Effect of Addition of Nitrogen to a Capacitively Radio-Frequency Hydrogen Discharge*

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Abstract A hybrid PIC/MC model is developed in this work for H\textsubscript{2}-xN\textsubscript{2} capacitively coupled radio-frequency (CCRF) discharges in which we take into account 43 kinds of collisions reaction processes between charged particles (e\textsuperscript{-}, H\textsuperscript{+}, H\textsuperscript{2+}, H\textsuperscript{+}, N\textsubscript{2}\textsuperscript{+}, N\textsuperscript{+}) and ground-state molecules (H\textsubscript{2}, N\textsubscript{2}). In addition, the mean energies and densities of electrons and ions (H\textsuperscript{+}, H\textsuperscript{2+}, H\textsuperscript{+}), and electric field distributions in the H\textsubscript{2}-N\textsubscript{2} CCRF discharge are simulated by this model. Furthermore, the effects of addition of a variable percentage of nitrogen (0-30\%) into the H\textsubscript{2} discharge on the plasma processes and discharge characteristics are studied. It is shown that by increasing the percentage of nitrogen added to the system, the RF sheath thickness will narrow, the sheath electric field will be enhanced, and the mean energy of hydrogen ions impacting the electrodes will be increased. Because the electron impact ionization and dissociative ionization rates increase when N\textsubscript{2} is added to the system, the electron mean density will increase while the electron mean energy and hydrogen ion density near the electrodes will decrease. This work aims to provide a theoretical basis for experimental studies and technological developments with regard to H\textsubscript{2}-N\textsubscript{2} CCRF plasmas.

Keywords: H\textsubscript{2}-N\textsubscript{2} capacitively coupled radio-frequency discharge, H\textsubscript{2} plasma, PIC/MC simulation

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(Some figures may appear in colour only in the online journal)

1 Introduction

H\textsubscript{2}-N\textsubscript{2} capacitively coupled radio-frequency (CCRF) plasmas are widely used in hydrogenated microcrystalline silicon film deposition, chemical synthesis of ammonia and nitridation of materials surface. In the synthesis of nitrogen-doped diamond-like carbon (DLC:N), the ratio of added N\textsubscript{2} to the hydrogen plasma is one of the important factors considered in this technology \cite{1}. Recently, H\textsubscript{2}-N\textsubscript{2} CCRF plasmas have been used to etch organic low dielectric constant (low-\kappa) films. As the size of ultra-large scale integrated-devices becomes smaller, several interconnection layers can be used to highly integrate the devices. In order to meet the requirement for low capacitance, low-\kappa materials are used as an interconnecting film. At present, there have been many efforts to establish an etching technology for low-\kappa materials using different gas plasmas. Currently, an N\textsubscript{2}-H\textsubscript{2} plasma is considered to be a promising candidate for etching low-\kappa materials because it is nontoxic, easy to process, permits independent control over the partial pressure of each of the constituent gases and because H or N radicals play important roles \cite{2,3}. Study on the characterization and microcosmic process mechanism of H\textsubscript{2}-N\textsubscript{2} CCRF plasmas is the basis for understanding the etching process of organic low-\kappa films, for the control of N and H radicals, and for achieving an anisotropic etching profile for low-\kappa materials.

A variety of applied technologies for H\textsubscript{2}-N\textsubscript{2} plasma are required to study the generation and behavior of active particles as well as to understand the microscopic mechanism in the plasma process. In H\textsubscript{2}-N\textsubscript{2} plasma research, theoretical simulation has been less extensive than experimental studies \cite{4,5,6}. Gordiets’ study group simulated the H\textsubscript{2}-N\textsubscript{2} DC glow discharge using a kinetic model and calculated relative densities of particles (N, H, NH\textsubscript{3}) that changed when the ratio of added H\textsubscript{2} \cite{7,8} was adjusted. Tatarova et al. theoretically and experimentally studied the dissociation of H\textsubscript{2} and N\textsubscript{2} molecules in H\textsubscript{2}-N\textsubscript{2} microwave discharges \cite{6}. We have previously studied the effects on electron behavior when H\textsubscript{2} was added to N\textsubscript{2} DC glow discharges using Monte Carlo (MC) modeling \cite{9}. Although theoretical simulations of RF plasmas have been reported for more than 20 years, these studies didn’t included numerical simulations of an H\textsubscript{2}-N\textsubscript{2} mixture gas in a capacitive

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RF plasma. Therefore, this paper presents an in-depth study to provide a more accurate quantitative description of the microscopic processes in H$_2$-N$_2$ CCRF plasmas and the effect of adding N$_2$ to an H$_2$ discharge on the characteristics of H$_2$ RF plasmas. The PIC/MC model is regarded as a good research method because it not only takes into account the advantage of collective interactions with PIC method and the particle collisions with the MC method, but also accurately simulates the details of the plasma process. In this paper, the H$_2$-N$_2$ CCRF discharge is simulated and the effects of adding small amounts of N$_2$ to a H$_2$ RF plasma is studied using the PIC/MC model. By changing the ratio of added N$_2$, change laws are described for the distribution of electric potential, gas temperature, secondary electron emission coefficient, and the energy profile. This work aims to provide a theoretical basis for experimental studies and technological innovations with regard to H$_2$-N$_2$ CCRF plasmas.

2 Description of the model

The discharge parameters used in our simulations are obtained from typical experimental discharge conditions used in various material processing [10]. The CCRF is sustained between two parallel plates, each is 12.8 cm in diameter and separated from the other by 2.2 cm. One of the electrodes is driven by a 13.56 MHz power source. The amplitude of applied voltage, $V_{\text{RF}}$, is 240 V, and the self-bias is $-15$ V. The other electrode is grounded. The gas pressure is 133.3 Pa, gas temperature is 300 K, secondary electron emission coefficient is 0.1, and the ratio of the added nitrogen to the H$_2$ discharge gas ranges from 0% to 30%.

2.1 The PIC/MC model

The following computations are based on a one-dimensional coordinate space and a three-dimensional velocity space (1d3v) PIC/MC algorithm. The charged species considered in the model are electrons (e$^-$), hydrogen ions (H$_2^+$, H$_3^+$, H$^+$) and nitrogen ions (N$_2^+$, N$^+$). The motion of the charged particles is simulated using the PIC method. Collisions between the particles are studied by combining the PIC model with a Monte Carlo procedure. To calculate collision probability, it is necessary to have the corresponding collision cross section data, which are not always available, especially the reaction between nitrogen-hydrogen particles. Hence, the present model uses several techniques to define the collision probabilities even when the collision cross sections are unknown.

The simulation grid is uniform and consists of 400 cells. The superparticles of electrons (e$^-$), hydrogen ions (H$_2^+$, H$_3^+$, H$^+$) and nitrogen ions (N$_2^+$, N$^+$) are set uniformly in a discrete discharge space. The size of each superparticle is of the same order as the grid size, and the charge of each superparticle is of the order of magnitude of 10$^{-12}$ C. The initial densities of the charged species in the model are assumed to be 10$^{16}$ m$^{-3}$; the initial velocities are calculated from the Maxwellian distribution with an average electron temperature of 1.8 eV and an average ion temperature of 0.0625 eV (300 K). Due to the electric field, a superparticle will follow a motion described by Newton’s laws in a discretized time interval, and the velocity and spatial location will constantly change. Poisson equation:

$$\frac{d^2\phi}{dz^2} = -\frac{e}{\varepsilon_0}n_j,$$

where $\phi$ is the potential, $\varepsilon_0$ is the dielectric constant in vacuum, $e$ is the basic charge, $n_j$ is the charge density:

$$n_j = n_{H^+} + n_{H^+_2} + n_{H^+_3} - n_e.$$

Boundary conditions for the equation is taken as follows:

$$\begin{align*}
V_{\text{RF}} \sin(\omega_{\text{RF}}t) - V_d & \quad (z = 0), \\
0 & \quad (z = d),
\end{align*}$$

where $\omega_{\text{RF}}$ is the angular frequency; $V_d$ is the self-bias, $d$ is the electrode gap. The potential and electric field at the grid points can be obtained by solving the poisson equation, and then are weighted to any position.

For each collision process of charged species, where we have obtained cross sections data (processes 1 to 33 in Tables 1 and 2), the probability of collision during a time step $\Delta t$ is calculated by:

$$P = 1 - \exp(-n\sigma_{\text{tot}}(\epsilon)V_i\Delta t), \quad (1)$$

where $n$ is the number density of background gas, $v_i$ is the three-dimensional velocity of species in the time step $\Delta t$ and $\sigma_{\text{tot}}(\epsilon)$ is the total collision cross section of charged particles with energy $\epsilon$. The electron time step is of the order of magnitude of 10$^{-11}$ s and the time step for an ion is equal to 25 electron time steps. The detailed description of 1d3v PIC/MC model can be found in our previous work [11].

For collisions between hydrogen ions (H$_2^+$, H$_3^+$, H$^+$) and nitrogen molecules as well as between nitrogen ions (N$_2^+$, N$^+$) and hydrogen molecules, we use Nanbu’s ion-neutral species collision model [12]. During the time step $\Delta t$, the ion-molecule collision probability is calculated by:

$$P = \left(\frac{\pi\alpha_p\rho^2}{\varepsilon_0\beta}\right)^{1/2} \beta_\infty n \Delta t,$$

where $\mu$ is the reduced mass, $\alpha_p$ is the polarizability, $\beta_\infty$ is the value of the dimensionless impact parameter $\beta$, for which the deflection angle is negligibly small. The value of $\beta_\infty$ is set to 3 [12] and $\alpha_p = a^3$ [13] where $a$ is the atom radius. The calculated probability is then compared with a random number ($R$). If $R < P$, a collision occurs. Finally, the kind of collision, an elastic collision or a charge transfer collision, is determined by $\beta$, and $\beta_\infty$ [12].
The total cross section of vibrational excitation is the kinds of N and H, respectively. There are a total of 14 primary and the triplet state are shown in Fig. 1(b) as numbers.

Electronic excitation states of H and e-H collisions as a functions of electron energy in Table 1 are shown in Fig. 1(a) and (b).

<table>
<thead>
<tr>
<th>Number</th>
<th>Reaction process</th>
<th>Type of collision</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>e⁻ + N₂ → N₂⁺ + e⁻</td>
<td>Elastic collision</td>
<td>[14,15]</td>
</tr>
<tr>
<td>2</td>
<td>e⁻ + N₂ → N₂⁺ (v) + e⁻</td>
<td>Total vibrational excitation</td>
<td>[14,15]</td>
</tr>
<tr>
<td>3</td>
<td>e⁻ + N₂ → N₂⁺ + e⁻</td>
<td>Total electronic excitation</td>
<td>[14,15]</td>
</tr>
<tr>
<td>4</td>
<td>e⁻ + N₂ → N⁺ + N + e⁻</td>
<td>Dissociation</td>
<td>[14,15]</td>
</tr>
<tr>
<td>5</td>
<td>e⁻ + N₂ → N₂⁺ + 2e⁻</td>
<td>Ionization</td>
<td>[14,15]</td>
</tr>
<tr>
<td>6</td>
<td>e⁻ + N₂ → N⁺ + N + 2e⁻</td>
<td>Dissociation ionization</td>
<td>[14,15]</td>
</tr>
<tr>
<td>7</td>
<td>e⁻ + H₂ → H₂⁺ + e⁻</td>
<td>Elastic collision</td>
<td>[16,17]</td>
</tr>
<tr>
<td>8</td>
<td>e⁻ + H₂ → H₂⁺ (v) + e⁻</td>
<td>Total vibrational excitation</td>
<td>[16,17]</td>
</tr>
<tr>
<td>9</td>
<td>e⁻ + H₂ → H₂⁺ + e⁻</td>
<td>Electronic excitation (singlet state)</td>
<td>[16]</td>
</tr>
<tr>
<td>10</td>
<td>e⁻ + H₂ → H₂⁺ + e⁻</td>
<td>Electronic excitation (triplet state)</td>
<td>[16]</td>
</tr>
<tr>
<td>11</td>
<td>e⁻ + H₂ → H₂⁺ + 2e⁻</td>
<td>Ionization</td>
<td>[16,17]</td>
</tr>
<tr>
<td>12</td>
<td>e⁻ + H₂ → H⁺⁺ + H + 2e⁻</td>
<td>Dissociation ionization</td>
<td>[16,17]</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Reaction process</th>
<th>Type of collision</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>N⁺⁺ + N₂ → N⁺⁺ + N₂</td>
<td>Elastic collision</td>
<td>[18]</td>
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<tr>
<td>14</td>
<td>N⁺⁺ + N₂ → N⁺⁺ + N₂⁺</td>
<td>Charge transfer</td>
<td>[18]</td>
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<tr>
<td>15</td>
<td>N⁺⁺⁺ + N₂ → N⁺⁺⁺ + N₂</td>
<td>Elastic collision</td>
<td>[18]</td>
</tr>
<tr>
<td>16</td>
<td>N⁺⁺⁺ + N₂ → N⁺⁺⁺ (v) + N⁺⁺⁺</td>
<td>Total vibrational excitation</td>
<td>[18]</td>
</tr>
<tr>
<td>17</td>
<td>N⁺⁺⁺ + N₂ → N⁺⁺⁺ + N⁺⁺⁺</td>
<td>Charge transfer</td>
<td>[18]</td>
</tr>
<tr>
<td>18</td>
<td>N⁺⁺⁺ + N₂ → N⁺⁺⁺ + N⁺⁺⁺</td>
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<td>[18]</td>
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<tr>
<td>19</td>
<td>N⁺⁺⁺ + H₂ → N₂H⁺⁺ + H</td>
<td>Binary processes</td>
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<td>20</td>
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<td>Elastic collision</td>
<td>[20-22]</td>
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<tr>
<td>21</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H₂ (0 → 1)</td>
<td>Vibrational excitation</td>
<td>[20-22]</td>
</tr>
<tr>
<td>22</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H₂ (0 → 2)</td>
<td>Vibrational excitation</td>
<td>[20-22]</td>
</tr>
<tr>
<td>23</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H₂ (0 → 3)</td>
<td>Vibrational excitation</td>
<td>[20-22]</td>
</tr>
<tr>
<td>24</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H⁺⁺</td>
<td>Asymmetric charge transfer</td>
<td>[20-22]</td>
</tr>
<tr>
<td>25</td>
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<td>[20,21]</td>
</tr>
<tr>
<td>26</td>
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<td>Ion conversion</td>
<td>[20,21]</td>
</tr>
<tr>
<td>27</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H⁺⁺</td>
<td>Ion conversion</td>
<td>[20,21]</td>
</tr>
<tr>
<td>28</td>
<td>H⁺⁺ + H₂ → H⁺⁺ + H⁺⁺</td>
<td>Vibration excitation</td>
<td>[20,21]</td>
</tr>
</tbody>
</table>

2.2 Collision processes and cross sections

The electron-neutral molecular collision processes considered in the model are listed in Table 1. The e-N₂ and e-H₂ collision cross sections as a functions of electron energy in Table 1 are shown in Fig. 1(a) and (b). Electronic excitation states of H for the singlet state and the triplet state are shown in Fig. 1(b) as numbers 9 and 10, respectively. There are a total of 14 primary kinds of N₂ electronic excitation state cross sections. The total cross section of vibrational excitation is the average of various cross sections of vibrational excitation (number 2 in Fig. 1(a)) [14,15].

The collision processes between nitrogen ions (N⁺⁺, N⁺⁺⁺) and nitrogen molecules, as well as the collision processes between hydrogen ions (H⁺⁺, H⁺⁺⁺, H⁺) and hydrogen molecules, which are listed in Table 2, are shown in Fig. 2(a)-(d) with respect to their collision cross sections as a function of ions energy. In addition, we also take into account the reaction processes between nitrogen ions and hydrogen molecules: N₂⁺ + H₂ → N₂H⁺⁺ + H (number 19), and the elastic collisions and charge transfer collisions between N₂⁺ - H₂, N⁺⁺ - H₂, H⁺⁺ - N₂, H⁺⁺⁺ - N₂ and H⁺⁺⁺ - N₂.
3 Results and discussions

3.1 Distribution of electric field

The time-averaged sheath thickness over one RF cycle near an RF electrode against the nitrogen ratios is shown in Fig. 3. By increasing the ratio of added N$_2$ to the H$_2$ discharge, the sheath thickness monotonously decreases. When the ratio of added N$_2$ is increased from 0% to 30%, the sheath thickness gradually drops from 0.89 cm to 0.76 cm. A great many properties of the plasma will change as the sheath thickness changes. The influence of the ratio of N$_2$ on RF sheath thickness is primarily due to the influence of the distributions of electric field and plasma density.

The electric field distribution along the axis averaged over one RF cycle is shown in Fig. 4 for N$_2$ ratios of 0%, 10%, 20% and 30%. Due to a self-bias of −15 V added to the driven electrode, the electric fields near the two electrodes are asymmetric. As the ratio of added N$_2$ is increased, the sheath thicknesses near the power electrode and the grounded electrode become narrower, and the electric field in these regions is strengthened. These results can be explained by the distribution of positive ion and electron densities, as described in detail in sections 3.3.
Fig. 3  Averaged sheath thickness in front of the RF electrode over one RF cycle as a function of the added nitrogen percentage into the H₂ discharge

Fig. 4  Time averaged distribution of the electric field along the axis of a H₂-N₂ CCRF discharge

3.2 Mean energy of particles

In Fig. 5, the electron mean energy profiles are shown for pure H₂ and for H₂ with added N₂ ratios of 10% and 20%. The results show that when the ratio of nitrogen increases, the electron mean energy in the discharge space decreases and the position of two peaks shifts toward two electrodes. There are two main reasons for the occurrence of the shift. The first reason is that the cross section of collision ionization between electron and H₂ molecule (e⁻ + H₂ → H₂⁺ + 2e⁻) is smaller than that between electron and N₂ (e⁻ + N₂ → N₂⁺ + 2e⁻)[14,16]. By increasing the ratio of nitrogen, the mean impact ionization rate between electrons and the background gas increases so that the mean electron energy decreases. The second reason is that the energy threshold for dissociation ionization between electron and H₂ (e⁻ + H₂ → H₂⁺ + H₂ + 2e⁻) is about 40 eV, but the energy threshold for dissociation ionization between electron and N₂ (e⁻ + N₂ → N₂⁺ + N₂ + 2e⁻) is about 28 eV. The cross section of the former is about one order of magnitude smaller than that of the latter [14,16]. When electron energy exceeds 28 eV, the electron impact dissociation ionization rate greatly increases. This impact can be effective for decreasing electron energy. Meanwhile, more secondary electrons are generated in the above two processes which increase the electron density (Fig. 9) and decrease the electron mean energy.

Although the sheath electric field strengthens with increasing ratio of nitrogen, the above two reasons are more effective.

Fig. 5  Electron mean energy profiles for pure H₂ and admixtures of 10% and 20% N₂ as a function of the axial position in the discharge

In Fig. 6, the distributions of electron mean energy along the axis for $\omega t = 0.5\pi, 1.0\pi, 1.5\pi, 2.0\pi$ are shown for an N₂ ratio of 20%. Electron motion varies with instantaneous electric field due to smaller mass. At $\omega t=0.5\pi$, electrons near the grounded electrode are accelerated by the electric field in sheath, so the electrons energy rapidly increases. Simultaneously, the collision rate with the background gas increases, and the electron energy is lost. Hence, the electron mean energy reaches a maximum at about 27 eV in front of the sheath boundary. And the distribution of the electron mean energy at $\omega t=1.0\pi$ and $2.0\pi$ are similar. The maximum electron mean energy is about 32 eV when $\omega t=1.5\pi$.

Fig. 6  Electron mean energy profiles along the axis at $\omega t=0.5\pi, 1.0\pi, 1.5\pi$ and $2.0\pi$ in H₂+20% N₂ mixture gas CCRF discharge

In Fig. 7, the distributions of H₃⁺ mean energies along the axis are shown for pure H₂, and for H₂ with added N₂ ratios of 10%, 20% and 30%. As can be seen, the mean energy of H₃⁺ bombarding the electrode increases when the N₂ ratio is increased. However, the mean energy of H₃⁺ is almost 0 in the bulk plasma. The energy of H₃⁺ bombarding the RF electrode as a
function of the ratio of $N_2$ is shown in Fig. 8. With an increased ratio of $N_2$ the sheath mean electric field strengthens, and the energy of $H_3^+$ obtained during the motion towards the two electrodes increases. In addition, the mean energy of $H_3^+$ may also be affected by the collision rate of $H_3^+-H_2$ and $H_3^+-N_2$. The mean energy at the RF electrode is higher than that at the grounded electrode due to the existence of self-bias at the RF electrode. The calculated results show that the variation of the mean energy of ions ($H_2^+$, $H^+$) bombarding electrode versus the ratio of $N_2$ is similar to that of $H_3^+$, which plays an non-negligible role in materials synthesis based on hydrogen radio-frequency discharge.

Fig.7  $H_3^+$ mean energy profiles for pure $H_2$ and for admixtures of 10%, 20% and 30% $N_2$

Fig.8  $H_3^+$ mean energy bombarding the RF electrode as a function of the percentage of added $N_2$

3.3 Density of particles

Time-averaged electron densities over one RF cycle are shown in Fig. 9 for different ratios of $N_2$ added to the hydrogen discharge. Increasing the ratio of $N_2$ broadens the electron density profile along the axis, i.e. the sheath thickness becomes narrower and the total electron density increases. The reason is that the e-$N_2$ collision cross sections of ionization and dissociative ionization are larger than those for e-$H_2$ in the same condition (as shown in Fig. 1(a) and (b)). Increase in the ionization rate leads to an increase in the electron densities and a decrease in the mean electron energy (as shown in Fig. 5).

The $H_3^+$, $H_2^+$ and $H^+$ ion mean densities for $N_2$ ratio of 20% as a function of the axial position can be seen in Fig. 10. It is clear that $H_3^+$ is the dominant ion, and $H_2^+$ and $H^+$ are primarily distributed in the bulk plasma. However, the density of $H_3^+$ is less in the bulk plasma, and two peaks appear in the sheath (Fig. 10(b)). This is because when a small amount of $N_2$ is added to $H_2$ gas, the reaction $H_3^+ + H_2 \rightarrow H_3^+ + H$ is still an important channel for converting $H_3^+$ to $H_4^+$. This reaction is especially dominant in the bulk plasma when the energy of $H_3^+$ is less than 3 eV. The densities of $H_2^+$ in the bulk plasma decrease due to the transformation of $H_3^+$ into $H_4^+$. However, since the e-$H_2$ ionization collision produces new $H_3^+$ in the sheath, there are two density peaks seen in Fig. 10(b).

Fig.9  Time-averaged electron density profiles for pure $H_2$ and for admixtures of 10% and 20% $N_2$

Fig.10  (a) Time-averaged hydrogen ion ($H_3^+$, $H_2^+$, $H^+$) density profiles, (b) Time-averaged $H_2^+$ density profile in an $H_2+20\%$ $N_2$ CCRF discharge
Fig. 11 shows the density of $H_3^+$ near the power electrode as a function of the percentage of $N_2$. The density of $H_3^+$ gradually decreases near the power electrode when the ratio of nitrogen is increased. The calculated results show that the densities of $H_3^+$ and $H^+$ are similar to that of $H_2^+$ as a function of the percentage of $N_2$. For $H_3^+$, increasing the ratio of nitrogen results in somewhat drop of the mean electron energy so that the energy of a fraction of the electrons is less than the threshold energy of the electron impact ionization ($e^- + H_2 \rightarrow H_3^+ + 2e^-$). In addition, the density of the background gas $H_2$ somewhat decreases which leads to a drop in the density of $H_3^+$. $H_3^+$ primarily derives from the charge transfer: $H_2^+ + H_2 \rightarrow H_3^+ + H$. Therefore, the density of $H_3^+$ drops when the density of $H_2$ decreases.

3.4 Comparison of simulated and measured results

In Fig. 12, the energy distribution of $H_3^+$ bombarding the RF electrode, measured by Numomura et al. [10] in the pure $H_2$ RF discharge, is presented by the solid line, and the dash line shows the results calculated in the corresponding conditions. It can be seen that the calculated outcome is generally in agreement with the experimental results. The number of low-energy ions distributed below 10 eV are almost 0. For the $H_3^+$ number distributed between 15 eV and 25 eV, the calculated result is a little higher than experimental result.

4 Conclusion

A hybrid PIC/MC model was developed for the $H_2-xN_2$ mixture gas capacitively coupled radio-frequency discharge, in which 43 kinds of collisions reaction processes were taken into account between charged particles ($e^-$, $H_3^+$, $H_2^+$, $H^+$, $N_2^+$, $N^+$) and ground-state molecules ($H_2$, $N_2$). The mean energy and densities of electrons and ions ($H_3^+$, $H_2^+$, $H^+$), and electric field distributions in the $H_2$-$N_2$ CCRF discharge are simulated. The effects of an added percentage of nitrogen (0%-30%) into $H_2$ discharge on the plasma processes and discharge characteristics were also studied with the conclusion that with increasing percentage of added nitrogen, the RF sheath thickness narrows, the sheath electric field is enhanced and the mean energy of hydrogen ions impacting the electrodes is increased. Because the cross sections of the $e^-$-$H_2$ collision ionization and dissociation ionization are less than those of $e^-$-$N_2$, the electron mean densities increase, and the electron mean energy decreases when the percentage of added $N_2$ increases. In the bulk plasma, $H_3^+$ is the most abundant ion, the density of $H_3^+$ is very small and the axial distribution has two peaks. Moreover, the densities of hydrogen ions near electrodes decrease when the ratio of nitrogen increases. Therefore, these simulation results make meaningful contributions to experimental studies and technological processing involving a capacitively coupled radio-frequency discharge in the $H_2$-$xN_2$ mixture gas.

References


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