Plasma boundary of nonlinear sheath dynamics for arbitrary waveforms in capacitive discharge

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Abstract. Capacitively coupled RF discharges (RF-CCPs) can offer a higher quality of semiconductor fabricating and processing thin film by applied fully arbitrary waveforms. Using different applied arbitrary voltage waveform, one can design varies distributions with specific tailoring features. Analyzing RF-CCPs dynamics using non-harmonically modulated sheath is more complicated. In this theoretical study of fluid model, various types of excitation waveforms, such as square, sawtooth, dual frequency, and pulse-like excitation were applied. Furthermore, different important semi-analytical descriptions, such as the particle density, instantaneous electric field distributions, the voltage and the effective charge-voltage of time characteristics of arbitrary waveforms are obtained. By applying the collision and collisionless self-consistent numerical solutions of the fluid model all complex dynamics are accomplished. In addition, by using the model of an ensemble in space-time (EST) it is found that arbitrary waveforms can offer more possibilities for tailoring IEDs for a purpose in collisionless regimes more than collisional regimes. Moreover, more control of RF-CCPs will be achieved for the different purpose of materials processing.

1. Introduction

The low-temperature plasma process is more applied in the Microelectronics fabrication. A plasma produces reactive ions at boundary sheath is the fundamental factors of the enhancement etching or deposition processes. Furthermore, boundary sheath controls flux, energy and angular distribution of the ions.

When the voltage drops fully across the sheath, the ions accelerate by the uniform electric field and affect the ion energy distribution (IED) in the sheath region. The details of sheath voltage characteristic and IED play important role in fabrication, for example for lower energy (lower sheath voltage of the electrode) ions, may enhance biomedical application and polymer deposition on the substrate, while higher energy ions (higher sheath voltage of the electrode) enhance etching and cleaning surface for semiconductor applications[1, 2, 3, 4, 5].

Since capacitive coupled radio frequency plasma discharges (RF-CCPs) present a considerable part in material processing. Several evolutions such as single (CCPs), dual (2f-CCPs), and the third generation of triple frequencies sources (3f-CCPs) are studied. These studies showed that the dual frequency (2f. CCPS) can cover the drawback of the single frequency of CCPs, which ion bombardment energy and ion flux can be controlled independently. However, the recent investigations have shown that the dual frequency (2f. CCPs) separate control is limited due to a coupling of frequencies. Therefore, in this manuscript the nonlinear sheath characteristics under the effect of different nonharmonic RF excitation such as sawtooth, triangle, square, dual frequency and pulse-like excitation are calculated where \( \omega_{RF} \gg \omega_{Pi} \) one may design voltage waveforms that make distributions with the specific countenance [6, 7, 8, 9, 10, 11, 12, 13]. The results may enhance the industrial applications.
However, an adequate experimental and simulations check these arbitrary waveforms study, but still, an important aspect of many questions is not fully answered, like what is the semi analytical descriptions of the sheath dynamics such as the particle density and instantaneous electric field distributions, the V(Q) characteristics of these different excitation waveforms. In this contribution, we will give a reasonable answer to many important questions by studying the collision and collisionless fluid model [14, 15, 16, 17, 18, 19, 20, 21]. The solution of the nonlinear integrodifferential equation of two regimes for a space-time dependent is obtain. The results of the potential $\phi(x, t)$ which includes all complex dynamics of the sheath are fed to EST simulation in order to obtain IED.

This paper is organized as follows: First, we will study collisionless and collision model of the exact fluid model of plasma boundary sheath. Second, we study the example of charge voltage $V(Q)$ distributions for different non-harmonic excitation of collisionless model. Third, find the voltage time depending in case of collision and collisionless model then fed it to EST model. Fourth, compare the results of IED in case of collision and collisionless regime. Finally, summary and conclusions is addressed.

2. Fluid model, specialized for an RF sheath

In the plasma boundary sheath region at high-frequency RF-regime, there is a depletion of electrons within the high electric field which replies the electrons to the bulk and extracts more ions to the sheath. There is an ambipolar field in the quasineutral bulk because of the diffusion of the negative and positive charge carriers. The analysis of RF-sheath dynamics is quite complicated, this study demonstrates the high complexity of this analysis, even after having simplified the assumptions and physical approximations [16, 17, 18, 19]. At the beginning fluid descriptions of the high RF regime are assumed to be $\omega_{\text{pi}} \ll \omega_{\text{RF}} \ll \omega_{\text{pe}}$, where the electrons are in Boltzmann equilibrium with the time-varying field, and the ions response to an average electric field. The model of the RF-plasma boundary sheath can be expressed using the following: electron model dynamics, ion model dynamics, field model Maxwell's equation, and one-dimensional geometry. In this approach we will use a scale length of Debye length $\lambda_D$, mean free path $\lambda$, reactor length $R$, sheath plasma $s$, scale time of electrons plasma frequency $\omega_{\text{pe}}$, ion plasma frequency $\omega_{\text{pe}}$, high applied radio frequency $\omega_{\text{RF}}$, collision frequency $\nu$. The equations can be summarized relative to accurate approximations and correlation of coupled sub-models as follows:

- Electron model:

$$c E n_e + T_e \frac{\partial n_e}{\partial x} = 0$$  \hspace{1cm} (1)

$$\frac{\partial n_e}{\partial t} + \frac{\partial}{\partial x} (n_e v_e) = 0$$  \hspace{1cm} (2)

- Ion model dynamics with continuity equation and equation of motion:

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x} (n_i v_i) = 0,$$  \hspace{1cm} (3)

$$v_i \frac{\partial v_i}{\partial x} = \frac{e}{m_i} E(x) - \nu_i (v_i) v_i.$$  \hspace{1cm} (4)

- Poisson’s equation via instantaneous electrical field:

$$\epsilon_0 \frac{\partial E(x, t)}{\partial x} = c(n_i(x) - n_e(x, t)).$$  \hspace{1cm} (5)
The instantaneous sheath surface charge which is not necessarily harmonic wave, typically a positive quantity, the parametric RF modulation determined by harmonic variation of the sheath charge can be calculated as follow:

\[
Q(t) = \int_0^\infty e(n_i - n_e) \, dx = Q + \frac{J_{f}}{\omega_{rf}} Q(\omega_{rf}t)
\]  

A function \(Q(\omega_{rf}t)\), refer to different type of functions such as pulse excitation (Gaussian function), square wave, sawtooth wave and double frequency

\[
Q(\omega_{rf}t) = \left\{ \begin{array}{ll}
-0.5 + \frac{1}{\sqrt{2\pi}\sigma} \sum_{n=-\infty}^{n=\infty} e^{-\frac{[\omega_{rf}t - (2n-1)\pi]^2}{2\sigma^2}} \\
\sum_{n=1}^{k} \frac{\sin(2n-1)\omega_{rf}t}{2n-1} \\
\sum_{n=1}^{k} \frac{2\sin(n)\omega_{rf}t}{n} \\
\cos[\omega_{rf}t] + \cos[n\omega_{rf}t]
\end{array} \right.
\]

\[
\int_{x_e}^{x_i} e(n_i - n_e) \, dx = Q(t).
\]

The final collected set of equations of the sheath model is still very difficult to solve. There are two general reasons for the difficulty of solving this equation. First, the Poisson's equation has no analytical solution to get the time-dependent field, hence the average electric field cannot be calculated. The second reason is that the ion equation of motion has also no analytical solution. If two different regime of collision and collisionless for the ion equation of motion is applied and the Poisson's equation is solved, the time-dependent electric field and its average can be calculated. Consequently, electron and ion densities can also be calculated and the self-consistent fluid model can be verified.

2.1. The collisionless sheath model

The sheath becomes collisional when it applies to discharges with a pressure \(p < 5\) Pa in argon, ion mean free path \(\lambda_i \gg s\) the sheath width [16]. It consists of coupled sub-models:

- Boltzmann equilibrium of electron model and Poisson equation:

\[
e\, E\, n_e + T_e \frac{\partial n_e}{\partial x} = 0 \quad (9)
\]

\[
\varepsilon_0 \frac{\partial E}{\partial x} = e(n_i - n_e) \quad (10)
\]

- Ion model:

\[
n_i v_i = -\Psi_i \quad (11)
\]

\[
\frac{1}{2} m_i v_i + e\phi = \frac{T_e}{2} \quad (12)
\]

Connection of the instantaneous to the phase-averaged field:

\[
E(x) = \frac{1}{T} \int_0^T E(x,t) \, dt \quad (13)
\]
To model our system with a set of dimensionless equations we need to normalize the dynamic fields such as density \(n\), ion speed \(v\), and Debye length \(\lambda_D\) with a set of values of same dimension to get the corresponding normalized fields the \(\hat{n}\), \(\hat{v}\), and \(\hat{\lambda_D}\), respectively, using the following relations:

\[
\begin{align*}
& x \rightarrow \hat{\lambda}_D x \\
& n_i \rightarrow \hat{n}_i, \quad n_e \rightarrow \hat{n}_e, \\
& \psi_i \rightarrow \psi_{i,\hat{\psi}}, \quad v_i \rightarrow \psi_{i,\hat{v}}, \\
& E \rightarrow (T_e/e \hat{\lambda}_D) \hat{E}, \quad Q \rightarrow \hat{\lambda}_D \hat{n} Q, \\
& J_e \rightarrow e \hat{n} \hat{\lambda}_D \omega_{RF} \hat{J}_e, \quad J_{RF} \rightarrow e \hat{n} \hat{\lambda}_D \omega_{RF} \hat{J}_{RF}.
\end{align*}
\]

For the dimensionless system of equations, the ion density, the electron and Poisson’s equation can be achieved by: The ion and electron densities in terms of the average potential

\[
\begin{align*}
\hat{n}_i &= \frac{1}{\sqrt{1 - 2\phi}} \\
\hat{n}_e &= e^{\phi(x,t)}
\end{align*}
\]  

(14)  

(15)  

The nonlinear differential equation of dimensionless field model is represented as follow:

\[
-\frac{\partial^2 \phi(x,t)}{\partial x^2} = \frac{1}{\sqrt{1 - 2\phi}} - \exp(\phi(x,t))
\]

(16)  

The differential Poisson’s equation is subject to two important boundary conditions, the first is at the electrode where the electric field is related to the sheath charge distribution and the second is at the bulk where the electric field is related to the ambipolar field.

\[
\begin{align*}
\frac{\partial \phi(x_{min},t)}{\partial x} \bigg|_{0} &= Q(t) = \hat{Q} - Q(\omega_{RF}t) \\
\phi(x_{max},t) &= \ln(n_i) = 0.
\end{align*}
\]  

(17)  

(18)  

lastly, the average electric field related to the instantaneous potential can be calculated as follows:

\[
E(x) = \frac{1}{2\pi} \int_{0}^{2\pi} \frac{\partial \phi(x,t)}{\partial x} dt.
\]

(19)  

- Exact numerical solution for collisionless fluid model (Newton relaxation scheme)

In order to solve the nonlinear differential Poisson’s equation of space time dependent \(\phi(x, t)\)[19], where \(j = 0\). A relaxation scheme was discretized between \([0, 2\pi]\). Suitable discretization for spatial interval \([x_{min}, x_{max}]\) was chosen at \([0, 100]\). At \(x_{min}\), the quasi-neutrality equation where,

\[
\phi - \text{Log}(n_i) = 0, \quad \text{with the modified condition} \quad \frac{d\phi}{dx|_{x_{min}}} = \hat{Q} - Q \cos(t), \text{was arbitrary}
\]

(but suitable chosen) positive number. The interval was discretized into 300 cells of size \(\Delta x = 1/3\); also the RF cycle \([0, 2\pi]\) was split into 32 intervals with \(\Delta t = \pi/32\). The relaxation scheme of current amplitude \(J = 3.75 = 8.52 \text{ mAcm}^{-2}\).  

(17)  

(18)  

(19)
Newton relaxation scheme

A relaxation of the collisional self-consisting numerical solution discretized the RF-cycle between scheme \([0 - 2\pi]\) into 32 intervals within time steps \(\Delta t = \frac{2\pi}{32}\), the spatial interval was chosen between \([-6.5 - 20]\). The interval was discretized into 350 cells of size \(\Delta x = 0.076\). Two essential boundary conditions are applied: one at the bulk \((x_{\text{max}} = 20)\) where the quasi-neutrality equation \(\Phi - \log(n_i) = 0\) is applied. However, the other condition at the electrode \((x_{\text{min}} = -6.5)\), where the modified condition of the field at the electrode is applied as follow

\[
\frac{\partial \Phi}{\partial x} \bigg|_{x_{\text{min}}} = Q^- - Q(t), \text{ where } Q^- \text{ is an arbitrary adequate positive number}
\]

Numerical results of collisionless fluid model

In the following example for a plasma processing discharge, we have a fixed parameters of a more fundamental model, namely a self-consistent one-dimensional fluid sheath model. The pressure was \(p = 1\) Pa at \(T_G = 300\) K. The applied voltage was \(V(t) = 100\) V cos\((\omega_{RF} t) + 100\) V cos\((3 \omega_{RF} t)\), with \(\omega_{RF} = 2\pi \times 13.56\) MHz. The results from PIC are shown such as, the electron temperature was estimated as \(T_e = 3\) eV, the ion current as \(e\psi_i = 1.27\) mA\(m^{-2}\). Furthermore, the temporal charge per area was calculated, where, \(J_{RF} = 2.3\) mA\(cm^{-2}\). The following figures shown the vital results of the temporal development of the charge per area, ion density distribution, and the charge voltage distribution of the RF-driven collisional sheath at modulation value of \(J_{RF} = 2.3\) mA\(cm^{-2}\).

Square wave excitation.

The following results of particle densities, instantaneous electric field and charge-voltage distributions for temporal case of \(j \neq 0\). The model amounts to the nonlinear integrodifferential equation for space-time dependent function \(\Phi(x,t)\) form driving parameter \(Q(t)\) of the square wave. The parameters are assigned as follow.

Sawtooth excitation wave

The following figures shown the sheath dynamics behaviors of the apply RF-driven sawtooth wave. The parameters are assigned as in the example of square wave.
The following figures shown the results for the sheath dynamics behaviors of the collisionless self-consisting numerical solution of the fluid model affected by applying RF-driven pulse-like excitation wave.

- **Pulse-like excitation wave**

The results are show for the example of the collisionless self-consisting numerical solution of the fluid model of applied dual frequency. Displayed in the figures below are dynamics of the sheath

- **Dual frequency excitation wave**

The results are show for the example of the collisionless self-consisting numerical solution of the fluid model of applied dual frequency. Displayed in the figures below are dynamics of the sheath
2.2. The collisional sheath model
The sheath becomes collisional when it applies to discharges with a pressure \( p > 5 \) Pa (in argon), ion mean free path \( \lambda_i \ll s \) the sheath width [17]. It consists of coupled sub-models:

- Electron model (Boltzmann equilibrium) and Poisson equation (field dynamics):
  \[
  e E n_e + T_e \frac{\partial n_e}{\partial x} = 0 \\
  \frac{\partial E}{\partial x} = e(n_i - n_e)
  \]

- Ion model:
  \[
  \frac{n_i v_i}{v_i} = -\Psi_1 \\
  v_i = \frac{2e\lambda_i}{\pi n_i |v_i|} E
  \]

Connection of the instantaneous to the average electric field:
\[
\bar{E}(x) = \frac{1}{T} \int_0^T E(x, t) \, dt
\]

Parametric RF modulation determined by harmonic variation of the sheath charge:
\[
Q = \int_0^\infty e(n_i - n_e) \, dx = \bar{Q} + \frac{J_{RF}}{\omega_{RF}} \sin(\omega_{RF} t)
\]

The boundary conditions subject to the nonlinear differential equation for \( \phi \), can be written as:
\[
\left. \frac{\partial \phi}{\partial x} \right|_0 = \bar{Q} - Q(t),
\]
\[
\lim_{x \to \infty} \exp(\phi) - \frac{1}{\sqrt{-E}} = 0.
\]

By using the dimensionless system of equations, the ion density \( n_i \) and the velocity \( v_i \) can be produced in terms of the average electric field:
\[
v_i = -\frac{1}{n_i} = -\sqrt{-E},
\]
\[
n_i = \frac{1}{\sqrt{-E}}
\]
Electron density $n_e$ and the electrical potential can be expressed as:

$$n_e = \exp(\phi),$$

$$E = -\frac{\partial \phi}{\partial x}.$$  \hfill (30)

The dimensionless nonlinear differential equation for $\phi$:

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{1}{\sqrt{-E}} - \exp(\phi)$$ \hfill (32)

subject to the boundary conditions

$$\left.\frac{\partial \phi}{\partial x}\right|_0 = \tilde{Q} - Q(t),$$

$$\lim_{x \to \infty} \exp(\phi) - \frac{1}{\sqrt{-E}} = 0.$$ \hfill (33)

- Newton relaxation scheme

A relaxation scheme of the collisional self-consisting numerical solution discretized the RF-cycle between $[0 - 2\pi]$ into 32 intervals within time steps $\Delta t = 2\pi/32$, and the spatial interval was chosen between $[-6.5 - 20]$. The interval was discretized into 350 cells of size $\Delta x = 0.076$.

Two essential boundary conditions are applied: one at the bulk ($x_{\text{max}} = 20$) where the quasi-neutrality equation $\Phi - \log(n_i) = 0$ is applied. However, the other condition at the electrode ($x_{\text{min}} = -6.5$), where the modified condition of the field at the electrode is applied as follow

$$\left.\frac{\partial \phi}{\partial x}\right|_{x_{\text{min}}} = \tilde{Q} - Q(t),$$

where $\tilde{Q}$ is an arbitrary (but suitably chosen) positive number.

- Numerical results of collisional fluid model

At collision regime where the discharge at pressure $p = 13.33$ Pa, The following figures shown the vital results of the temporal development example of nonlinear dynamic of dual frequency nonharmonic wave at the same previous example of collision regime.

- Dual frequency excitation wave

The results are show for the example of the collision self-consisting numerical solution of the fluid model of applied dual frequency. Displayed in the figures below are dynamics of the sheath

![Figure 9](image-url)
2.3. Ion Energy distribution form EST

Many recent studies which have considered arbitrary waveforms such as dual frequency and square waves. The sheath voltage as a function of time $V_{sh}(t)$ of arbitrary waveforms can be calculated. The data of the sheath voltage as a function of the time are then fed into the ensemble in spacetime model EST where, EST is a fast, kinetically self-consistent boundary sheath model which covers the requirements of the technology-oriented computer aided design (TCAD)-suited simulator [20, 21]. Starting with, the sheath charge $t(k)$ can be calculated as follows:

- $t = \frac{2\pi}{64}$
- $s(k) = k(\frac{2\pi}{64})$, $k$ changes from 0 to 64

Sheath voltage $V_{sh}(t)$ can be determined through the electrode distance of the sheath (minimal distance $x_E$) where, $n_e(x, t) = \mu$ and the maximal distance of sheath expansion $x_{Top}$. At certain time, the sheath charge can be found using the difference between the potential at maximum value $\Phi(x_{Top})$ and the minimum value of the potential $\Phi(x_E)$, where $V(Q) = \Phi(x_{Top}, t) - \Phi(x_E, t)$. In the following study, collision and collisionless regimes of the ion energy...
distributions results from EST will be investigated. At collision regime, figure 12, shows the time varying sheath voltage of the reference quantities as follows: the discharge at pressure $p = 13.33$ Pa, with applied dual frequency $\omega_{LF} = 2\pi \times 13.56$ MHz and $\omega_{HF} = 3\omega_{LF}$, the mean free path is $\lambda_i = 0.1$ cm, the electron temperature is $T_e = 3$ eV, the ion current is $e\psi_i = 1.27$ mA m$^{-2}$. Ion energy distribution IED from EST at collisional is then obtained. See figure.

- Ion energy distribution of the example of collision regime model

At collision regime where the discharge at pressure $p = 13.33$ Pa, we will focus only on the example of the dual frequency.

Figure 12. Charge-voltage distributions $V_{sh}(t)$ distribution of the dual frequency excitation at collisional case where, $p = 13.33$ Pa.

- Ion energy distribution of collisionless regime model

At collisionless regime where the discharge at pressure $p = 1$ Pa, the below figure show the time varying sheath voltage and the related ion energy distribution from EST at the same set parameters of previous example.

Figure 13. Normalized sheath voltage distributions $V_{sh}(t)$ and the related ion energy distributions of the dual frequency excitation wave of collisionless regime where, $p = 1$ Pa.

Figure 14. Normalized sheath voltage $V_{sh}(t)$ and the related ion energy distributions of the square excitation wave of collisionless regime where, $p = 1$ Pa.
3. Summary and conclusion

In fact, there are several important theoretical studies in case of collision and collisionless regime are accomplished. The complex dynamics of the plasma boundary sheath with higher accuracy is studied. In addition, a wide range of significant different applied sheath voltage waveforms and how they affect the ion energy distributions are achieved to obtain the desired distribution. By applying fluid sheath model in case of two regimes collision and collisionless of different excitation signals, we can obtain important parameters: the sheath voltage distribution with time, which control the IED more than the sinusoidal case. Based on the results of different variable sheath voltage from fluid sheath model and that can be used as input parameters to EST, the comparisons between the results shown in figures, prove that the tailoring of IED is more effective in collisionless regime than collision regime.

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