Dynamic effects in dual-frequency capacitively coupled discharges

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Abstract. Investigations of the discharge current shape in a low frequency single frequency discharge and in a dual frequency discharge are performed in this paper. For this purpose a Particle in cell with Monte-Carlo Collisions numerical simulation of the capacitively coupled discharge in argon, operated at frequencies of 1.76 MHz & 81 MHz, is carried out. As a result the non-sinusoidal, close to triangle shape of the discharge current is obtained even for the case of a symmetric discharge. The physical reason of such non-sinusoidal behavior of the discharge current is the dynamic structure of the discharge sheaths. Corresponding to the discharge current, the sheath edge motion is also non-sinusoidal and non-symmetric. These results may be important for the appropriate choice of the current and voltage waveforms in analytic modeling of single and dual frequency discharges.

1. Introduction
Radio-frequency capacitively coupled plasma (CCP) discharges have been intensively studied both experimentally and theoretically due to their wide application in plasma processing and technology.

In modern plasma processing devices the CCP discharge is usually driven by two rf sources. Such dual-frequency excitation allows achieving more flexibility in the control of plasma properties. The typical value of the low-frequency is about 2 MHz and lower. Thereby there is additional interest in the study of the plasma dynamic properties in low-frequency (LF) discharges and the influence of the LF on the plasma in dual-frequency (DF) discharges.

Recent experimental investigations in DF discharges were performed for argon plasmas [1] and hydrogen plasmas [2]. These experiments showed the significant influence of the low-frequency on the discharge behavior.

Single frequency LF discharges have been studied for a long time [3–7], but some physical phenomena are still poorly understood.

In [3] an equivalent circuit model was presented to obtain voltage and current waveforms in the LF CCP discharge. These waveforms were nonsinusoidal for both symmetric and asymmetric discharges, and were explained by the nonlinear properties of the plasma sheaths. However, the physical reasons of this specific current shape were beyond the framework of the equivalent circuit model.

Different analytical and numerical approaches have been developed for analysis of CCP discharges. Such approaches usually use the discharge current or the electrode voltage as an input parameter, and the sinusoidal discharge current is often assumed in single frequency (SF) and DF
discharges [6 – 11]. However, since the DF CCP discharge is a strongly non-linear system, the question about the discharge current waveform is very important.

In view of the great interest in modeling dual frequency discharges and the importance of the appropriate choice of the current and voltage waveforms, the numerical investigation of the discharge current in the LF 1.76 MHz SF discharge and the 1.76 MHz & 81 MHz DF discharge is performed in this paper.

2. Particle in Cell model

A numerical simulation of SF and of DF CCP discharges based on the Particle in cell with Monte-Carlo collision method (PIC MCC) is performed.

The used PIC MCC model of RF discharge was described in detail in [12]. The one dimensional model of CCP discharge with an electrode gap of 2.4 cm and electrode radii of 5 cm is applied. The ion and electron behaviors are kinetically simulated by solving Newton’s equations and with a MC treatment of collisions processes. The sets of electron-neutral and ion-neutral collision cross sections for Ar were described in [12]. In addition, in this work we take into account ionization of Ar by Ar+ ions and the cross section for this process is taken from [13].

Since the large applied voltages are considered, the secondary electron emission from electrodes may play an essential role. The probability for secondary emission induced by the ion impact, γi, depends on the electrode material and on the energy of impinging ions. We use the energy dependence of the coefficient γ that is suggested in [14]. Besides Ar+ ions, high energy argon atoms, Arfast, generated in the sheaths due to charge transfer collisions of Ar+ ions, may cause secondary electron emission at the electrode surface. As the following calculations have shown, in the conditions under study the relative contribution of the secondary electron emission by Arfast atoms may be comparable with the secondary emission due to ion impact. That is why we track motion of fast atoms in the present PIC MCC simulation. The initial velocities of the generated Arfast atoms are equal to the “parent” ions velocities. Then fast atoms move in the sheaths and lose their energy in elastic and ionization collisions with “cold” Ar atoms. The momentum transfer and ionization cross-section of Arfast were taken from [13]. According to [14] the probability of the secondary electron emission induced by the fast argon atoms, γα, depends on the energy of the Arfast, and this process is not effective for low energies. The used in this work the analytical expression for γα from [14] and an energy threshold of 32 eV. Therefore we stop tracking the Arfast atom if its energy drops below 30 eV. It is an irreversible process since neutral atoms are not accelerated in the electric field. As a result, Arfast are distributed mainly in the sheaths and the total number of super particles representing Arfast atoms is only about 10-15% of the total numbers of super particles for electrons and ions at the same particle weights. In that way the kinetic description of Arfast atoms does not slow down the PIC MCC simulation.

The anisotropic scattering of electrons in collisions due to high electron velocities is taken into account [15].

2.1. Single frequency discharge

The numerical simulation of the SF discharge was performed for the following discharge parameters: rf frequency is \( f = 1.76 \) MHz, the input power is \( P = 60 \) W, the gas pressure is \( P = 45 \) mTorr. In figure 1 the discharge current is shown along with the electron, ion and displacement currents to the left electrode. It can be seen that the total current has the non-sinusoidal, close to triangle shape.

The physical reason of such nonsinusoidal behavior of the discharge current is caused by dynamic structure of the discharge sheaths.

The main temporal characteristic of the sheath is the relation between the ion transit time through the sheath, \( \tau_{ion} \), and the rf period, \( \tau_{RF} \). There are two limit regimes for the SF discharge: the low frequency regime (\( \tau_{ion} \ll \tau_{RF} \)) and the high frequency (HF) regime (\( \tau_{ion} \gg \tau_{RF} \)) [16]. In the HF regime ions pass the sheath for many rf periods and respond to the average sheath potential [16]. In the
LF regime ions cross the sheath during the small part of the rf period and trace the instantaneous value of the electric field in the sheath.

![Image of discharge current and electrode sheath](image)

**Figure 1.** The total discharge current and the electron, ion and displacement currents at the electrode obtained from the PIC MC simulation.

As it follows from [17], in the LF case the ion velocity is close to the Bohm velocity during a considerable part of the rf period. And as the PIC MCC simulation has shown, the time when the ions move with Bohm velocity is about half of the rf period. Therefore considering the LF case of the SF discharge (or the DF discharge, where one frequency is relatively low) the following additional temporal characteristic should be taken into account:

\[
\tau_B = \frac{s_m}{\sqrt{T_e / M}},
\]

where \( \tau_B \) is the Bohm time, \( s_m \) is the electrode sheath width, \( T_e \) is the electron temperature in the plasma-sheath edge region, and \( M \) is the ion mass. The Bohm time describes the time which is necessary for the ion flow from the plasma bulk to maintain the ion concentration profile in the sheath region.

When

\[
\omega \tau_B \ll 1,
\]

or \( \tau_B \ll \tau_{RF} \), the quasi-stationary case takes place. In this case the ion flow from plasma maintains the ion profile in the sheath and at each phase of the rf period the plasma is screened by the positive space charge in the sheath. The sheath edge motion corresponds to the sinusoidal electrode voltage.

When inequality (2) fails, or \( \tau_B >> \tau_{RF} \), the low-frequency dynamic case takes place [17]. In this case the electrode sheath doesn’t correspond to the ordinary Child-Law sheath and the ion flow to the electrode varies during rf period.

In the studied discharge conditions, the sheath temporal characteristic may be evaluated as follows:

\[
\tau_{RF} = \frac{1}{f} = 0.5682 \times 10^{-6} \text{ s},
\]

\[
\tau_{ion} \approx \frac{s_m}{\sqrt{eU_{pl} / M}} = 0.26 \times 10^{-6} \text{ s},
\]

\[
\tau_B \approx \frac{s_m}{\sqrt{kT_e / M}} = 5.8 \times 10^{-6} \text{ s},
\]
where $U_{pl} = 680$ V is the plasma potential; the sheath width is $s_m = 0.9$ cm; the electron temperature is $T_e = 1$ eV. The used numerical values are taken from the PIC MCC calculation.

It can be seen that in the discharge conditions under study the inequality (2) fails and the low-frequency dynamic case takes place.

In the dynamic case the ion flow from the plasma has no time to restore the ion concentration profile as the electrode potential changes relatively fast. As a result the sheath edge moves away from the electrode during the one half of the rf period to screen the plasma by the positive space charge in the sheath. When the electrode voltage change its sign in the middle of the rf period the sheath edge moves very rapidly towards the electrode. This is illustrated by the PIC MC simulation results in figure 2. In comparison with the quasistationary case, where the sheath edge moves away and towards the electrode with equal velocities, in this dynamic case the sheath edge moves towards the sheath 3 times faster than it moves away from the sheath.

As a result of the fact that sheath edge moves very rapidly towards the electrode, the electron current to the electrode has the triangle shape which can be seen in figures 3, 4. The sheath resistivity becomes higher when the rf frequency decreases. At the present frequency of 1.76 MHz the ion and electron currents are of the same order as the total discharge current, and during a part of the LF period the electron current becomes equal to the total discharge current. Thus in this dynamic case the discharge current takes the non-sinusoidal form, close to the triangle one.

![Figure 2](image-url)

**Figure 2.** The sheath edge motion during rf period in the LF dynamic case. The discharge parameters are the same as in figure 1.

We should note once again that this phenomenon is caused by the temporal effects of the ion motion in the sheath, because there are also several different cases when the non-sinusoidal discharge current is possible. First, it is the case of an asymmetric discharge with electrodes of different areas. But in this paper we consider the symmetric discharge. Second, the secondary electrons emitted from the electrode may cause the non-sinusoidal shape of the current [18]. But this case takes place at higher gas pressures of several hundreds mTorr [18]. To prove that secondary electrons do not affect much the current shape for the case discussed in this paper, we performed the calculation without secondary electron emission from the electrode at the following discharge parameters: the rf frequency is 1.76 MHz; the pressure is 100 mTorr (since the discharge at 45 mTorr does not turn on without secondary electron emission taken into account), and the input power is 60 W. The results are presented in figure 3. It can be seen that the total discharge current is non-sinusoidal, close to triangle. In comparison with figures 1, 2, the electron current to the electrode has positive value everywhere since electrons are not emitted from the electrode.
The discharge parameters for the quasi-stationary LF case are far from the typical parameters for the real applications of CCP discharges. Therefore in order to illustrate the case of the sinusoidal discharge current, the discharge in argon at a rf frequency of 13.56 MHz, pressure of 45 mTorr, and input power of 30 W is simulated. Such parameters correspond to the HF regime for the ion motion in the sheath. The sheath edge moves sinusoidal in this case and the electron current has a symmetrical shape. Certainly its value is smaller and the electrons reach the electrode during a smaller part of the rf period in comparison with the 1.76 MHz discharge. The electron current does not disturb the total discharge current and the last one is close to sinusoidal as it can be seen in figure 4.

2.2. Dual frequency discharge

The numerical simulation of the DF discharge is performed for the following discharge parameters: $f_l = 1.76$ MHz; $f_h = 81$ MHz; $p = 45$ mTorr; the input power at low frequency is $P_l = 10$ W, the input power at high frequency is $P_h = 11$ W.

The total discharge current, and electron and ion currents to the electrode are shown in figure 5. It can be seen that in spite of the high frequency oscillation the envelope curve of the total current (or the current averaged over the high frequency) has the non-sinusoidal shape. The electron current to
the electrode is not equal to the total current at its maximum, but nevertheless the electron current is high enough to disturb the shape of the total current.

We can test the error that the sinusoidal approximation of the total current brings in this case. We have taken a Fourier analysis of the total current to find the amplitude of the oscillation at low frequency and at high frequency. In figure 6 the total discharge current is compared with the sum of sinusoidal functions at HF and LF. The maximal total current is 1.5 times higher than sum of LF and HF sinusoidal component. So, the usage of the sinusoidal current shape may lead to errors in the treatment of the discharge processes. The sheath dynamics discussed in this paper may be important also for the treatment of electron heating and resonance phenomena [19] in SF and DF discharges.

3. Conclusion
The low frequency 1.76 MHz discharge and the dual frequency 1.76 MHz & 81 MHz discharge were investigated with the PIC MCC model. The resulting “triangle” form of the discharge current is explained on the base of the ion dynamics in the sheath. It is shown that the sinusoidal approximation of the discharge current is not valid in these regimes.

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