Ion Energy and Angular Distribution in Biased Inductively Coupled Ar/O₂ Discharges by Using a Hybrid Model

De-Qi Wen, Yu-Ru Zhang, Michael A. Lieberman, You-Nian Wang*

In this work, a global bulk plasma model coupled bi-directionally with a Monte-Carlo/fluid sheath model was developed for electronegative Ar/O₂ inductive discharges, to explore the ion energy function (IEDF) and angular distribution function (IADF) bombarding an rf-biased electrode. At low bias voltage, the IEDF of Ar⁺ shows a single energy peak that transforms into a bimodal distribution with increasing bias voltage. The IEDFs of O₂⁺ and O⁺ are always bimodal. The ion energy peak separation width largely depends on the ion masses. The IADFs are affected by the bias voltage, pressures and coil powers. The results at different coil powers indicate the importance of considering the collisions induced by atoms, especially in a molecular gas.

1. Introduction

Inductively coupled plasma (ICP) has played critical roles for etching and depositing devices in the microelectronics industry,[1] as well as in other applications, such as materials surface modification.[2] In order to improve the plasma performance, computer modeling has been employed as a powerful tool for fundamental investigations and chamber design. The computer models can be divided into two main categories: spatially resolved models[3–9] and volume averaged models.[10–15] The former needs to solve a series of partial differential equations. As we know, in an ICP discharge, multi-time scale and multi-space scale processes happen simultaneously, which brings large challenges in the simulation. Generally, for a physical process within given time or space scale, one specific model has to be developed. By combining several models, the total discharge system can be investigated. This approach allows us to capture the space transport of plasma composition, the distribution of the induced and static electric fields, local electron heating, etc. For example, in the hybrid plasma equipment model (HPEM),[3–5] a finite volume method is applied to deal with the spatial differences and the electromagnetic fields and wave propagation are solved in frequency or time domain. Zhao et al.[6,7] developed a 2D fluid/electron Monte-Carlo hybrid model to investigate mode transition phenomenon. Such a model could be used...
to study many physical and chamber design problems, but requires much computer time. Kawamura et al.\cite{8,9} developed a fast 2D hybrid model, in which an analytical method is applied to address the sheath, and particle-in-cell simulation is used as an interface to track the ion energy distribution function (IEDF). These works suggest means for speeding the simulations.

Volume-averaged models were developed and applied to capture the scaling of plasma parameters with major external control parameters, such as pressure, input power, and chamber size,\cite{10–15} as well as to investigate the effect of neutral species and chemistry dynamics\cite{15} on the overall discharge properties. For this reason, many researchers employ a global model, which has the advantage of saving time. Unfortunately, the ion energy distribution function, a key plasma parameter, especially when a bias source is mounted, can not be obtained, by a global model. Thus, a model, which can show the IEDFs self-consistently, considering the interaction between the bulk plasma and sheath above the biased electrode,\cite{16} is needed.

In previous work,\cite{17} we developed a hybrid model for argon in biased ICP discharges. To validate the model, both bulk plasma density and IEDF on the bias electrode were compared with experimental measurements, and a good agreement was obtained. In this work, we extend that model to electronegative Ar\textsubscript{2}/O\textsubscript{2} discharges. We introduce the model and examine the ion energy and angle distributions versus rf bias amplitudes, pressures, and coil powers. The bias frequency is fixed at 13.56 MHz. In current work, we consider the important chemical dynamics as described in refs.\cite{10,11,18}. The plasma species are shown in Table 1.

### Table 1. The plasma species considered in the Ar/O\textsubscript{2} discharge model.

<table>
<thead>
<tr>
<th>Neutral species</th>
<th>Positive ions</th>
<th>Negative ions and electron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar, Ar\textsuperscript{+}, O\textsubscript{2}(X\textsubscript{1}S\textsubscript{g}\textsuperscript{+}), O\textsubscript{3}, O\textsubscript{3}P, O\textsubscript{1}D</td>
<td>Ar\textsuperscript{+}, O\textsuperscript{+}, O\textsubscript{2}\textsuperscript{+}</td>
<td>O\textsuperscript{-}, e</td>
</tr>
</tbody>
</table>

2. Model

We consider an inductively coupled plasma driven by a planar coil source and a radio frequency bias source. A cylindrical chamber with radius $R$ and height $L$ is assumed. A schematic of the configuration for our model is shown in Figure 1. The chamber is subdividing into two main parts, i.e., the plasma bulk and the sheath zone. The former is completely filled by plasma and is modeled by a global (volume-averaged) model, assuming all the plasma species have nearly uniform profiles. The ions and neutrals are assumed to be separately in thermal equilibrium and described by different temperatures, in general, different from the electron temperature. The sheath zone is modeled by a set of fluid equations for ions. To obtain an accurate IEDF and ion angle distribution function (IADF), we employ a random Monte-Carlo collision model to examine the ion collision dynamics. In the following subsections, these models and the main governing equations in an electronegative Ar\textsubscript{2}/O\textsubscript{2} discharge are described.

2.1. Global Bulk Plasma Model

Volume-averaged (global) models have been well known in research on electropositive and electronegative inductively coupled plasmas.\cite{16–19} These models consider the two basic principles: the volume-averaged particle balance and power balance. More specifically, for a steady-state plasma discharge, the number of generated particles equals the number of lost particles induced by chemical reactions, surface processes and pumping etc; and the absorbed power equals the consumed power due to elastic and inelastic collisions and ions flowing to the walls. In electronegative plasmas, due to the existence of negative ions, the ion fluxes to the walls are different from those in electropositive plasmas and need modification as shown in the following. As the negative ion temperature is much lower than electron temperature, negative ions are confined in plasma bulk by the positive space potential and do not flow to the walls. The
The particle balance equation for species \( l \) is given by\,[27]

\[
\frac{L - d_s}{L} \left( \sum_j R_{ij} - \sum_j R_{ji} \right) + R_{in,l} - R_{out,l} + \sum_s R_{is} - \sum_s R_{si} = 0
\]

where \( L \) is the chamber height, \( d_s \) is the maximum sheath width obtained from the sheath model, and \( R_{ij} = \sum_k k_{ij} n_j n_i \) is the sum of the chemical reaction rates of different generation and loss processes of species \( l \) with \( k_{ij} \) rate coefficient of the \( k \)th reaction between species \( l \) and \( j \), and \( n_i \) and \( n_j \) are the reactant densities. Note that three body collisions are not included in the model. The detailed chemical reactions are found in ref.[19] In this model, we updated the rate coefficients of positive-negative ion neutralization reactions for \( \text{Ar}^+ \), \( \text{O}^+ \), and \( \text{O}^- \).[11,20] \( R_{in,l} = 4.48 \times 10^{17} Q_{in,l} / V \) \( \text{m}^{-3} \text{s}^{-1} \), where \( Q_{in,l} \) is the fixed flow of ground state atoms \( \text{Ar} \) and molecules \( \text{O}_2 \) into the chamber in units of sccm, and \( V \) is the chamber volume. \( R_{out,l} = 1.27 \times 10^{-5} n_j Q_{in,l} / V \) \( \text{m}^{-3} \text{s}^{-1} \)[12,19,15] with \( Q_{in} \) the total inflow, gives to the pumping of gas out of the chamber. Here \( p \) is the out-flow pressure in Torr. In the present work, the total inflow is fixed at 45 sccm with a ratio \( Q_{in,Ar} : Q_{in,O_2} = 4 : 1 \). The negative ion \( \text{O}^- \) is confined in the plasma bulk and is not pumped out. In addition, the surface processes indicated by \( R_{ij} \) also contribute to the variation of the particle number. In our global model, the species considered are listed in Table 1.[12,18–20] At the walls, the metastable state atoms \( \text{Ar}^* \) and \( \text{O}^*(\text{D}) \) and molecules \( \text{O}_2(a^3\text{Ag}) \) are assumed to be de-excited to the ground state with certain probability,[20] and two \( \text{O} \) atoms recombine and generate an oxygen molecule \( \text{O}_2 \). \( R_{ej} = K_{loss} n_i \) is the surface reaction rate, and the rate coefficient for neutral species is given by\,[20,21]

\[
K_{loss} = \left( \frac{A_0^2}{D_l} + \frac{2V(2 - \gamma_l)}{A\nu\gamma_l} \right)^{-1} \text{s}^{-1}
\]

where \( \lambda_0 \) is the effective diffusion length of a cylindrical chamber and \( D_l \) is the diffusion coefficient for species \( I \) and \( V \) are the surface area and volume of the reactor chamber, respectively. \( v \) is the mean thermal velocity, \( \gamma_l = 1 \) for \( \text{Ar}^* \) atoms and \( \gamma_l = 0.007 \) for \( \text{O}_2(a^3\text{Ag}) \).[22] The recombination coefficient of \( O^+(\text{P}) \) is related to wall materials[23] and gas pressure,[24] and affects the densities of atomic oxygen, ionic components and electrons[20] we use a coefficient of 0.26.[25]

For positive ions, the loss rate \( R_{ej} = \beta_{ij} A_{eff} n_i / V \) is estimated from the Bohm speed \( \beta_{ij} \) and the effective loss area \( A_{eff} = 2 m k (h_{ij} + h_{j} + L) \). Due to the existence of negative ions, the axial and radial edge to center ion density ratios \( h_{ij} \), \( h_{j} \), are different from the electropositive case, and are related to the central degree of electronegativity[15,21]

\[
h_{ij} = \left( h_{ij}^2 + h_{j}^2 \right)^{1/2}
\]

\[
h_{j,a,l} \approx \frac{0.86}{1 + \alpha_0} \left( 3 + \frac{l}{2\lambda} \left( \frac{0.86 l F_{ij}^2}{\pi D_l} \right) \right)^{1/2} - 1/2
\]

\[
h_{j,e,l} \approx \frac{0.8}{1 + \alpha_0} \left( 4 + \frac{R}{\lambda} \left( \frac{0.86 l F_{ij}^2}{\pi D_l} \right) \right)^{1/2} - 1/2
\]

\[
h_{j,c} \approx \left( \gamma_{ij}^2 + \gamma_{ij}^1 n_{j} n_{i}^{-3/2} \right)^{-1}
\]

where \( \alpha_0 = 3 \alpha / 2 \) is the central degree of electronegativity with \( \alpha \) the averaged electronegativity, \( D_l \) is ambipolar diffusion coefficient, \( \lambda = 1 / n_i \sigma \) is the ion mean free path, \( \lambda_0 \approx 2 \text{.}405 \) is the first zero of the zero order Bessel function, and \( \lambda_1(\lambda_0) \) is the first order Bessel function. We assume that the positive and negative ions have the same temperature, \( \gamma = T_e / T_i \) and \( n_e = 15 v_i / 56 k_i \lambda_i \), where \( v_i \) is the mean ion thermal velocity, and \( k_i \) is the rate coefficient of the ion-ion recombination process. In this work, the neutral molecules and atoms temperature are assumed to be 330 K, and ion temperature is a function of gas pressure \( P \) as \( T_i(\text{eV}) = 0.063 / P(\text{Pa}) + 0.028 > 0.133 \text{ Pa} \), i.e., 1 mTorr. The electron density is determined by quasi-neutrality. In the power balance equation

\[
P_c + \frac{1}{V} P_{wall} - \frac{1}{V} (P_{coil} + P_{bias}) = 0
\]

\[
P_c = en_e \sum_l n_l n_{c,l} k_{el}^{i,l}
\]

where \( P_c \) is the power loss per unit volume due to the electron inelastic/elastic collisions, \( P_{wall} \) is the power loss due to the charged particles flowing to the walls, and \( P_{coil} \) and \( P_{bias} \) are the absorbed power from the coil source and the rf bias source. In our system, the power provided by the coil source is assumed to be mainly absorbed by electrons with a power transfer efficiency of 0.75 neglecting the capacitive coupling. The electron power loss \( P_c \) is given by

\[
P_c = en_e \sum_l n_l n_{c,l} k_{el}^{i,l}
\]

This sum is over all neutral species \( l \) having density \( n_l \), ionization rate \( k_{el}^{i,l} \), and equivalent collisional energy loss \( e_{el}^{i,l} \) per electron-ion pair created. Here \( e_{el}^{i,l} \) is given by

\[
e_{el}^{i,l} = e_{el}^{i,l} + \sum_j e_{ex}^{j,l} \left( k_{el}^{i,l} / k_{el}^{j,l} + 3 m_i T_e / M_i^3 \right)
\]

where \( e_{ex}^{j,l} \) and \( k_{el}^{j,l} \) represent the ionization and the excitation threshold energy of \( f \)th collision process of species \( l \)[23] and \( M_i^3 \) is the mass of species \( l \). The wall power is
The power absorbed by electrons from the rf bias source calculated in the sheath model (see the next subsection).

where \( \nu_p \) is the plasma presheath potential drop,

\[
\nu_p = \frac{1}{2} \frac{1 + \alpha_s}{1 + \alpha_s T_e} T_e
\]

with \( \alpha_s \) the degree of the electronegativity at the sheath edge. \( \alpha_s \) and \( \alpha_0 \) satisfy the following relationship

\[
\alpha_s = \alpha_0 \exp \left[ \frac{(1 + \alpha_s)(1 - \gamma)}{2(1 + \alpha_s \gamma)} \right].
\]

2.2. Fluid Sheath and Monte-Carlo Collision Models

In biased ICP discharges, a sheath will be formed above the biased electrode, whose thickness is small compared with the electrode radius. Thus, a one-dimensional sheath model is adopted. Assuming Boltzmann electron and negative ions, the spatiotemporal variation of the positive ion density \( n_i(z, t) \), ion drift velocity \( \mathbf{u}_i(z, t) \), negative ion density \( n_e(z, t) \), electron density \( n_e(z, t) \), and the electric potential \( V(z, t) \) inside the sheath are described by the following equations:

\[
\frac{\partial n_{i+}}{\partial t} + \frac{\partial n_{i+} \mathbf{u}_{i+}}{\partial z} = 0
\]

\[
\frac{\partial \mathbf{u}_{i+}}{\partial t} + \mathbf{u}_{i+} \frac{\partial \mathbf{u}_{i+}}{\partial z} = -\frac{e}{M_{i+}} \frac{\partial V}{\partial z} n_{i+} n_{l+} + n_{i+} \mathbf{u}_{i+} \left[ n_{j+} \sigma_{i+} (|\mathbf{u}_{i+}|) |\mathbf{u}_{i+}| \right]
\]

\[
n_{l+} = n_{l+0} \exp \left( \frac{e(V_p - V(z, t))}{k_B T_L} \right)
\]

\[
n_e = n_{e0} \exp \left( \frac{e(V_p - V(z, t))}{k_B T_L} \right)
\]

\[
\frac{\partial^2 V}{\partial z^2} = -\frac{1}{\varepsilon_0} \left( \sum_{l+} q_{l+} n_{l+} + \sum_{l-} q_{l-} n_{l-} - e n_e \right)
\]

where \( n_{i0} \) and \( n_{e0} \) are the negative ion density and the electron density at the plasma bulk, respectively, and obtained from the global model. \( \sigma \), as a function of the ion drift velocity, is the collision cross section of ion. \( T_{l+} \) is the temperature of the negative ions. At the electrode, continuous (zero slope) boundary conditions are chosen for the positive ion density and drift velocity. To calculate the potential on the bias electrode and the time averaged dc voltage, a current balance equation is applied. The total current passing through the sheath equals the source current, i.e., \((1 + \gamma) I_I + I_e + I_d = I_0 \sin(\omega t)\), where \( I_I, I_e, \) and \( I_d \) represents, respectively, the ion current, electron current and displacement current. Negative ions are confined in the plasma bulk and do not flow to the bias electrode.
\[ I_e = -\frac{e\bar{u}_t n_{i0} A}{4} \exp \left( -\frac{(V_p - V_e)}{k_b T_e} \right) \]
\[ I_t = eA \sum_{i} u_i(t) n_i(0, t) \]
\[ I_d = C_s \frac{d}{dt} (V_p - V_e) + (V_p - V_e) \frac{dC_s}{dt} \]

where \( A \) is the biased electrode area, \( V_p \) and \( V_e \) are the potential of the plasma and at the biased electrode, respectively, \( u_i(0, t) \) and \( n_i(0, t) \) are the \( i \)th positive ion drift velocity and density at the electrode, \( C_s(t) = \frac{\epsilon_0 A}{d_s(t)} \) is the temporal sheath capacitance, and the sheath width \( d_s(t) \) is determined by \( \bar{u}_t |_{t=d_s(t)} = \bar{u}_B \). Note that we will examine the effect of voltage amplitude on the ion energy and angular distribution. After every global model-sheath model solve, the amplitude of the the waveform is obtained and compared with the desired amplitude. If they are different, the applied rf current amplitude \( I_0 \) is adjusted and the voltage amplitude is calculated again. These steps are repeated until we obtain the desired voltage amplitude.

These two models are coupled in the following way: the initial species densities \( n_i \) (including ions and neutrals) and electron temperature \( T_e \) are obtained from the global model and then are delivered to the sheath model as boundary conditions. Utilizing these conditions, the sheath width, the absorbed power from the bias electrode and the averaged potential drop through the sheath are calculated in the sheath model. Subsequently, these physical quantities are redelivered to the global model.

A Monte-Carlo collision model is executed when the global model and the sheath model reach the convergence. At this time, the temporal electric field is periodically repeated, and \( 10^5 \) particles of each positive ion species are sprinkled randomly at the computation boundary.

These particles arrive at the electrode under the electric field force and collide with neutral species. Finally, by recording the direction and the value of the velocity, the ion energy distribution and the ion angle distribution are obtained. In this model, the updating of the particle position and velocity is similar to that in PIC simulations. A detailed description of the collision process between ions and neutrals is given in our recent publication.

The ion-neutral reactions considered in the Monte Carlo collision model are shown in Table 2. The main collision processes are reactions 1, 2, and 7, which have large cross sections. The cross section of reaction 11 is assumed to be one half of reaction 9.

### 3. Results and Discussion

The IEDFs of \( \text{Ar}^+ \), \( \text{O}_2^+ \), and \( \text{O}^+ \) at various rf bias voltage amplitudes are presented in Figure 2. The total gas pressure is fixed at 2 Pa. The inflow ratio of argon and oxygen is 4:1 and the applied coil power is kept at 150 W. As mentioned above, the actual power transfer efficiency is assumed to be 75\%.[12–14] It is clear that when the voltage amplitude is low, i.e., 13 V, the IEDF of \( \text{Ar}^+ \) exhibits a nearly single energy peak and it transforms into a bimodal distribution as the bias voltage amplitude increases. This can be interpreted by the relationship between the ion transit time across the sheath \( t_i \) and the rf bias period \( t_{rf} \). When \( t_i \) is much larger than \( t_{rf} \), the ions are accelerated by the time-averaged voltage drop across the sheath. Estimating the ion transit time across the sheath at 13 V by \( t_i = \frac{3\delta (M_i/2eV_e)^{1/2}}{1} \) with time-averaged sheath

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Types</th>
<th>Cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \text{Ar}^+ \rightarrow \text{Ar} \rightarrow \text{Ar}^+ + \text{Ar} )</td>
<td>ES(^a) and CX(^b)</td>
<td>Ref.[1]</td>
</tr>
<tr>
<td>2</td>
<td>( \text{O}_2^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{O}_2 )</td>
<td>ES(^a) and CX(^b)</td>
<td>Ref.[30,33]</td>
</tr>
<tr>
<td>3</td>
<td>( \text{O}_2^+ + \text{O} \rightarrow \text{O}_2^+ + \text{O} )</td>
<td>CX(^b)</td>
<td>Ref.[30]</td>
</tr>
<tr>
<td>4</td>
<td>( \text{O}_2^+ + \text{O} \rightarrow \text{O}^+ + \text{O}_2 )</td>
<td>Dissociation</td>
<td>Ref.[30]</td>
</tr>
<tr>
<td>5</td>
<td>( \text{O}^+ + \text{O}_2 \rightarrow \text{O}^+ + \text{O}_2 )</td>
<td>ES(^a)</td>
<td>Ref.[30]</td>
</tr>
<tr>
<td>6</td>
<td>( \text{O}^+ + \text{O}_2 \rightarrow \text{O}^+ + \text{O}_2 )</td>
<td>CX(^b)</td>
<td>Ref.[30]</td>
</tr>
<tr>
<td>7</td>
<td>( \text{O}^+ + \text{O}_2 \rightarrow \text{O}^+ + \text{O}_2 )</td>
<td>ES(^a) and CX(^b)</td>
<td>Ref.[30]</td>
</tr>
<tr>
<td>8</td>
<td>( \text{Ar}^+ + \text{O}_2 \rightarrow \text{Ar}^+ + \text{O}_2 )</td>
<td>ES(^a)</td>
<td>Ref.[34]</td>
</tr>
<tr>
<td>9</td>
<td>( \text{O}_2^+ + \text{Ar} \rightarrow \text{O}_2^+ + \text{Ar} )</td>
<td>ES(^a)</td>
<td>Ref.[34]</td>
</tr>
<tr>
<td>10</td>
<td>( \text{O}_2^+ + \text{Ar} \rightarrow \text{O}_2^+ + \text{Ar} )</td>
<td>CX(^b)</td>
<td>Ref.[34]</td>
</tr>
<tr>
<td>11</td>
<td>( \text{O}^+ + \text{Ar} \rightarrow \text{O}^+ + \text{Ar} )</td>
<td>ES(^a)</td>
<td>Ref.[34]</td>
</tr>
</tbody>
</table>

\(^a\)ES represents elastic scattering collision. \(^b\)CX represents charge exchange collision. "The neutrals \( \text{O}_2(a^1\Delta g), \text{O}(^1\text{D}), \text{O}(^3\text{P}), \text{Ar}^+ \) are assumed to be same as the ground states."
Furthermore, the slope peak separation width of \( O^+ \) transit time across the sheath, as we estimated above, IEDFs of Ar\(^+\) energy moves to a larger value. Due to the shorter ion bimodal distribution appears and the time-averaged ion single energy peak. When the sheath voltage drop increases, the rf period. As a result, ion energy distribution shows a bimodal distribution even at low voltage.

Due to the larger percentage of \( O^+ \) and \( O_2^+ \) also qualitatively agree with measurements in a pure oxygen discharge. Therefore, we conclude that the increasing rate of the ion energy peak separation width versus rf bias amplitude depends largely on the ion mass. Figure 4 shows the IADFs of Ar\(^+\), \( O_2^+ \), and \( O^+ \) at various rf bias voltages. As the rf voltage increases, more ions are incident on the electrode with a smaller deflection angle due to the smaller effects of the ion-neutral scattering at higher energies. Note that there is larger percentage of \( O_2^+ \) than Ar\(^+\) and \( O^+ \) in the deflection angle ranging from 4\(^\circ\)–16\(^\circ\), due to large cross section of elastic and charge exchange collisions between \( O_2^+ \) and feed gas \( O_2 \). In order to show the effect of gas pressure on IADFs, the rf bias amplitude is fixed at 200 V and other conditions are the same as above. From Figure 5, it is clear that the ions bombard the bias electrode within a small deflection angle, typically smaller than 2\(^\circ\) both at 2 and 6.67 Pa. In ref.\([32]\) the IADFs were measured for the pressure of 4–20 mTorr, similar to the gas pressure scope in this work. The scope of deflection angle and variation trend agree with our results. Figure 6(a) and (b) shows the densities of all plasma components at Pa and 6.67 Pa. In ref.\([32]\) the results, we can see the densities of neutrals, such as ground state Ar, \( O_2 \), \( O^+ \), and \( O(\text{D}) \), at 6.67 Pa are higher than at 2 Pa. The higher neutral species lead to more
collisions, and therefore more ions have large deflection angles.

By fixing the pressure at 2 Pa, Figure 7 shows the effect of the coil power on IADFs of Ar$^+$, O$_2^+$, and O$^+$. The evolution of the IADF of O$^+$ with coil power is different from Ar$^+$ and O$_2^+$. A larger percentage of Ar$^+$ and O$_2^+$ ions have small deflection at 300 W than at 150 W, whereas O$^+$ ions show an opposite trend. This is mainly attributed to the chemical dynamics as shown in Figure 8(a) and (b), in which we show the densities of plasma species and the ground state O$_2$ dissociation rate at different coil powers. In our model, the total particle number of different species satisfy ideal gas equation, i.e., $p = \sum n_i k_B T_i$. Here $n_i$ and $T_i$ are the density and temperature of the $i^{th}$ plasma species. Comparing Figures 6(a) and 8(a), at 300 W, more O$_2$ are dissociated into O(3P) and O(1D). The O$_2$ density decreases from $3.27 \times 10^{18}$ m$^{-3}$ at 150 W to $2.26 \times 10^{18}$ m$^{-3}$ at 300 W. The corresponding O$_2$ dissociation rate, as shown in Figure 8(b), is about 0.42 at 150 W larger than 0.64 at 300 W. The O(3P) and O(1D) densities become higher at
Since the collision cross section for O$^+$ with O is larger than with other neutral species, O$^+$ has more collisions at higher power, thus the amount of O$^+$ with small deflection angles becomes lower. This also indicates the importance of chemical dynamics in modeling the IADF, especially in molecular gases, which may have higher dissociation rates and lead to different IADFs at higher power.

4. Conclusions

In this work, we extended our previous hybrid model of biased ICP discharges for argon to electronegative ArO$_2$ discharges. The ion energy and angular distributions versus bias amplitude were examined at a coil power of 150 W, and gas pressure of 2 Pa. The IEDF of Ar shows a single energy peak distribution at low voltage that shifts into a bimodal distribution with increasing voltage amplitude. The IEDFs of O$_2^+$ and O$^+$ are characterized by bimodal distribution for all investigated bias voltages. In addition, the bimodal energy width $\Delta E$ increases with the bias amplitude, and the rate of increase, to a great extent, depends on the ion masses. As the bias voltage increases, the IADs indicates that more ions are incident on the electrode with a smaller deflection angle. The results at different pressures and coil powers indicate that the collisions significantly affect the IADF. Especially, the atoms from dissociated reactions may play an important role in determining the IADs in a molecular gas. In the future, a trench etching model could be added to simulate the evolution of an etching process.

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