added dc bias voltage,\(^10\) for \(H \gg 1\)

\[
\tilde{V}_s = \frac{9\pi^2 H^2}{32} T_e, \tag{4}
\]

and the amplitude of the fundamental voltage between the two electrodes is

\[
\frac{\tilde{V}_{ab1}}{T_e} = \frac{\pi}{4} \left[ 8 + H \left( \frac{12\pi}{3} \frac{\alpha_0}{T_e} \right) \right]. \tag{5}
\]

Equation (4) is divided by Eq. (5)

\[
\tilde{V}_s \approx 0.4138 \tilde{V}_{ab1} \approx 0.83 V_1. \tag{6}
\]

The ion sheath voltage \(\tilde{V}_s\) is obtained by the Child law for collisionless rf/dc sheaths, for \(H \gg 1\),

\[
\tilde{V}_s = \frac{9\pi^2 H^2}{32} T_e + \frac{0.83}{2} |V_0|, \tag{7}
\]

\[
\frac{\tilde{V}_{ab1}}{T_e} = \frac{\pi}{4} \left[ 8 + H \left( \frac{12\pi}{3} \frac{4096}{675\pi} \right) \right] + \frac{0.83 |V_0|}{2 T_e}. \tag{8}
\]

The second item in Eq. (7) is the item added on the basis of Eq. (4), which is not previously mentioned in relevant literatures; the mention of sheath voltage error is given in in the abstract. We think the second item is because of adding DC bias. Equation (7) is the average sheath voltage for collisionless rf/dc sheaths. Equation (7) is divided by Eq. (8)

\[
\frac{\tilde{V}_s}{\tilde{V}_{ab1}} = \frac{\pi}{4} \left( \frac{8 + H \left( \frac{12\pi}{3} \frac{4096}{675\pi} \right) T_e + \frac{0.83 |V_0|}{T_e}}{8 + H \left( \frac{12\pi}{3} \frac{4096}{675\pi} \right) T_e + \frac{0.83 |V_0|}{T_e}} \right). \tag{9}
\]

as \(H \gg 1\), then we obtain

\[
\frac{\tilde{V}_s}{\tilde{V}_{ab1}} \approx \Delta + \sigma, \tag{10}
\]

where \(\Delta = \frac{9\pi^2 H^2}{32} / \left( \frac{8 + \sigma}{\sigma} \right)\) and \(\sigma = \frac{0.83 |V_0|}{2 T_e} / \left( \frac{8 + \sigma}{\sigma} \right)\).

We estimate the parameters in Table I using Eqs. (4), (6), and (10).

According to calculation made from Table I, we obtain the following new sheath voltage:

\[
\tilde{V}_s = (\Delta + \sigma) \tilde{V}_{ab1} \approx 0.437 \tilde{V}_{ab1} \approx 0.88 \tilde{V}_1. \tag{11}
\]

The parameter 0.88 is larger than 0.83 in Eq. (6), because of the added dc bias voltage on rf power electrode. Obviously, this parameter is obtained with an increase in dc bias voltage and is composed of two parameters: the first parameter \(\Delta\) changes a little, and the second parameter \(\sigma\) with the change of voltage becomes larger, as \(\Delta \gg \sigma\) and \(\sigma\) is considered as sheath voltage errors. This is our new proposed collisionless sheath voltage scaling parameters obtained if rf sheath voltage is not fixed to 0.83,\(^10\) and it will be larger (0.83–0.92) with increasing dc bias (100 V–300 V), the average value being 0.88.

<table>
<thead>
<tr>
<th>(\tilde{V}_s/(V))</th>
<th>(V_0/(V))</th>
<th>(V_1/(V))</th>
<th>(T_e/(eV))</th>
<th>(H)</th>
<th>(\Delta)</th>
<th>(\sigma)</th>
<th>(\Delta)</th>
<th>(\sigma)</th>
<th>(\tilde{V}<em>s/\tilde{V}</em>{ab1})</th>
<th>(\tilde{V}_s/V_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>-100</td>
<td>249</td>
<td>3.3</td>
<td>5.214</td>
<td>0.356</td>
<td>0.059</td>
<td>0.356</td>
<td>0.081</td>
<td>0.415</td>
<td>0.830</td>
</tr>
<tr>
<td>500</td>
<td>-200</td>
<td>290.5</td>
<td>3.3</td>
<td>5.631</td>
<td>0.355</td>
<td>0.082</td>
<td>0.356</td>
<td>0.081</td>
<td>0.437</td>
<td>0.874</td>
</tr>
<tr>
<td>500</td>
<td>-300</td>
<td>332</td>
<td>3.6</td>
<td>6.020</td>
<td>0.358</td>
<td>0.102</td>
<td>0.356</td>
<td>0.081</td>
<td>0.460</td>
<td>0.920</td>
</tr>
</tbody>
</table>
C. IEDs $f(E)$, energy width $\Delta E_i$, and sheath $s_m$ for only rf and combination of rf/dc

We can obtain a self-consistent model of ion energy distributions $f(E)$, energy width $\Delta E_i$, and sheath $s_m$ in a collisionless sheath on combination of dc/rf voltage sources electrode according to above analysis and previous theories.

$$f(E) = \frac{2n_i}{\omega \Delta E_i} \left[1 - \frac{4}{(\Delta E_i)^2} (E - eV_s)^2\right]^{-1/2}, \quad (12)$$

$$\Delta E_i = \frac{2eV_s}{\cos \theta_m} \left( \frac{2eV_s}{M} \right)^{1/2}, \quad (13)$$

$$s_m \approx 0.91 \left( \frac{2e}{kT_v} \right)^{1/4} \left( \frac{\epsilon_0}{0.61n_0e} \right)^{1/2} \frac{V_s^{3/4}}{C}, \quad (14)$$

where Eq. (12) is an expression for the IEDF ($f(E)$), $f(E) \propto 1/\Delta E_i$, its physical dimension is $[1/eV]$. $n_i$ is the ion density with time rate of change, $\omega$ is the RF source frequency. $[1 - 4(E - eV_s)^2/(\Delta E_i)^2]^{-1/2}$ is bimodal peaks, IED dimensionless factor with energy center at $eV_s \pm \Delta E_i$. $\Delta E_i$ is ion energy width, it is in proportion to sheath voltage, and it is inversely proportional to frequency and sheath width in Eq. (13). Equation (14) is derived from Eq. (2) with ion current density $j_i \approx 0.61n_0u_B$ and Bohm velocity $u_B = \sqrt{kT_v/M}$.

When the same frequency

$$\frac{s_m}{s_1} = \left( \frac{V_s}{\tilde{V}_1} \right)^3,$$  \quad (15)

$$n_i/n_1 = (s_1/s_m)^2 \left( \frac{V_s}{\tilde{V}_1} \right)^{3/2},$$  \quad (16)

when $V_0 = 0$

$$\tilde{V}_s \approx 0.83\tilde{V}_1 = 0.415\tilde{V}_{cr},$$  \quad (17)

when $V_0 \neq 0$

$$\tilde{V}_s \approx 0.88\tilde{V}_1 = 0.437(\tilde{V}_{cr} + |V_0|).$$  \quad (18)

Equation (18) is the first time we proposed, because we think that the sheath voltage is composed of the rf sheath voltage and dc sheath voltage, and the dc sheath voltage is proportional to dc bias voltage. Where $\tilde{V}_s = \tilde{V}_{cr}$, $\tilde{V}_1$, and $s_1, n_1$ are, namely, the sheath voltage, the sheath width, and the sheath density of only rf power source without dc voltage source. We can calculate $f(E)$, $\Delta E_i$, and $s_m$ in a collisionless sheath on a combination of different dc/rf voltage sources electrode by Eqs. (12)–(18). These calculation parameters are listed in Table II.

According to Table I and Eqs. (12)–(18), we plot ion energy distributions function IEDF (or $f(E)$) on combination of dc/rf voltage sources electrode (see Figs. 2–4).

III. PIC SIMULATIONS

The simulations are performed using a one-dimensional (1D) particle-in-cell code XPPD1. Starting from the initial conditions, particle and field values are sequentially advanced in time. The particle equations of motion are advanced one time step, using fields interpolated from the discrete grid to the continuous particle locations. Next, particle boundary conditions such as absorption are applied. The Monte Carlo collision scheme is applied for electron-neutral collisions. Ion-neutral and neutral-neutral collisions are not considered here.

After the simulation becomes steady state, the IED is collected over many cycles of the lowest frequency and normalized to unity. The PIC IED results are then compared with the self-consistent model. In the simulation, the discharge gap $L = 0.1$ m, and area $A = 0.01$ m², consistent with typical processing applications. The gap width is divided into 500 cells, ion and electron temperature are, respectively, $T_i = 0.03$ eV and $T_e = 3$ eV, and the simulation time step is $\Delta t = 7.2 \times 10^{-11}$ s, ion velocity range $v_s = 3.5 \times 10^5$–$1.5 \times 10^6$ m/s, and therefore, ion mean free path $\Delta x = 2.5 \times 10^{-5}$–$1.1 \times 10^{-4}$ m, ion Debye length $\lambda_D \approx 69000 \sqrt{T_i/n_i} = 2.4 \times 10^{-5}$ m. $\Delta x \geq \lambda_D$, argon gas is used with $p = 3$ mTorr, ratio of physical particles to computer particles $np/c = 10^5$, and initial density of particles $n_0 = 2.5 \times 10^{15}$ m⁻³. These parameters chosen are in order conditions.
to resolve the Debye length and fulfill simulation stability criteria.

A RF steady state of ion and electron number density described by PIC simulation on a rf 13.56 MHz (\(V_{\text{rf}} = 500 \text{ V}, V_0 = 0 \text{ V}\)) source electrode is shown in Figure 5. The PIC simulation analytical results are shown as a, b, c, and d curves of bimodal peaks IEDF in sheath collisionless on a rf 13.56 MHz, rf voltage (\(V_{\text{rf}} = 500 \text{ V}\)) source electrode, added different dc bias voltages (\(V_0 = 0 \text{ V}, 100 \text{ V}, 200 \text{ V}, 300 \text{ V}\)) in Figure 6, on a rf 7 MHz in Figure 7, and on a rf 4 MHz in Figure 8.

IV. COMPARISON BETWEEN THEORY AND SIMULATION, SHEATH VOLTAGE ERROR ANALYSIS

We analyzed comparatively these IEDFs between the self-consistent model and PIC simulation in the sheath on a rf (respectively, 13.56 MHz, 7 MHz, and 4 MHz) voltage source electrode added a dc bias voltage (respectively, 0 V, \(-100 \text{ V}, -200 \text{ V}, \text{ and } -300 \text{ V}\)).

FIG. 5. Ion and electron number density analyzed by PIC simulation on a rf 13.56 MHz, (\(V_{\text{rf}} = 500 \text{ V} \text{ and } V_0 = 0 \text{ V}\)) source electrode.

\(V_0 = 0 \text{ V}, -100 \text{ V}, -200 \text{ V}, \text{ and } -300 \text{ V}\)) in Figures 6–8. The bimodal IEDs of the lines (solid, dashed, dotted, and dashed-dotted lines) by the self-consistent model are corresponded to their bimodal peaks of curves (a, b, c, and d lines) by PIC simulation, and the analytical results are shown \(V_{\text{rf}}/V_0: 500 \text{ V}/0 \text{ V}, 500 \text{ V}/-100 \text{ V}, 500 \text{ V}/-200 \text{ V}, \text{ and } 500 \text{ V}/-300 \text{ V}\) cases reasonably well, the error voltage of \(500 \text{ V}/-300 \text{ V}\) case is larger, these sheath voltage errors are 15.6 eV for rf 13.56 MHz, 57.57 eV for rf 7 MHz, and 53.6 eV for rf 4 MHz between the upper limits peaks. The reason may be that the sheath voltage calculation used average sheath voltage \(V_s = 0.88V_1 = 0.437(V_{\text{rf}} + |V_0|)V_0 \neq 0\). In fact, sheath voltage varies with dc bias voltage and rf voltage, when \(V_0 = -300 \text{ V}, V_s = 0.92V_1 = 0.46(V_{\text{rf}} + |V_0|)\) from Table I, so the energy center of IEDF \(e\) should be 368 eV rather than 352 eV, their energy widths \(\Delta E_i\) are modified for 322.67 eV, 592.72 eV, and 653.57 eV, therefore sheath voltage errors are reduced to 5.6 eV, 4.01 eV, and 6.12 eV. Of course, the energy width increases with the addition of dc bias voltage (see Eqs. (13) and (18)), resulting in the increase in sheath voltage and sheath thickness (see Eqs. (14), (15), and (18)); this primary cause may be more high-energy directional electrons originating by particle bombardment of the dc
electrode and secondary electrons, and such electrons offer the possibility to decrease the bulk plasma thickness and lead to increase high energy part ions in sheath. In Figure 5, ion and electron number density analyzed by PIC simulation on a rf 13.56 MHz, \( V_{\text{rf}} = 500 \text{ V} \), \( V_0 = 0 \text{ V} \) source electrode, and different dc bias voltages added.

V. CONCLUSIONS

IEDs in collisionless sheaths are performed on combination of dc/rf voltage sources electrodes discharge using argon as the process gas. The incident ions on the grounded electrode are separated, according to their different radio frequencies and dc voltages on a separated electrode, and the IEDs and widths of energy in sheath and the plasma sheath thickness are discussed. In this paper, we propose the self-consistent model, the binodal IEDs can be better described, and the analytical results for different combined dc/rf capacitive coupled plasma discharge cases, including sheath voltage errors analysis, are compared with the results of numerical simulations using a 1D plane-parallel PIC code. The IEDs, the IED widths, and sheath voltages by the theoretical model are investigated, which show good agreement with PIC simulations.

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