

Fluid simulation for influence of metastable atoms on the characteristics of capacitively coupled argon plasmas

Yu-Ru Zhang, Xiang Xu, and You-Nian Wang^a

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Received 15 January 2010; accepted 1 March 2010; published online 29 March 2010

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I. INTRODUCTION

Capacitively coupled plasma CCP is vitally important to manufacture the very large scale integrated circuits used by the electronics industry.¹ It can be widely used to sustain the discharge for stripping of photoresist, deposition of thin films and etching of semiconductor and metal surfaces. Argon is particularly important in the discharge, because it can be used to dilute the reactive gas and enhance the physical etching, for instance. It is well known that, for the argon discharge, there exist much more long-lifetime metastable atoms, which will affect significantly the plasma properties, due to the obvious energy dissipation caused by them. To control the discharge parameters and improve the plasma processes, it is important to understand the mechanisms involved by the metastable atoms.

During the past decades, significant progress has been achieved in theoretical studies^{2–8} and experimental researches^{9–15} of the metastable effects in CCP. From early on, Yamaguchi *et al.*^{2,3} employed a relaxation continuum model to observe the metastable atom density, and came to a conclusion that the profile was controlled by the diffusion loss mechanism, with a maximum at the center. Lymberopoulos and Economou^{4,5} used a fluid model to simulate the CCP plasma characteristics in the case including metastable atoms in a parallel plate geometry, explaining that the profile of metastable atom density had two peaks when the pressure was high. After that, Rauf and Kushner⁶ placed their emphases on the metastable atom density in different gas mixtures. They discovered that the addition of O₂ or CF₄ could decrease the metastable density, or even change the profile. Roberto *et al.*⁷ and Lauro-Taroni *et al.*⁸ surveyed the dependence of the metastable atom density profiles on various pressures in a particle-in-cell/Monte Carlo model, and discussed the importance of the different production and loss mechanisms. It should be stressed that in the above studies,

the frequency of the radio-frequency RF power is almost equal to 13.56 MHz.

In addition, some experiments have been put forward to investigate the properties and effect of metastable atoms. As early as 1988, Scheller *et al.*⁹ measured the quenching rate for argon metastable at 20–100 KHz by the plasma-induced emission and laser-induced fluorescence spectroscopy technique. Sansonnens *et al.*¹⁰ compared the metastable density for a pure argon plasma with that for an argon plasma containing 4% silane, detecting that the density was substantially decreased by molecular quenching on silane. Whereafter, McMillin *et al.*^{11,12} obtained the argon metastable density as a function of pressure and voltage in the pure argon RF plasma reactor by planar laser-induced fluorescence imaging, and then they added a few percent of the electron attaching gases, such as O₂ to the pure argon, observing a decrease in density. Collard *et al.*¹³ and Ishimaru *et al.*¹⁴ investigated the metastable atom density in a single-frequency and dual-frequency CCP by optical emission spectroscopy and laser absorption spectroscopy, respectively. Last year, Hebner *et al.*¹⁵ clarified that the metastable density became more peaked in the center when the frequency is up to 150 MHz, which demonstrated the spatial change in the electron temperature, by means of the optical measurements.

For other plasma sources, the effect of metastable atoms also have been widely reported experimentally and theoretically, for instance, in positive column discharges,^{16,17} in an electron cyclotron resonance plasma,¹⁸ and chiefly in an inductively coupled plasma,^{19,20} which indicates that investigating the mechanisms with regard to the metastable effect contributes significantly to developing our comprehension and optimizing the plasma techniques.

However, there remain some questions regarding the theoretical studies of the metastable effects in the CCP. For instance, the plasma characteristics have been studied in different frequencies, especially in the very-high-frequency by experimental approach. Yet, in most of those models mentioned above, the emphasis is mainly placed on the discharge in different pressures and voltages, while the frequency is

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Citation: [Physics of Plasmas \(1994-present\)](#) **17**, 033507 (2010); doi: 10.1063/1.

View online: <http://dx.doi.org/10.1063/1>.

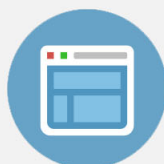
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TABLE I. The important reactions in argon discharge, where T_e represents the electron temperature, and E_e represents the electron energy in Kelvin.

Process	H_i eV	Rate coefficient cm^3/s	Reference
Ground state excitation ^a	11.56	$k_{ex}=3.71 \cdot 10^{-8} e^{-15.06/T_e}$	21
Ground state ionization	15.7	$k_i=8.7 \cdot 10^{-9} - 5.3 e^{-4.9/T_e - 5.3}$, 5.3	22
Step-wise ionization	4.14	$k_{si}=6.8 \cdot 10^{-9} T_e^{0.67} e^{-4.2/T_e}$	23
Superelastic collisions	11.56	$k_{sc}=4.3 \cdot 10^{-10} T_e^{0.74}$	23
Quenching to resonant ^b		$k_r=2 \cdot 10^{-7}$	4
Metastable pooling		$k_{mp}=6.2 \cdot 10^{-10}$	4
Two-body quenching		$k_{2q}=3 \cdot 10^{-15}$	4
Three-body quenching		$k_{3q}=1.1 \cdot 10^{-31}$	4

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usually fixed at 13.56 MHz. Whereas, the discharge modes in different frequencies may be different, which Yamaguchi *et al.*² has been explored, and consequently the influence of metastable atoms at high frequency may be distinct from the results obtained under the RF. The purpose of this article is to establish a fluid model, including metastable atoms, to examine the effect of metastable atoms in different discharge conditions systematically, especially in different frequencies.

This paper is outlined as follows. In Sec. II, the fluid model for the CCP which includes the metastable atoms, as well as the boundary conditions used in the model, is presented. The influence of metastable atoms in different frequencies on the plasma characteristics is shown in Sec. III. The results obtained from the simulation in various voltages are also shown in the section. Finally, we give a summary in Sec. IV.

II. DESCRIPTION OF THE FLUID MODEL

In this section, the equations for the fluid model, together with the boundary conditions, are presented. Above all, some approximations should be put forward that the plasma parameters are uniform along the radial axis. In addition, the discharge is sustained by Ohmic heating at high pressures, and there are hardly any energetic electrons due to the sufficient collisions with neutral atoms. Therefore, the electron energy distribution function obeys the Maxwellian distribution. In our model, there are two electrodes that separate from each other with a gap L . The upper electrode $x=L$ is grounded and the lower electrode $x=0$ is driven with a sinusoidal RF voltage, $V = V_{\text{RF}} \sin 2\pi ft$, where V_{RF} is the peak RF voltage, and f is the RF.

The fluid model, which treats the plasma as a continuum media, consists of electron, ion and metastable atom continuity equations and momentum balance equations. Electron energy balance equation and Poisson's equation are also included. The continuity equations for electrons, positive ions and metastable atoms are:

$$\frac{dn_e}{dt} + \nabla \cdot j_e = k_i N n_e + k_{si} n_e + k_{mp} n^2, \quad (1)$$

$$\frac{dn_i}{dt} + \nabla \cdot j_i = k_i N n_e + k_{si} n_e + k_{mp} n^2, \quad (2)$$

$$\frac{dn}{dt} + \nabla \cdot j = k_{ex} N n_e - k_{si} n_e - k_{sc} n_e - k_r n_e - 2k_{mp} n^2 - k_{2q} N n^2 - k_{3q} N^2 n. \quad (3)$$

Here n_e , n_i , n , and N are electron density, ion density, metastable atom density, and neutral gas density, respectively; u_i is ion velocity; j_e and j are electron flux and metastable atom flux, respectively.

Since the electron mass is very small, we can ignore the inertial term, so the electron flux can be given in the drift-diffusion form:

$$j_e = - \frac{1}{m_e} \frac{n_e T_e}{\nabla x} - \frac{en_e}{m_e} E, \quad (4)$$

where ν_{en} is electron-neutral collision frequency, m_e is electron mass, and T_e is the electron temperature. Since the metastable atoms are not charged, the drift term disappears in the equation determined the flux of metastable atoms,

$$j = - D \frac{dn}{dx}, \quad (5)$$

where D is the metastable atom diffusivity. For ions, we adopt the momentum balance equations in disregard of the pressure gradient term to calculate the ion velocity, based on the cold fluid approximation:

$$\frac{du_i}{dt} + u_i \frac{du_i}{dx} = \frac{eE}{m_i} - \nu_{in} u_i. \quad (6)$$

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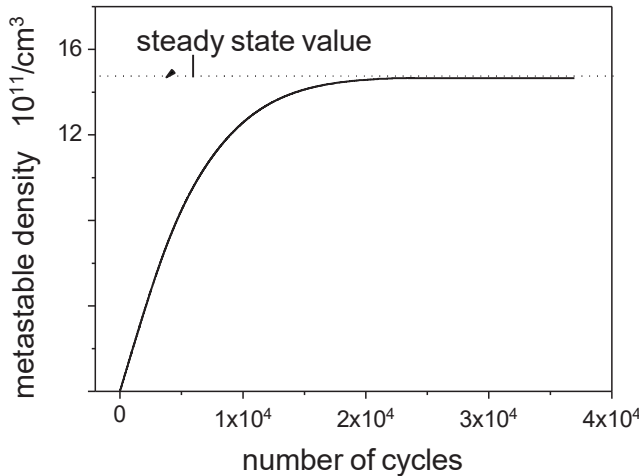


FIG. 1. The bulk metastable density at the end of each RF cycle at 1 Torr, 100 V.

$$\frac{\frac{5}{2}n_e T_e}{t} = -\frac{q_e}{x} - eEj_e - \sum_j H_j R_j, \quad (7)$$

where R_j and H_j are the reaction rate coefficient and the energy change in each collision. The reactions that are taken into account are shown in Table I. The flux of energy q_e is given by:

$$q_e = \frac{5}{2}T_e j_e - \frac{5}{2} \frac{n_e T_e}{m_e} \frac{T_e}{x}. \quad (8)$$

The self-consistently calculated electric field is obtained from the Poisson's equation, which is solved by coupling the Eqs. 1–8,

$$\frac{\partial^2 V}{\partial x^2} = \frac{e}{\epsilon_0} (n_e - n_i), \quad (9)$$

where e and ϵ_0 are electron charge and the permittivity of the vacuum. The relation between the electric field E and the electric potential V is

$$E = -\frac{\partial V}{\partial x}. \quad (10)$$

The boundary conditions of j_e and q_e used in the fluid simulation are as follows:

$$j_e = \frac{1-\gamma}{4} n_e \frac{8T_e}{m_e} j_i \quad (11)$$

$$q_e = \frac{5}{2} j_e T_e, \quad (12)$$

where γ and j_i are electron reflection coefficient and secondary electron emission coefficient, respectively. Meanwhile, we assume that the ion density and the ion velocity do not change substantially near the wall, so the gradients of its density and velocity are set to zero at the electrodes, as

$n_i / x = 0$, and $u_i / x = 0$, where the metastable atom density is equal to zero, as $n = 0$.

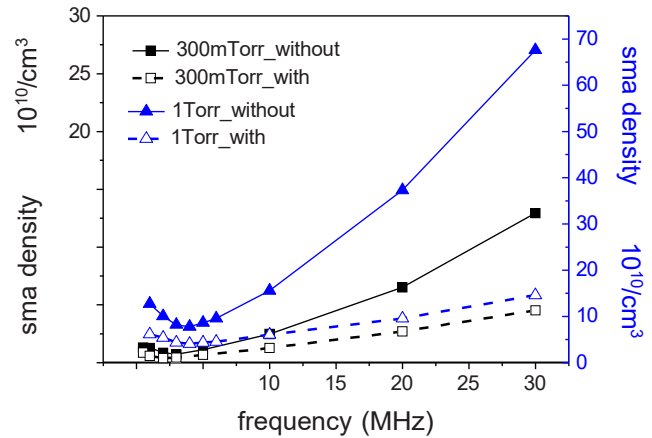


FIG. 2. Color online The plasma density at the discharge center between two electrodes in different frequencies at 300 mTorr and 1 Torr.

It is noteworthy that since metastable atoms respond on a long time scale, we indicate that convergence based on n is sufficient to ensure convergence of other plasma parameters. The bulk metastable density at the end of each RF cycle is shown in Fig. 1. It can be observed that 10^5 RF cycles are required to achieve the convergence.

III. RESULTS AND DISCUSSIONS

In this part, the discharges in various frequencies and voltages both at two different pressure values have been simulated, and the influence of metastable atoms on the bulk plasma density and the bulk electron temperature, as well as the distribution of metastable density are presented. The neutral gas temperature is fixed at 300 K, and the two electrodes separate from each other by 3 cm.

A. Frequency effect

In Fig. 2, the trends of bulk plasma density with frequency at different pressures are shown. The applied voltage is set to 300 V. It is obvious that there is a distinct difference between the case of including metastable atoms and the case without them. The plasma density decreases significantly when metastable atoms are included in the model both at 300 mTorr and 1 Torr. The result can be understood by examining the electron temperature between two cases, which may influence the ground state ionization rate greatly. From Fig. 3, it is seen that the temperature of electrons in the case with metastable atoms is noticeable lower than that in the case without metastable atoms, which means lower ground state ionization rate in the case with metastable atoms. Therefore, though in the case including metastable atoms, the step-wise ionization reaction and metastable pooling reaction can produce electrons and ions, the fraction generated by these two reactions cannot compensate the loss due to the lower ground state ionization rate. Thus the plasma density becomes lower in the case with metastable as a whole. Moreover, it is clearly seen that the decline in the plasma density is greater at higher frequency or higher pressure; in other words, the metastable effect on the plasma density is greater

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$$\frac{\partial n_e}{\partial t} + \nabla \cdot j_e = k_i N n_e + k_{si} n_* n_e + k_{mp} n_*^2, \quad (1)$$

$$\frac{\partial n_i}{\partial t} + \frac{\partial(n_i u_i)}{\partial x} = k_i N n_e + k_{si} n_* n_e + k_{mp} n_*^2, \quad (2)$$

$$\begin{aligned} \frac{\partial n_*}{\partial t} + \nabla \cdot j_* = & k_{ex} N n_e - k_{si} n_* n_e - k_r n_* n_e \\ & - 2k_{mp} n_*^2 - k_{2q} N n_* - k_{3q} N^2 n_*. \end{aligned} \quad (3)$$

Here n_e , n_i , n_* , and N are electron density, ion density, metastable atom density, and neutral gas density, respectively; u_i is ion velocity; j_e and j_* are electron flux and metastable atom flux, respectively.

Since the electron mass is very small, we can ignore the inertial term, so the electron flux can be given in the drift-diffusion form:

$$j_e = -\frac{1}{m_e \nu_{en}} \frac{\partial(n_e T_e)}{\partial x} - \frac{e n_e}{m_e \nu_{en}} E, \quad (4)$$

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$$j_* = -D_* \frac{\partial n_*}{\partial x}, \quad (5)$$

where D_* is the metastable atom diffusivity. For ions, we adopt the momentum balance equations in disregard of the pressure gradient term to calculate the ion velocity, based on the cold fluid approximation:

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The energy conservation equation for electron is:

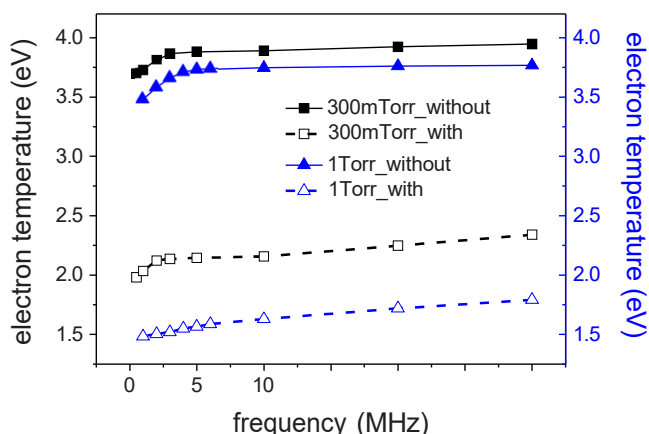


FIG. 3. Color online The electron temperature at the discharge center between two electrodes in different frequencies at 300 mTorr and 1 Torr.

by reason that the ground state ionization rate is influenced obviously by the metastable atoms, especially at higher frequency or higher pressure.

It is interesting that there is a minimum on the curve of the variation in bulk plasma density with frequency. The plasma density decreases with the raise in frequency in the range of low frequency; but as the frequency increases further, the density rises rapidly. The different trend of plasma density is due to the different discharge modes. When the frequency is high, the discharge is sustained by the Townsend discharge in the bulk plasma, i.e., α mode. As we all know the scaling $n \propto V_{RF}^2$, with a constant voltage, the plasma density is in proportion to the square of the frequency, and therefore the plasma density increases with frequency rapidly. However, when the frequency is low, the discharge is sustained by secondary electrons, i.e., γ mode. In other words, if there are not any secondary electrons, the discharge cannot be stable. A transition of discharge mode happens at the minimum. In the range of low frequency, the secondary electron emission becomes less predominant with the increasing frequency, and meanwhile, the bulk ionization mechanism does not contribute to the production of electrons and ions, so the plasma density decreases as the frequency rises in the low range. Both in the two discharge modes, the metastable atoms play an important role on the discharge and result in a significant decrease in plasma density.

To show the influence of metastable atoms more clearly, the results of bulk electron temperature in the cases including and without metastable atoms in different frequencies at 300 mTorr and 1 Torr are presented in Fig. 3. Compared with the result simulated in the case without metastable atoms, it can be clearly seen that the bulk electron temperature becomes lower when metastable atoms are included. It is because that, on one hand, the metastable atoms may cause obvious energy dissipation; on the other hand, the electrons may undergo more collisions caused by metastable; moreover, the weaker electric field due to the thicker sheath will also consequently limit the energy gain.

Besides, the bulk electron temperature increases monotonously with the increasing frequency, but the rising rate is different at different discharge modes. When the frequency

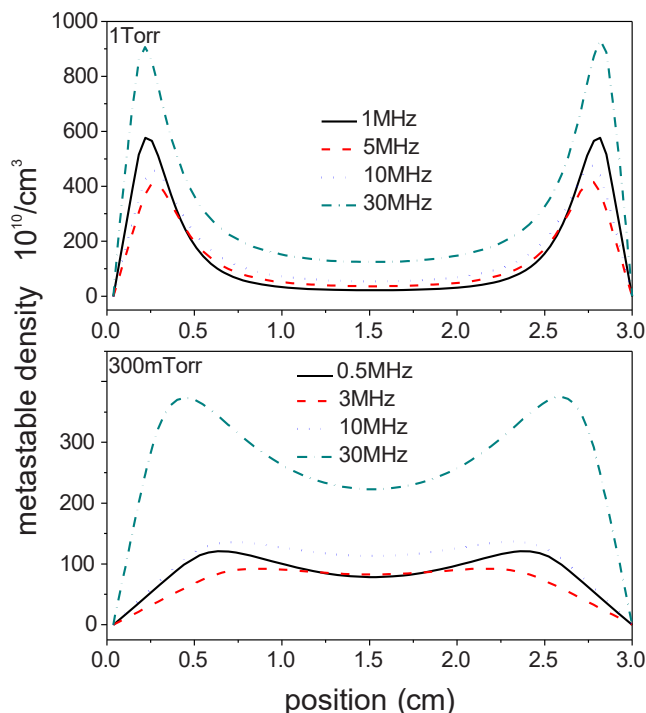


FIG. 4. Color online The metastable atom density between two electrodes in different frequencies at 300 mTorr and 1 Torr.

is low, the discharge is in γ mode. With the increase in frequency, the plasma density decreases and the electrons have a longer distance to be accelerated and gain energy during the thicker sheath. In addition, the secondary electron heating is more effective at low frequency, therefore the electrons can gain energy from the energetic secondary electrons more efficient, so the bulk electron temperature increases rapidly.

When the frequency is higher than the frequency threshold, the discharge is maintained by the α mode. The electron temperature increases gently with the increase in frequency.

The spatial metastable atom density profiles in different frequencies at 300 mTorr and at 1 Torr are shown in Fig. 4. It can be seen that the peaks of metastable atom density decrease with the raise in frequency first and then increase when the frequency is higher than the minimum. The trend is the same as that of the plasma density, for that the metastable atoms are created by the collisions between electrons and Ar atoms, which is in proportion to the plasma density in the discharge region. Moreover, it should be noted that the peaks of the metastable density move away from the electrodes with the rise of frequency first and then move toward, which also indicates the sheath variation with frequency. It is also found that at the conditions of high pressure or high frequency, the density of metastable atoms presents a saddle profile due to that the resonant reaction and step-wise ionization reaction take place more frequently in the bulk, which leads to more loss in the metastable atoms. When the pressure and frequency are low, the metastable atom density profile spreads out in the entire discharge region, because the diffusion has a predominant influence on the loss process of metastable atoms.

The distribution of ion density with frequency in the

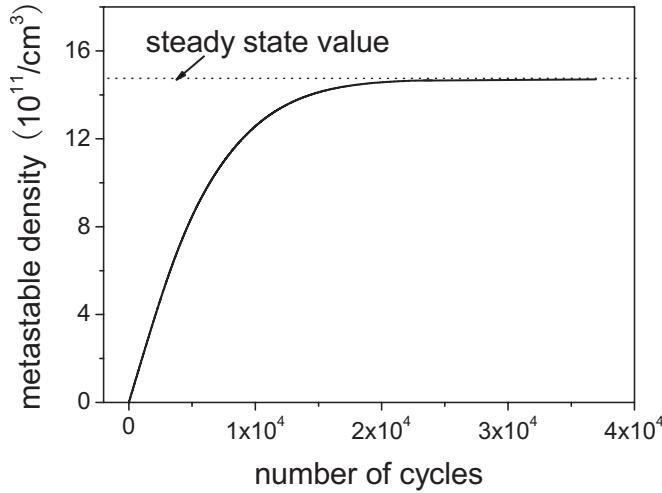


FIG. 1. The bulk metastable density at the end of each RF cycle at 1 Torr, 100 V.

$$\frac{\partial}{\partial t} \left(\frac{1}{2} n_e I_e \right) = - \frac{\partial q_e}{\partial x} - e E j_e - \sum_j H_j R_j, \quad (7)$$

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The self-consistently calculated electric field is obtained from the Poisson's equation, which is solved by coupling the Eqs. (1)–(8),

$$\frac{\partial^2 V}{\partial x^2} = \frac{e}{\epsilon_0} (n_e - n_i), \quad (9)$$

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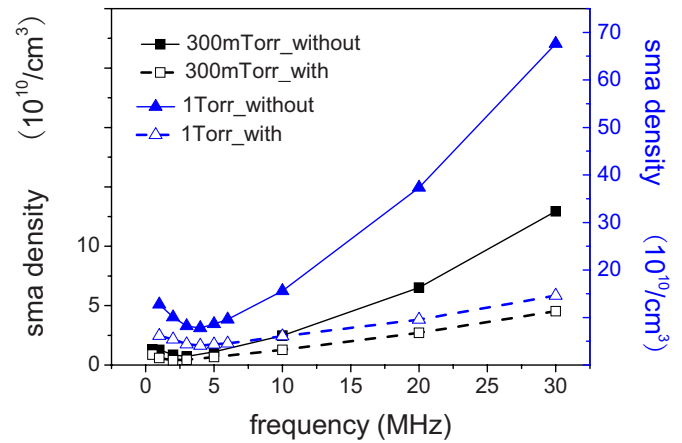


FIG. 2. (Color online) The plasma density at the discharge center between two electrodes in different frequencies at 300 mTorr and 1 Torr.

It is noteworthy that since metastable atoms respond on a long time scale, we indicate that convergence based on n_* is sufficient to ensure convergence of other plasma parameters. The bulk metastable density at the end of each RF cycle is shown in Fig. 1. It can be observed that $\sim 10^5$ RF cycles are required to achieve the convergence.

III. RESULTS AND DISCUSSIONS

In this part, the discharges in various frequencies and voltages both at two different pressure values have been simulated, and the influence of metastable atoms on the bulk plasma density and the bulk electron temperature, as well as the distribution of metastable density are presented. The neutral gas temperature is fixed at 300 K, and the two electrodes separate from each other by 3 cm.

A. Frequency effect

In Fig. 2, the trends of bulk plasma density with frequency at different pressures are shown. The applied voltage is set to 300 V. It is obvious that there is a distinct difference between the case of including metastable atoms and the case without them. The plasma density decreases significantly when metastable atoms are included in the model both at 300 mTorr and 1 Torr. The result can be understood by examining the electron temperature between two cases, which may influence the ground state ionization rate greatly. From Fig. 3, it is seen that the temperature of electrons in the case with metastable atoms is noticeable lower than that in the case without metastable atoms, which means lower ground state ionization rate in the case with metastable atoms. Therefore, though in the case including metastable atoms, the step-wise ionization reaction and metastable pooling reaction can produce electrons and ions, the fraction generated by these two reactions cannot compensate the loss due to the lower ground state ionization rate. Thus the plasma density becomes lower in the case with metastable as a whole. Moreover, it is clearly seen that the decline in the plasma density is greater at higher frequency or higher pressure; in other words, the metastable effect on the plasma density is greater

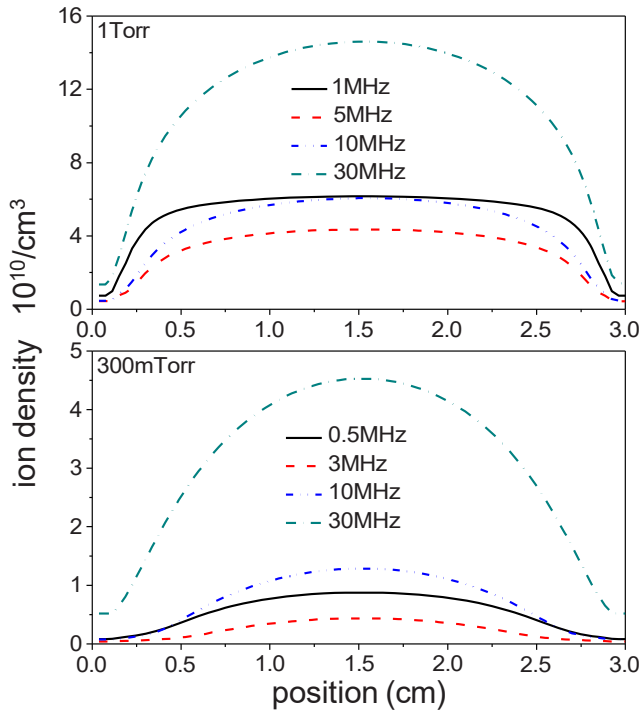


FIG. 5. Color online The ion density including metastable atoms between two electrodes in different frequencies at 300 mTorr and 1 Torr.

case including metastable atoms is shown in Fig. 5. It is discovered that the ion density is characterized by a parabolic profile at both of the considered pressure values, which is similar to the profile in the case without metastable atoms, but with a lower value. There is also a trend reverse of density with the increase in frequency. The reason of that is the same as that explained in Fig. 2.

B. Voltage effect

Figure 6 shows the evolution of bulk plasma density with voltage at 300 mTorr and 1 Torr, respectively, and the frequency of the power is set to 13.56 MHz. It is obviously that the bulk plasma density decreases when metastable at-

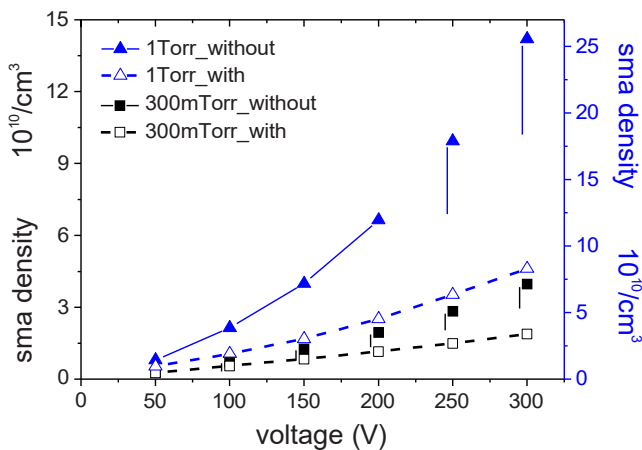


FIG. 6. Color online The plasma density at the discharge center between two electrodes in different voltages at 300 mTorr and 1 Torr.

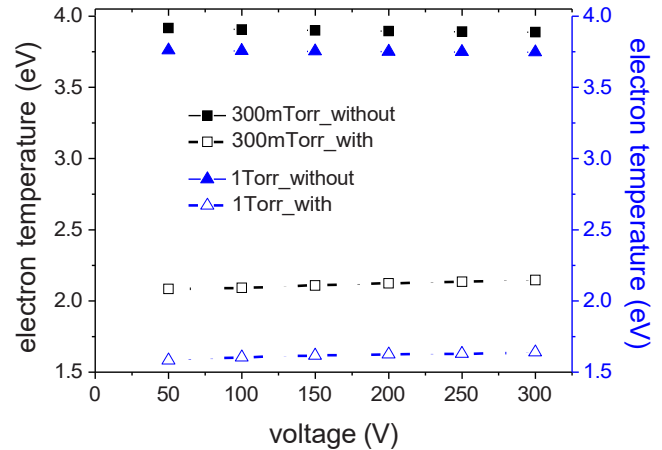


FIG. 7. Color online The electron temperature at the discharge center between two electrodes in different voltages at 300 mTorr and 1 Torr.

oms are included for both of the considered pressure values. Moreover, the decline in plasma density is more notable when the pressure or the voltage is high, for the same reason as that explained in Fig. 2. The plasma density rises with the increase in voltage, for that when the frequency is a constant, the plasma density is in proportion to the applied voltage, which is based on the well-known scaling $n \propto V_{RF}$.

In Fig. 7, the bulk electron temperature in different voltages at 300 mTorr and 1 Torr are shown. It can be seen clearly that when metastable atoms considered, the bulk electron temperature decrease obviously, due to the weaker electric field and more frequent collisions, as we have analyzed in Fig. 3. It is also shown that the electron temperature in the center decreases a little with the increase in voltage in the case without the metastable atoms, but increases slightly in the case including the metastable atoms. It might be the reason that the energy loss by ionization slightly increases faster than the energy gain from the Ohmic heating in the case without metastable atoms. In the case with metastable atoms, the energy loss process is more complicated, and the total energy loss increases slower than the energy gain.

The spatial metastable atom density profiles in various voltages under both of the selected pressure values are presented in Fig. 8. It can be observed that the metastable atom density increases with the raise in voltage, for the reason that the plasma density becomes higher with the increase in voltage, and then more ground state atoms are excited. When the pressure and the voltage are low, the density spreads out more in the entire discharge region due to the diffusion, and is characterized by a parabolic profile. With the increase in voltage and pressure, the density profile begins to flatten at the center. It shows that other loss processes, i.e., quenching to resonant reaction and step-wise ionization reaction, are becoming important. As the voltage increases further, a dip appears at the center, and two peaks are formed near the electrodes. Finally, it becomes a saddle profile.

In Fig. 9, it is discovered that the ion density has an rising trend with the increase in voltage due to that the sheath electric field is enhanced and then the discharge power increases. It is characterized by a parabolic profile at both

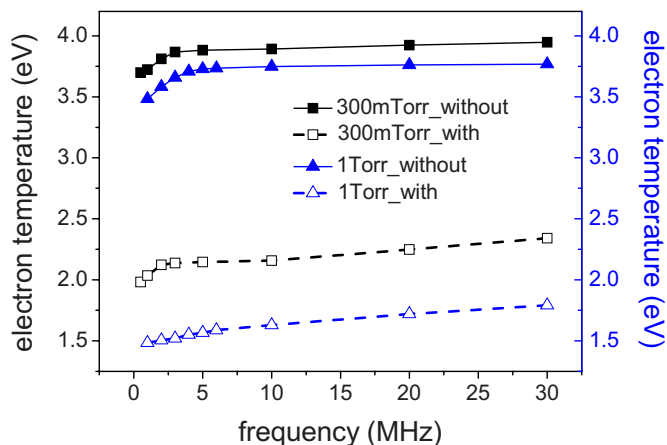


FIG. 3. (Color online) The electron temperature at the discharge center between two electrodes in different frequencies at 300 mTorr and 1 Torr.

by reason that the ground state ionization rate is influenced obviously by the metastable atoms, especially at higher frequency or higher pressure.

It is interesting that there is a minimum on the curve of the variation in bulk plasma density with frequency. The plasma density decreases with the raise in frequency in the range of low frequency; but as the frequency increases further, the density rises rapidly. The different trend of plasma density is due to the different discharge modes. When the frequency is high, the discharge is sustained by the Townsend discharge in the bulk plasma, i.e., α mode. As we all know the scaling $n \propto \omega^2 V_{RF}$, with a constant voltage, the plasma density is in proportion to the square of the frequency, and therefore the plasma density increases with frequency rapidly. However, when the frequency is low, the discharge is sustained by secondary electrons, i.e., γ mode. In other words, if there are not any secondary electrons, the discharge cannot be stable. A transition of discharge mode happens at the minimum. In the range of low frequency, the secondary electron emission becomes less predominant with the increasing frequency, and meanwhile, the bulk ionization mechanism does not contribute to the production of electrons and ions, so the plasma density decreases as the frequency rises in the low range. Both in the two discharge modes, the metastable atoms play an important role on the discharge and result in a significant decrease in plasma density.

To show the influence of metastable atoms more clearly, the results of bulk electron temperature in the cases including and without metastable atoms in different frequencies at 300 mTorr and 1 Torr are presented in Fig. 3. Compared with the result simulated in the case without metastable atoms, it can be clearly seen that the bulk electron temperature becomes lower when metastable atoms are included. It is because that, on one hand, the metastable atoms may cause obvious energy dissipation; on the other hand, the electrons may undergo more collisions caused by metastable; moreover, the weaker electric field due to the thicker sheath will also consequently limit the energy gain.

Besides, the bulk electron temperature increases monotonously with the increasing frequency, but the rising rate is different at different discharge modes. When the frequency

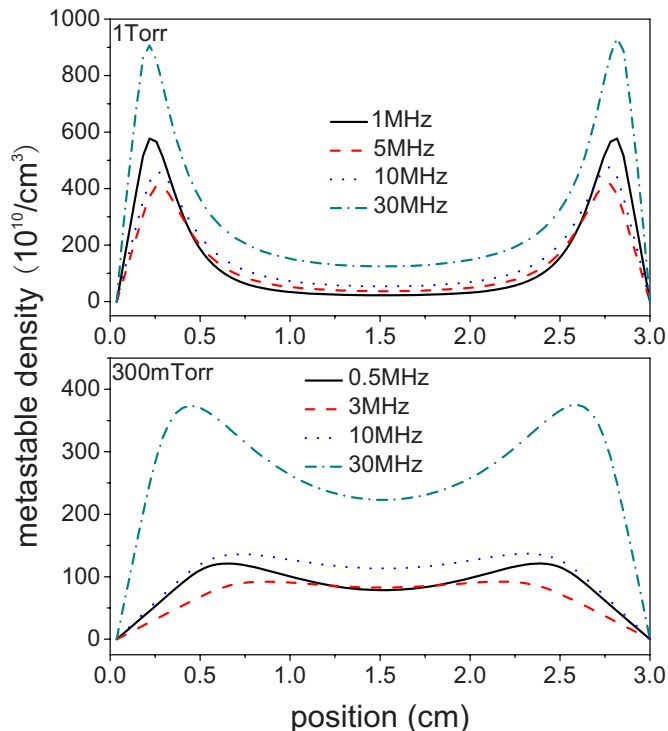


FIG. 4. (Color online) The metastable atom density between two electrodes in different frequencies at 300 mTorr and 1 Torr.

is low, the discharge is in γ mode. With the increase in frequency, the plasma density decreases and the electrons have a longer distance to be accelerated and gain energy during the thicker sheath. In addition, the secondary electron heating is more effective at low frequency, therefore the electrons can gain energy from the energetic secondary electrons more efficient, so the bulk electron temperature increases rapidly. When the frequency is higher than the frequency threshold, the discharge is maintained by the α mode. The electron temperature increases gently with the increase in frequency.

The spatial metastable atom density profiles in different frequencies at 300 mTorr and at 1 Torr are shown in Fig. 4. It can be seen that the peaks of metastable atom density decrease with the raise in frequency first and then increase when the frequency is higher than the minimum. The trend is the same as that of the plasma density, for that the metastable atoms are created by the collisions between electrons and Ar atoms, which is in proportion to the plasma density in the discharge region. Moreover, it should be noted that the peaks of the metastable density move away from the electrodes with the rise of frequency first and then move toward, which also indicates the sheath variation with frequency. It is also found that at the conditions of high pressure or high frequency, the density of metastable atoms presents a saddle profile due to that the resonant reaction and step-wise ionization reaction take place more frequently in the bulk, which leads to more loss in the metastable atoms. When the pressure and frequency are low, the metastable atom density profile spreads out in the entire discharge region, because the diffusion has a predominant influence on the loss process of metastable atoms.

The distribution of ion density with frequency in the

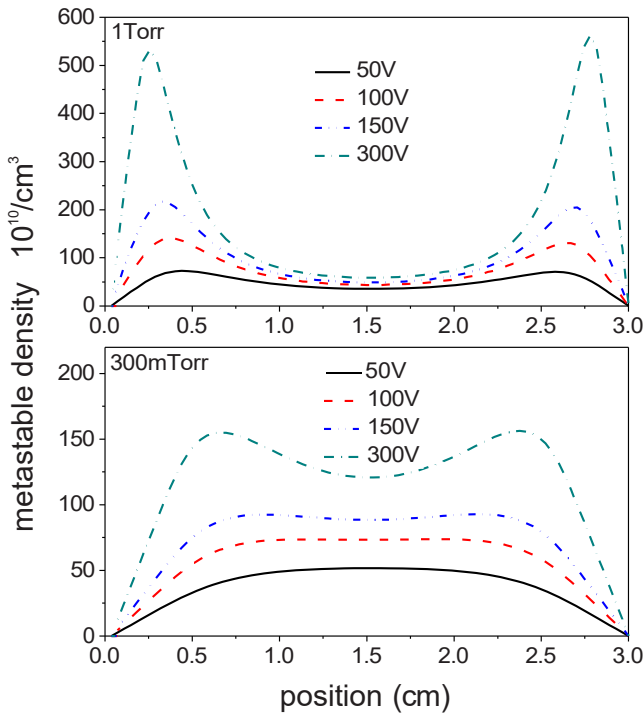


FIG. 8. Color online The metastable atom density between two electrodes in different voltages at 300 mTorr and at 1 Torr.

300 mTorr and 1 Torr, which is similar to the result in the case without metastable atoms, but the amplitude of density is lower due to the metastable effect.

Figure 10 shows the metastable density comparison between our fluid simulation result and the corresponding

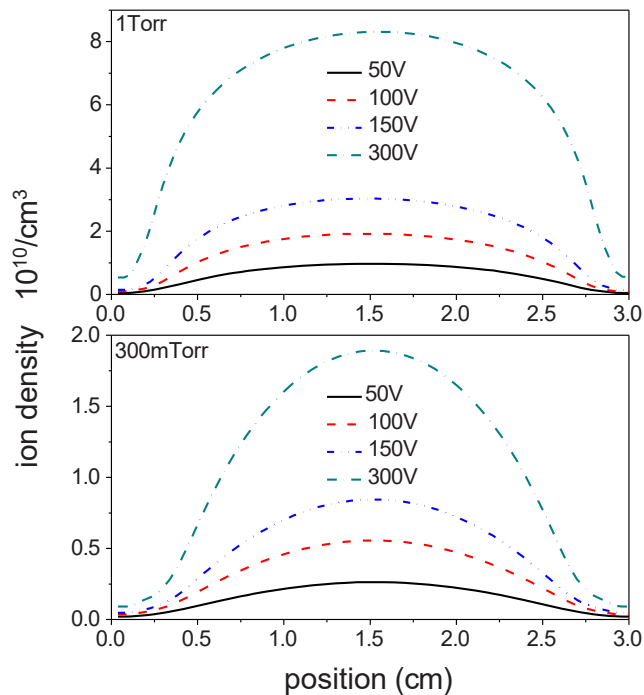


FIG. 9. Color online The ion density including metastable atom between two electrodes in different voltages at 300 mTorr and 1 Torr.

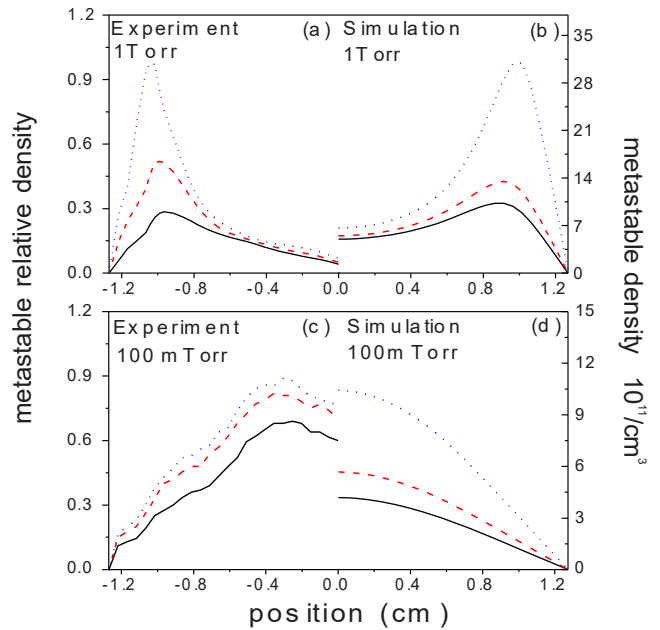


FIG. 10. Color online The metastable density comparison between a and c experimental data measured by McMillin *et al.* Ref. 11 and b and d our simulation results in 75 V solid line, 100 V dashed line, and 200 V dotted line at pressures of 100 mTorr and 1 Torr.

experimental data measured by McMillin *et al.*¹¹ with planar laser-induced fluorescence imaging. The selected discharge parameters are the same as experiment, which are $f = 13.56$ MHz, $L = 2.54$ cm, voltage = 75, 100, and 200 V, at pressures of 100 mTorr and 1 Torr. It is clearly shown that a satisfyingly qualitative agreement between the computed and measured profiles, as well as their evolutions with voltage, is obtained, which prove the reliability of this fluid model we used.

IV. CONCLUSIONS

In this article, we develop a one-dimensional self-consistent fluid model to investigate the influence of metastable atoms on the characteristics of a capacitively coupled Ar plasma. By altering the frequency, pressure and voltage, the metastable effect in various discharge conditions has been studied, and the detailed distributions of the ion density, electron temperature, and metastable atom density in the cases including metastable atoms and without them are obtained.

It is shown that the source term of ground state ionization has a greater impact on the plasma density than step-wise ionization, due to the fact that metastable atom density is still far too low compared to ground state neutral density for step-wise ionization to contribute significantly to plasma production. At all conditions, the bulk plasma density in the case with the metastable atoms is significantly lower than that in the case without the metastable atoms, and the difference is more obvious at high pressure, high frequency, and high voltage. Meanwhile, the bulk electrons have lower temperature in the case with metastable atoms, due to more frequent collisions and the weaker electric field. Moreover,

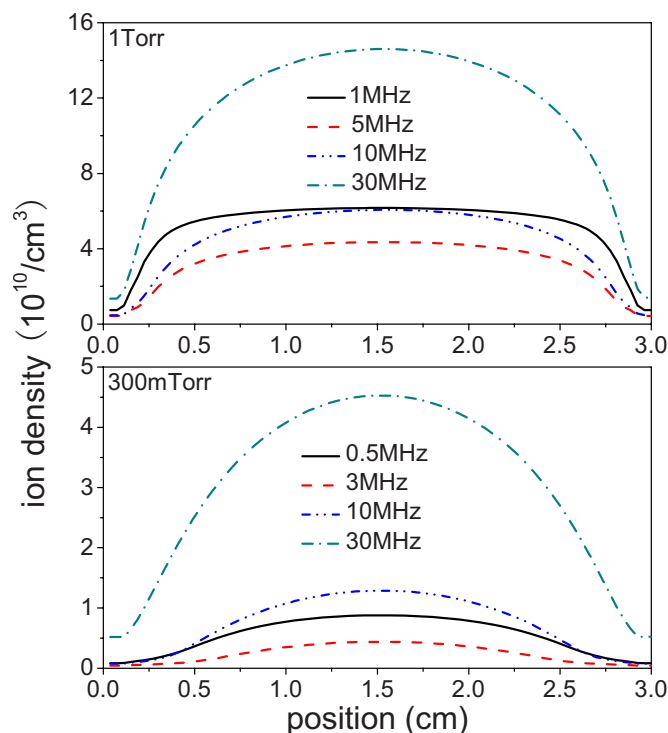


FIG. 5. (Color online) The ion density (including metastable atoms) between two electrodes in different frequencies at 300 mTorr and 1 Torr.

case including metastable atoms is shown in Fig. 5. It is discovered that the ion density is characterized by a parabolic profile at both of the considered pressure values, which is similar to the profile in the case without metastable atoms, but with a lower value. There is also a trend reverse of density with the increase in frequency. The reason of that is the same as that explained in Fig. 2.

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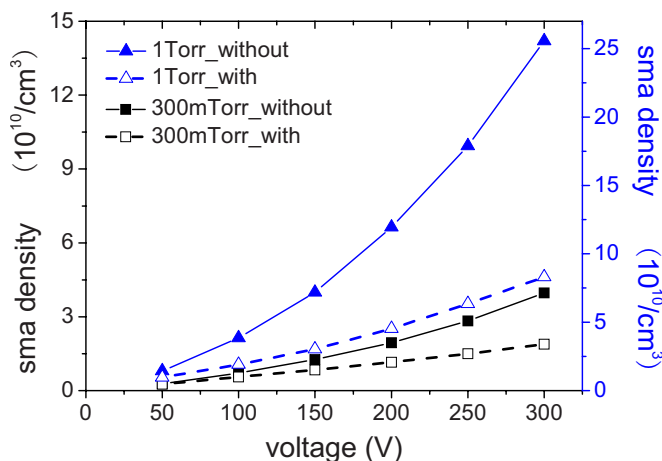


FIG. 6. (Color online) The plasma density at the discharge center between two electrodes in different voltages at 300 mTorr and 1 Torr.

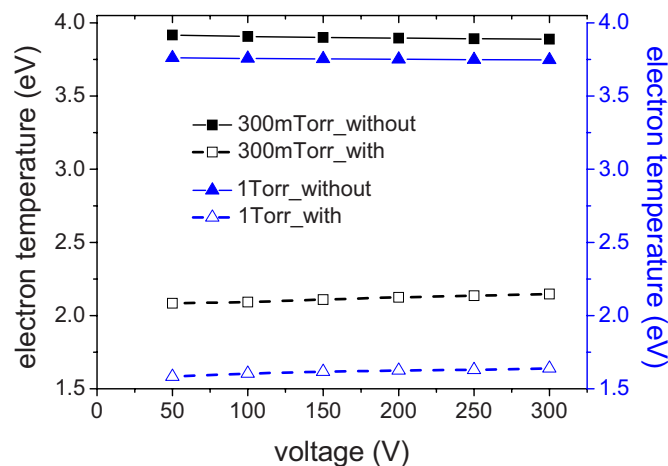


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