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Characteristics of single and dual radio-frequency (RF) plasma sheaths

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Abstract The characteristics of radio-frequency(RF) plasma sheaths have been topics of much scientific study for decades, and have also been of great importance in the manufacture of integrated circuits and fabricating microelectromechanical systems (MEMS), as well as in the study of physical phenomena in dusty plasmas. The sheaths behave special properties under various situations where they can be treated as collisionless or collisional, single- or dual-RF, one- or two-dimensional (1D or 2D) sheaths, etc. This paper reviews our recent progress on the dynamics of RF plasma sheaths using a fluid method that includes the fluid equations and Poission's equation coupled with an equivalent circuit model and a hybrid method in which the fluid model is combined with the Monte-Carlo (MC) method. The structures of RF sheaths behave differently in various situations and plasma parameters such as the ion density, electron temperature, as well as the external parameters such as the applied frequency, power, gas pressure, magnetic field, are crucial for determining the characteristics of plasma sheaths.

Keywords plasma, sheath, ratio-frequency, fluid model, Monte-Carlo method, simulation

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1 Introduction

Rf gas discharges currently play a critical role in fabricating the new generation ultralarge-scale integrated circuits and microelectromechanical systems (MEMS), as well as in

investigating dusty plasmas. The typical plasma discharges that have been used for decades are capacitively coupled plasma (CCP) and induced coupled plasma (ICP). The CCP has two electrodes, the lower one is RF powered on which a process substrate is usually placed, while the upper one is grounded. An ICP utilizes RF electric fields generated by planar, cylindrical, or hemispherical induction coils to maintain high-density discharges.

For capacitively driven RF discharges, positive ions are accelerated and the electrons are decelerated by the electric field near the powered electrode, correspondingly, a space charge sheath will be formed. For an ICP, in order to control the ion impact energy and obtain better plasma uniformity, the electrode that a substrate is placed upon is often independently RF biased so that the region where the plasma is generated is separated from the region where the plasma is processed, also causing an RF sheath adjacent to the substrate electrode.

In plasma processing, the ion energy distribution functions (IEDs) and ion angular distribution functions (IADs) on the substrate are significant because they determine etch rates and etch profiles in the etching processes as well as deposition rates and microstructures in deposition. IEDs and IADs describe respectively the probability of ion impact at a process surface for a given ion impact energy and the probability of ion impact for given ion impact angles about normal incidence to the surface. Ion behaviors are modulated by the RF sheath field sheath when they cross the sheath. Thus, IEDs and IADs are determined mainly by the characteristics of the space-charge sheath. Meanwhile, the behavior of the sheath is essential to studying dusty plasmas. Therefore, it is significant to better understand the physical process in the sheath.

In the case of a plane substrate on which there are no topographical features and in the low pressure case (<50 mTorr) where the ion mean free path may be greater than the sheath thickness, the 1D collisionless sheath model is adequate for describing the spatial variation of the sheath assuming that the underlying electrode is an infinite plane with the sheath electric field perpendicular to the surface. The characteristics of collisionless sheath in a

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single-frequency driven plasma will be discussed in Section 3.

In the field of film deposition, however, discharge pressures can be up to hundreds of mTorr, which could lead to the ion mean free path getting close to the sheath thickness. Thus, positive ions can suffer collisions in the sheath such as elastic scattering or charge exchange collisions. Collisions will reduce the energy of ions bombarding the substrate and result in a nonzero impact angle. In this case, the effects of collision on the sheath properties should be taken into account in describing the ion dynamics. The collisional sheath in a single-frequency (SF) driven plasma will be discussed in Section 4.

When the surface contains topographical features and the size of features can be comparable to or larger than the sheath thickness, the sheath profile is drastically distorted by the surface structure of the electrode in such a way that it tends to wrap around the contour of the electrode features, which is the effect known as characteristic plasma molding. Sometimes, a set of optional multipole permanent magnets can be used to surround the substrate chamber to minimize plasma losses to the walls and improve plasma uniformity, which is particularly important in the experiments on dusty plasmas. Under these circumstances, multi-dimensional sheath dynamic simulations are indispensable in addressing the important issue of plasma uniformity and the spatio-temporal sheath dynamics. Section 5 discusses the structures of a 2D sheath and those with a static magnetic field applied perpendicular to the surface.

The most important issue to be solved is the independent control of the flux and energy distribution of the ions bombarding the substrate, because high plasma density and controllable energy of the ions are needed to increase etch rates, uniformity and selectivity. A disadvantage of the traditional capacitive plasma driven by a single industrial standard frequency of 13.56 MHz is that the plasma density cannot be controlled independently of the ion bombardment energy. The plasma density can be increased by increasing the applied RF voltage amplitude, and also the sheath potential and consequently the ion bombardment energy. Excessive ion energy is not beneficial as it can give rise to undesired sputtering and radiation damage. Also, the plasma density can be increased by increasing the applied frequency [1], however, the width between the high energy and the low energy peak of the IED bombarding the substrate shrinks, which will decrease selectivity [2]. On the other hand, although an ICP has an advantage of being able to achieve high density (10^{11} – 10^{12} cm⁻³), and can accomplish (quasi) independent control of plasma density and ion bombardment energy by decoupling plasma generation from substrate bias, it is difficult for an ICP to promote uniformity over large diameter substrates due to a more nonuniform electric field compared with a CCP. In the last few years, the use of a dual frequency capacitively coupled plasma (DF-CCP) operated with an additional power supply driven by a different frequency attracted much attention as a mainstream plasma source for etching. This makes it possible to obtain

the desired independent control of plasma density and the ion bombardment energy, which is crucial for material processing. In general, the lower frequency source mainly determines the sheath parameters and consequently the ion bombardment energy while the higher frequency source mainly controls the bulk plasma parameters [3,4] (details in Section 6).

The outline of the paper is as follows. In Section 2, the basic dynamic model of the RF sheath is formulated in terms of ion fluid equations and the equivalent circuit model. Section 3 discusses the characteristics of collisionless sheath in a single RF biased plasma. In Section 4, the characteristics of collisional sheath in a single RF driven plasma are presented. Section 5 proposes a 2D sheath and a magnetic sheath. In Section 6, a dual RF sheath will be shown. A summary is given in Section 7.

2 Sheath model descriptions

The modelling of ion transport in RF sheaths is fundamental to understand the exact details of the spatio-temporal variations of parameters within the sheath such as the potential, electric field, ion density as well as the time dependence of the sheath thickness, sheath potential, and ion flux. We use a fluid model to study the transport of ions in a RF driven sheath. The ion transport is described by the continuity and momentum transfer equations. The electrons are assumed inertialess and respond to the instantaneous electric field, hence obey Boltzmann distribution, because the electron plasma frequency ω_{pe} is much higher than the applied frequency. The electric potential in the sheath is determined by Poisson's equation. In addition, we introduce an equivalent circuit model to define the relationship between the sheath potential and sheath thickness as well as the applied RF current. Moreover, we can neglect the ion thermal motion effects since the ion temperature is much smaller than the directional kinetic energy in the sheath regions. Thus, the spatiotemporal variation of the ion density, n_i , the ion drift velocity, \mathbf{u} , and the electric potential inside the sheath, Φ , are described by the cold ion fluid equations,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial (n_i \mathbf{u})}{\partial t} + \nabla \cdot (n_i \mathbf{u} \mathbf{u}) = -\frac{en_i}{m_i} \nabla \Phi + \frac{1}{c} \frac{en_i}{m_i} \mathbf{u} \times \mathbf{B} - \nu n_i \mathbf{u} \quad (2)$$

where \mathbf{B} is the static magnetic field, $\nu = u N_n \sigma_c$ is the frequency of the charge exchange collisions between the ions and neutral particles, with N_n being the neutral gas density and σ_c the collision cross section [1,5], and the Poisson's equation,

$$\frac{\partial^2 \Phi}{\partial r^2} = -\frac{e}{\epsilon_0} (n_i - n_e) \quad (3)$$

where m_i is ion mass, e is the electronic charge, ϵ_0 is the

permittivity of free space, and $n_e(x,t)$ is the electron density.

We consider that the electron density in the sheath is given by Boltzmann's distribution

$$n_e(r,t) = n_0 \exp\left(\frac{e\Phi(r,t)}{k_B T_e}\right) \quad (4)$$

where n_0 is the plasma density, T_e is the electron temperature, and k_B is the Boltzmann's constant.

Through conservation of current, the currents passing through the sheath which include the ion current $I_i(t)$, electron current $I_e(t)$ and displacement current $I_d(t)$, should equal to the applied sinusoidal RF current [2,10]

$$I_i(t) - I_e(t) - I_d(t) = I_{\max} \sin \omega t \quad (5)$$

where $I_{\max}(t)$ and ω are respectively the amplitude of the applied current and the frequency of RF source, and $I_i(t) < I_e(t)$ and $I_d(t)$ can be found in Ref. 2. For a dual RF-biased sheath, the right side of Eq.(5) should be the sum of two sinusoidal RF currents, i.e., $I_1 \sin(\omega_1 t) + I_2 \sin(\omega_2 t)$, where the suffixes 1 and 2 refer to the low- and high-frequencies, respectively.

Equations (1)–(5) form a set of closed nonlinear equations that determine the spatio-temporal dependence of the RF biased-sheath which can be obtained by using a finite difference scheme with an iterative process with the appropriate boundary conditions [2,13,20,24,25]. The iteration is repeated until the solutions converge to a self-consistent periodic steady state.

3 Collisionless sheaths in a single RF-driven plasma

In this section, we focus on the 1D collisionless sheath in which the magnetic field and collision effects in Eq.(2) are neglected.

In general, it is difficult to get analytical solutions for the RF sheath due to its strongly nonlinear processes. A crucial parameter of the RF sheath dynamics is the ratio of the RF frequency to the ion plasma frequency, $\beta = \omega / \omega_{pi}$. When the RF frequency is much smaller than the ion plasma frequency ($\beta \ll 1$), the ions in the sheath respond to the instantaneous sheath potential and cross the sheath in a small fraction of a RF cycle. A quasi-static model [6], in which the sheath properties at different times in a RF cycle are the same as those of a direct-current (dc) sheath with a potential equal to the instantaneous value, can be used to describe the processes in the low frequency range.

In the high-frequency range ($\beta \gg 1$), the ions will take many RF cycles to cross the sheath and can no longer respond to the instantaneous sheath potential. Instead, the ion dynamics is governed by a time-averaged field in the sheath. The time-averaged model, which ignores all time-dependent terms in the ion fluid equations, has been proposed by Lieberman *et al.* [7]. It uses an electron steplike model in which the electron density drops abruptly to zero at the electron sheath boundary. With the time-averaged model, analytical expressions can be obtained for various sheath

parameters such as the dc sheath voltage, the sheath capacitance, and the stochastic heating power. Making use of suitable boundary conditions, Gierling and Riemann [8] introduced a consistent step model. Beyond the step model, Riemann [9] gave an improved description of the RF sheath by taking into account the distribution function of ions entering the RF sheath. It should be noticed [7] that although a sinusoidal RF current source is applied on the electrode, the voltage on the electrode is not exactly sinusoidal due to the effects of the sheath loading. In fact, both the forms and amplitudes of the voltage on the electrode are unknown and should be determined consistently by the current balance condition on the electrode. Edelberg and Aydil [10] introduced an equivalent circuit model for predicting consistently the time-dependent potential on the electrode.

In the intermediate frequency range ($\beta \sim 1$), it is nearly impossible to obtain an analytical representation of the sheath because the ion inertia allows it to only partially respond to the fields in the sheath. In this frequency range, one should take into account all the time-dependent terms in the ion fluid equations. A "damped potential" was introduced to model the ion dynamics assuming that the ions respond to the damped potential [11]. Containing all time-dependent terms in the ion fluid equations, Bose *et al.* [12] found that the ion flux oscillates significantly in an RF cycle for values of $\beta \sim 1$ rather than remaining constant as that in the high frequency range of $\beta \gg 1$, although they assumed that a sinusoidal voltage is applied on the electrode.

The fluid sheath model [2] including all time-dependent terms in ion fluid equations and using the current balance condition [10] can study self-consistently the spatiotemporal characteristics of the sheath and predicting the energy distributions of ions impinging on a RF-biased electrode over a wide range of frequency ratio β . It has been shown from the numerical results (Fig. 1) that in the low RF-frequency

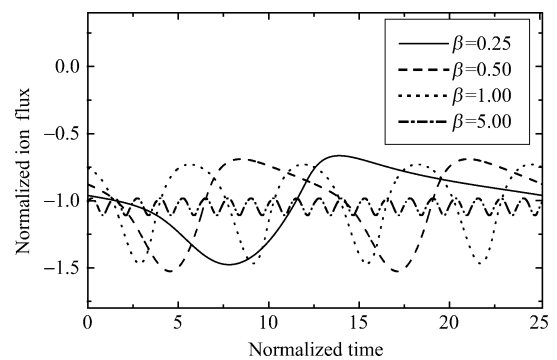


Fig.1 The time-dependent ion flux nu_i incident onto the RF-biased electrode for different values of the frequency ratio β [2]. In the simulation, an argon discharge is used in which the plasma density, the electron temperature, the RF-biased power, and the electrode area are chosen as $2.1 \times 10^{11} \text{ cm}^{-3}$, 3 eV, 50 W, and 325 cm^2 , respectively.

regime ($\beta \leq 1$) the ion flux on the electrode oscillates strongly with the time and its amplitude drops gradually as

increasing the frequency ratio β , while the ion flux approaches the constant flux $n_0 u_B$ at the high-frequency limits ($\beta \gg 1$) which is the same as the time-average sheath model mentioned above. Figure 2 displays that the IED on the substrate has a bimodal shape and the width of the IED shrinks and the two peaks of the IED approach each other with increasing the RF-frequency. It is can be seen from Fig. 3 that the spatiotemporal variations of the electric field vary significantly near the electrode and the temporal profile of it oscillate periodically with the time. With the multiple ion sheath dynamics model [13], considering the existence of multi-ion species, it has been found that multiple peaks appear in the ion energy distributions, i.e., the low- and high-energy peaks split up into many small peaks due to the existence of ions with different mass, as

Fig.3 The spatiotemporal variation of the electric field inside the sheath during one RF cycle [2]. The frequency ratio is 0.25 and the parameters are the same as in Fig. 1.

illustrated in Fig. 4, similar to the experimental results [14].

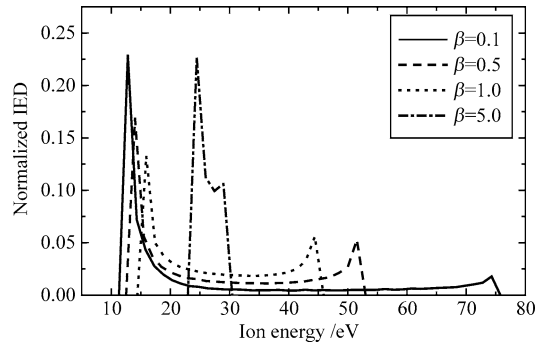


Fig.2 The effect of the frequency ratio β on the ion energy distributions [2] for the same input parameters as in Fig. 1.

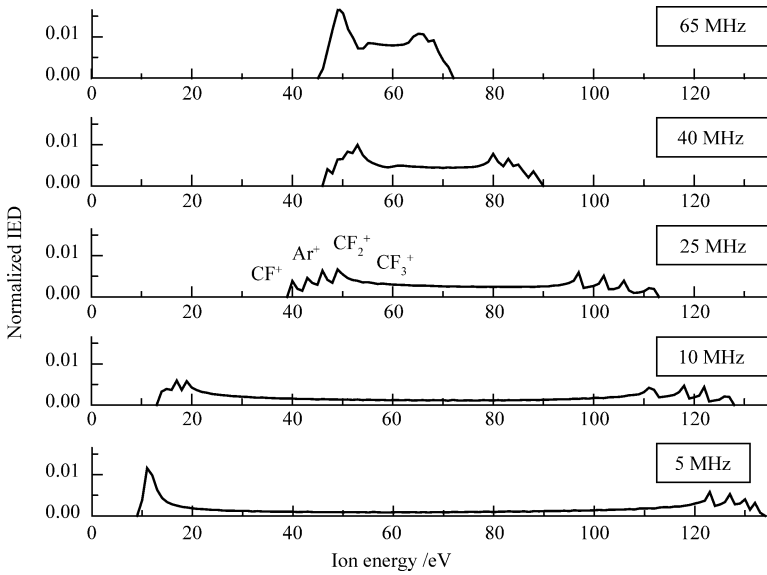
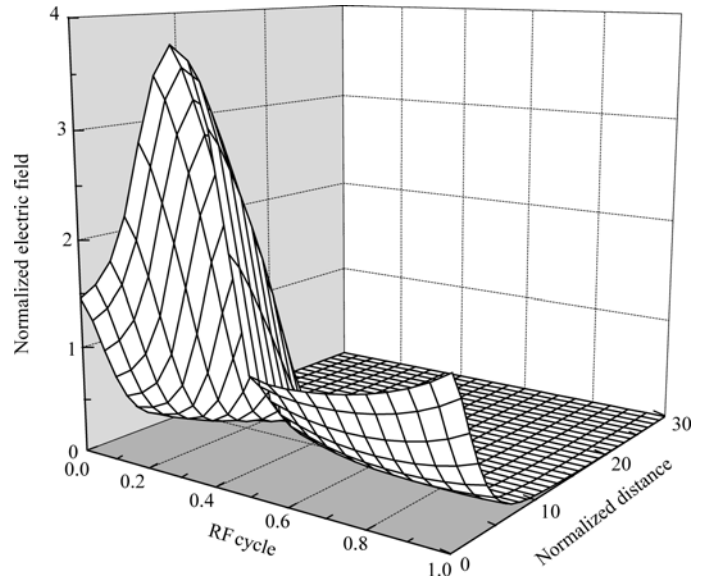


Fig.4 The effect of the RF-biased frequency on ion energy distributions [13] for the sheath with multi-ions such as A^+ , CF^+ , CF_2^+ and CF_3^+ . The RF-biased power, the bulk plasma density, electron temperature, and the electrode area are kept constant at 150 W, $2.0 \times 10^{11} \text{ cm}^{-3}$, 2 eV, and 325 cm^2 , respectively.

4 Collisional sheaths in a single RF-driven plasma

The electron-neutral and ion-neutral collisions play a key role in the momentum and energy transfer in a partially ionized plasma. Their role on sheath formation is also significant. On physical grounds one can expect that the ion collision in the sheath may reduce the ion impact energy to the substrate. Consequently, ion dynamics must encompass the entire range of collisionality. The characteristics of collisional sheath and effects of collision on IEDs and IADs will be discussed in this section where the magnetic field is also neglected in Eq.(2).

It is well-known that a stationary collisionless sheath exists only if the ion flow velocity satisfies the Bohm criteria at the plasma-sheath boundary, i.e., the plasma drift speed must exceed the Bohm velocity. Thus, the value of ion velocity at the plasma-sheath interface is usually chosen as the Bohm velocity in order to reduce the amount of computation, which is appropriate for collisionless sheath. For a collisional sheath, however, there are no finite location of a sheath edge under the influence of collision [15]. If the Bohm velocity is still chosen as the boundary condition, this would lead to inconsistency in physics. In this case, we have to consider a transition layer, i.e., a space charge neutral presheath that is of the order of mean free path of plasma-neutral interaction and in which the ions are accelerated so that they enter the sheath with the minimum energy required for a stable sheath.

With an extended Lieberman's time-averaged model [16], which assumes that the average ion potential energy gains from the RF electric field dissipate fully in the charge-exchange collisions between the ions and the neutral particles based on the step model, it is found that the

increase of the pressure can result in a reduction of the ion bombardment energy and the thinning of the sheath [17].

Theoretically and experimentally, investigations [18–20] show that IEDs also have the bimodal shape just as those in collisionless sheaths for $\beta \leq 1$ or $\beta \sim 1$. The effects of the collision processes on the IEDs and IADs have been simulated with the Monte Carlo method [18,19] assuming parametric sheath electric fields which depend on the sheath thickness and the potential on the electrode. Dai *et al.* [20] proposed a self-consistent hybrid model including a fluid model by which the spatial-temporal electric field in the sheath is determined self-consistently, and a Monte-Carlo model by which the ion trajectories, IEDs and IADs can be simulated. In these works, the presheath and sheath region are considered as a whole in order to avoid singularities and discontinuities in some physical quantities that usually occur using Bohm's criterion as the boundary condition at the sheath-plasma interface. It is found from Fig. 5 (a) that at low pressures, a significant number of ions experience no collision when crossing the sheath, causing a wide IED. As the pressure is increased, however, due to the ions going through a great deal of charge-exchange collisions, the heights of both peaks decrease, especially for the high-energy peaks, and the location of the high energy peak decreases. In addition, as the discharge pressure increases, the IADs spread to large angle regions, which results from the ions undergoing a number of collisions with neutrals in the sheath, as shown in Fig. 5 (b). The spreading in angle of the IADs has important consequences in plasma etching where an anisotropic delivery of activation energy to the surface is required to obtain vertical etches.

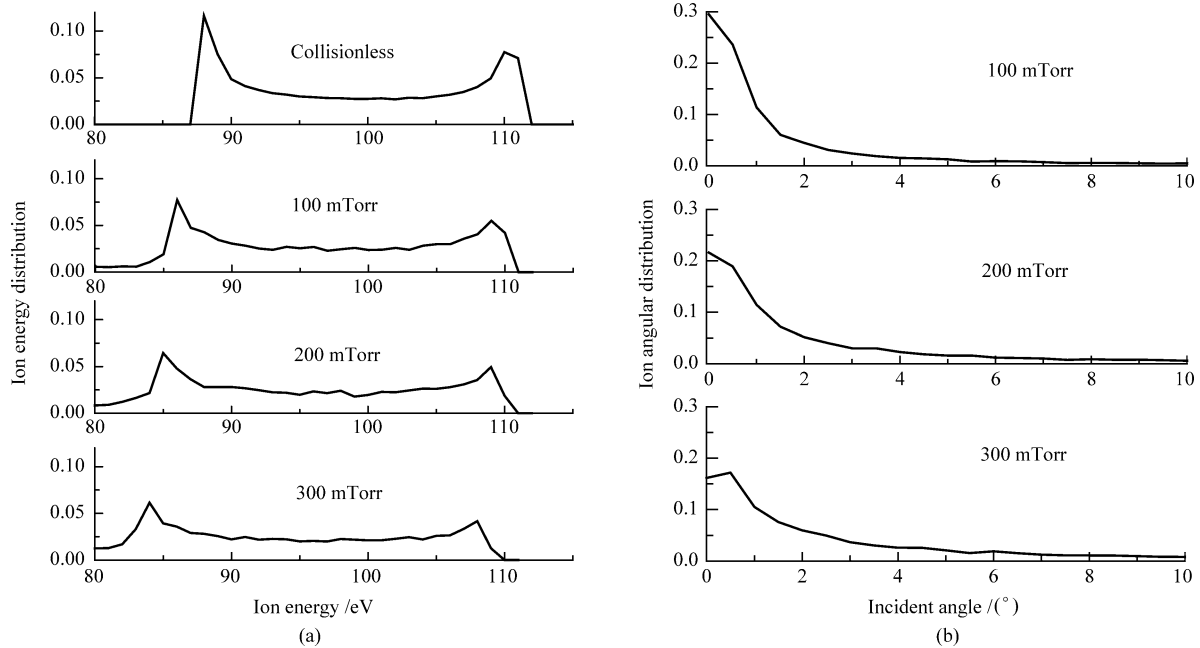


Fig.5 The effect of the discharge pressure on (a) the ion energy distributions and (b) ion- angular distributions for an Ar plasma [20]. The RF-biased frequency, RF-biased power, plasma density and electron temperature are kept at 13.56 MHz, 50 W, $1.0 \times 10^{10} \text{cm}^{-3}$, and 3 eV, respectively.

5 2D sheaths in a single RF-driven plasma

This section will report on the structures of a 2D collisional sheath and those with a static magnetic field applied perpendicular to the surface. A RF-powered electrode with an azimuthal symmetric cylindrical hole is used in the simulation.

Recently, Kim and Economou studied [21–23] a 2D sheath model, developed to simulate plasma molding over micron-sized steps, trenches or rings. In the model, the electrode is grounded while the plasma potential is assumed sinusoidal.

In a self-consistent manner, i.e., using current balance condition to self-consistently determine the relationship between the sheath potential and the applied current, Hou *et al.* [24] studied a 2D sheath model, obtaining the time dependence of instantaneous potential, as shown in Fig. 6. The results [24] show that the existence of the cylindrical hole on the electrode significantly affects the sheath structure and generates a potential trap in the horizontal direction, which is particularly strong when the sheath thickness is comparable to the depth of the hole. It [24] also has been found that, with increasing discharge pressure or with decreasing RF bias power, the sheath becomes thinner and its profile follows more closely the profile of the hole in the electrode. In particular, strong radial ion fluid velocity and the radial electric field were found close to the surface of the hole.

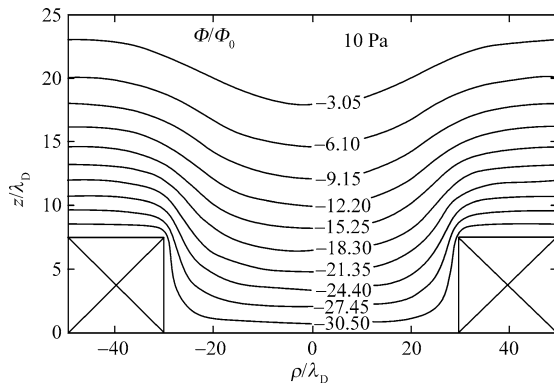


Fig. 6 Contour lines of the time-averaged sheath potential over the powered electrode [24]. The base values of the discharge parameters are given as follows: the plasma density is $1 \times 10^9 \text{ cm}^{-3}$, the electron temperature 3 eV, the rf source frequency 13.56 MHz, the discharge pressure 10 Pa, the RF powers 1 W, the diameter of the electrode 10 cm, the diameter $2R$ of the hole 2.4 mm, and the hole depth being $4 \lambda_D$ (λ_D being the Debye length, which is about 0.04 cm under the present discharge conditions).

In a subsequent work, Hou *et al.* simulated the 2D magnetized sheath dynamics over a RF-biased electrode with a magnetic field applied perpendicular to it [25]. The results obtained show that such an electrode gives rise to a strong radial component of the electric field, which distorts the distribution of the plasma and generates a radial component of the ion flow. It has been found that the

azimuthal ion flow by the $\mathbf{E} \times \mathbf{B}$ drift can be significant when the discharge pressure is relatively low. The azimuthal velocity of the ion flow has been found to increase in proportion to the increasing magnetic field. Figure 7 displays the spatial distribution of the time-averaged sheath potential ϕ , and radial component of the electric field E_ρ . From Fig. 8, one can see that the radial component of the ion flow u_ϕ starts from zero at the axis and rapidly grows larger towards the wall of the hole, reaching a peak value just above the edge of the hole.

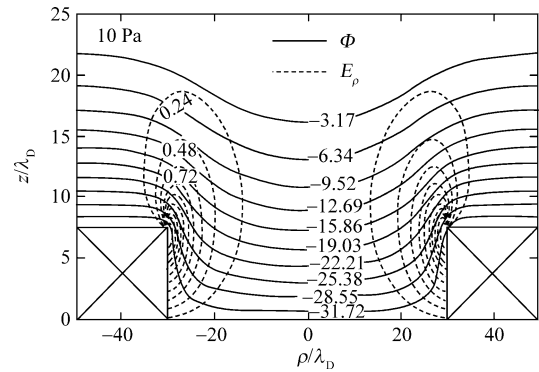


Fig. 7 Contour lines of the time averaged normalized sheath potential Φ and radial 15 component of electric field E_ρ over the electrode with the plasma density is fixed at $1.0 \times 10^9 \text{ cm}^{-3}$, electron temperature 3 eV, frequency 13.56 MHz, diameter of the electrode 10 cm, the diameter of the hole 2.4 cm, the depth of the hole 3 mm, the RF power 2 W, discharge pressures 10 Pa, and the magnetic field 100 G, respectively.

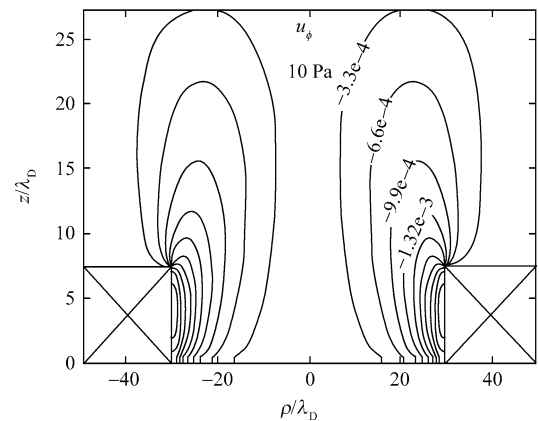


Fig. 8 Contour lines of the time averaged azimuthal component of ion velocity u_ϕ field (normalized by Bohm velocity u_B) over the electrode [25]. The same parameters are used as the same as in Fig. 7.

6 Collisionless sheaths in a dual RF-driven plasma

Although DF-CCPs operated with an additional power supply driven by a different frequency attracted much attention as a mainstream plasma source for etching, the physics of DF-CCP has not been fully investigated as that of

SF-CCP. The characteristics of the 1D dual RF sheath and IEDs on the dual biased substrate without collision and magnetic field will be presented in this section.

With simplified models, some authors got analytical expressions for dual frequency-biased sheaths and found that the sheath thickness is modulated by high-frequency [26–28]. With a homogeneous plasma model for a dual RF discharge, Kim [29] introduced a concept of effective frequency to understand DF-CCP by treating it as SF-CCP that is a simpler and well-known system. Using a fluid model for dual RF sheaths, Guan *et al.* [30] discovered that the structure of a dual RF biased sheath is more complex than that of a single RF biased sheath. Besides, the potential

within a dual RF sheath and sheath thickness as well as ion flux not only have a slow oscillating contour modulated by the low-frequency similar to that in a single frequency biased sheath, but also has many rapid oscillations modulated by the high-frequency in one low frequency cycle, as illustrated in Fig. 9. So far, few self-consistent works have been done for the effect of dual frequencies on IEDs. It has been presented from Guan’s work (Fig. 10.) that the IEDs have multiple peaks because the potential on the dual RF-biased electrode oscillates many times, which just demonstrates that the frequencies of the Low-and high-frequency source are crucial for controlling the energy of ions bombarding the substrate.

Fig.9 The effect of low frequency on the instantaneous sheath potential for an Ar plasma [30]. The frequency and power of the high frequency source are fixed at 60 MHz and 300 W, the power of the low frequency source is fixed at 900 W, the plasma density, electron temperature, and electrode diameter are kept at $5.0 \times 10^{11} \text{cm}^{-3}$, 3 eV, and 30 cm, respectively.

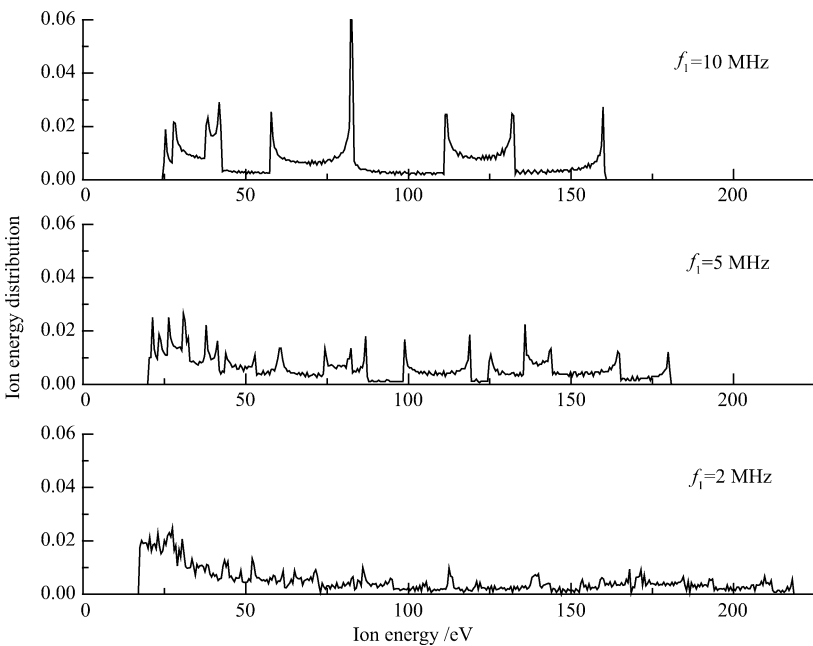
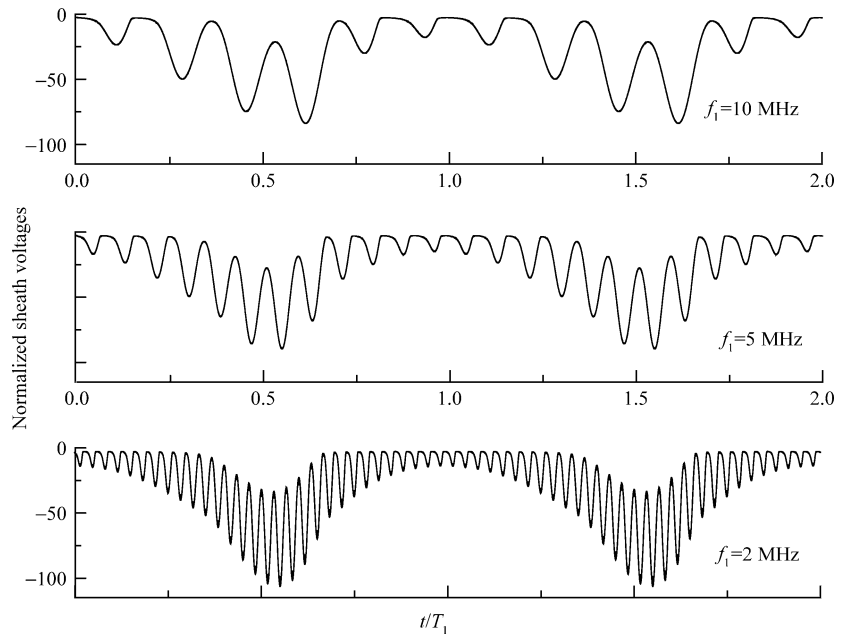


Fig.10 The effect of lower frequency on the IEDs impinging on the dual RF electrode [30]. The input parameters are the same as those used in Fig. 9.

7 Conclusions

This paper provides an overview of the dynamics of the RF sheath. It is found that the collisionless sheath, collisional sheath, 2D sheath, and dual RF sheath behave uniquely, consequently, and in different shapes from IEDs. Also, we found that the frequency is the most important parameter that determines the structure for any kinds of sheath. In addition, the properties of the sheath depend on the ion density, electron temperature, applied frequency, power, pressure, magnet field and so on. For the most attractive and promising technique, DF-CCP showed that both a high- and low-frequency sources modulate the structure of the sheath. Therefore, the urgent task is finding a way to solve decoupling between the two frequencies by studying plasma dynamics in a whole reactor scale.

It should be stressed that the plasma parameters such as the ion density and electron temperature are given for studying the sheath dynamics, which inevitably leads to inconsistent in physics. In order to resolve the issue, we need to investigate the plasma characteristics within the whole plasma scale instead of just the sheath scale. However, it is a challenging multiscale task in which many technical problems remain unresolved. The more accurate method for obtaining the IEDs may be the particle-in-cell (PIC) method in spite of its computational burden.

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