Two-dimensional Fluid Simulation of an RF Capacitively Coupled Ar/H$_2$ Discharge

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- Effect of small amount of \( \text{H}_2 \) added to Ar
- Charge accumulation of the focus ring
- DC-bias generated by the blocking capacitor
RF discharge and CCP plasma (1)

- RF discharge is important in the plasma CVD for the fabrication of thin film or in the field of plasma chemistry. In microwave plasma, a high ionization rate exists so that the plasma density is high.

- In RF plasma processing, the discharge threshold voltage is low. The discharge can be easily sustained and the electrode can be covered with dielectric materials.

- Types of RF plasma reactors
  - Inductively coupled plasma (ICP)
  - Microwave plasma (MWP)
  - Capacitively coupled plasma (CCP)
  - Combined ICP/CCP reactor
RF discharge and CCP plasma (2)

Capacitively coupled radio-frequency discharges are still among the most powerful and flexible plasma reactors, widely used both in research and in industry.

One-dimensional model


Among the different modelling approaches available to characterize CCP discharges, two-dimensional fluid models provide a good compromise solution within acceptable calculation runtimes.

High frequency

Very high frequency (180 MHz)

Gas heating


The computational model (1)

Model geometry

Computational conditions:
- Gases: Ar/H₂ mixtures (pure Ar, 1%H₂)
- Species: \(e^-\), Ar, H₂, Ar⁺, H⁺, H₂⁺, H₃⁺, ArH⁺, Ar⁺, H, H(2p), H(2s)
- RF frequency: 13.56 MHz
- RF voltage: 200 V, applied to the bottom electrode
- Temperature: 300 K
- Gas pressure: 100 Pa
- Inter-electrode gap: 3.2 cm
- Blocking capacitor: 100 nF
- Focus ring: Silicon
- Dielectric: SiO₂

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
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<tbody>
<tr>
<td>1</td>
<td>(\text{Ar} + e^- \rightarrow \text{Ar} + e^-)</td>
</tr>
<tr>
<td>2</td>
<td>(\text{Ar} + e^- \rightarrow \text{Ar}^* + e^-)</td>
</tr>
<tr>
<td>3</td>
<td>(\text{Ar} + e^- \rightarrow \text{Ar}^+ + 2e^-)</td>
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<tr>
<td>4</td>
<td>(\text{Ar}^* + e^- \rightarrow \text{Ar}^+ + 2e^-)</td>
</tr>
<tr>
<td>5</td>
<td>(\text{Ar}^* + \text{Ar}^* \rightarrow \text{Ar}^+ + \text{Ar} + e^-)</td>
</tr>
<tr>
<td>6</td>
<td>(\text{Ar}^* + \text{Ar} \rightarrow \text{Ar} + \text{Ar})</td>
</tr>
<tr>
<td>7</td>
<td>(\text{H}_2 + e^- \rightarrow \text{H}_2 + e^-)</td>
</tr>
<tr>
<td>8</td>
<td>(\text{H}_2 + e^- \rightarrow \text{H} + \text{H} + e^-)</td>
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<tr>
<td>9</td>
<td>(\text{H}_2 + e^- \rightarrow \text{H} + \text{H}(2s) + e^-)</td>
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<tr>
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<td>(\text{H}_2 + e^- \rightarrow \text{H}(2p) + \text{H}(2s) + e^-)</td>
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<td>(\text{H}_3^+ + e^- \rightarrow \text{H}_2 + \text{H})</td>
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<td>(\text{H} + e^- \rightarrow \text{H}_2 + e^-)</td>
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<td>21</td>
<td>(\text{H}(2p) \rightarrow \text{H} + \hbar \nu)</td>
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<tr>
<td>28</td>
<td>(\text{Ar}^* \rightarrow \text{Ar} \text{ (wall loss)})</td>
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<td>29</td>
<td>(\text{H}_2^+ \rightarrow \text{H}_2 \text{ (wall loss)})</td>
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<tr>
<td>30</td>
<td>(\text{H}_3^+ \rightarrow \text{H} + \text{H}_2 \text{ (wall loss)})</td>
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<td>31</td>
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<td>(\text{H} + \text{H}_2 \text{ (wall loss)})</td>
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<tr>
<td>33</td>
<td>(\text{H}(2p) \rightarrow \text{H} \text{ (wall loss)})</td>
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<tr>
<td>34</td>
<td>(\text{H}(2s) \rightarrow \text{H} \text{ (wall loss)})</td>
</tr>
</tbody>
</table>
The computational model (2)

Drift-diffusion equations for electrons

\[
\frac{\partial}{\partial t} (n_e) + \nabla \cdot \Gamma_e = R_e \\
\Gamma_e = -n_e (\mu_e E) - D_e \nabla n_e
\]

Source term

\[
R_e = \sum_{j=1}^{M} x_j k_j N_n n_e
\]

Reaction rate

\[
k_j = \gamma \int_{0}^{\infty} \varepsilon \sigma_j(\varepsilon)f(\varepsilon)d\varepsilon
\]

\[
\gamma = (2q/m)^{1/2}
\]

Cross sections for electron collisions

Boundary conditions:

\[
-n \cdot \Gamma_e = \left(\frac{1}{2} v_{e,th} n_e\right) - \sum_{p} \gamma_p (\Gamma_p \cdot n)
\]

\[
-n \cdot \Gamma_\varepsilon = \left(\frac{5}{6} v_{e,th} n_\varepsilon\right) - \sum_{p} \varepsilon_p \gamma_p (\Gamma_p \cdot n)
\]
The computational model (3)

**Modified Maxwell-Stefan equation for ion and neutral species**

\[
\rho \frac{\partial}{\partial t} (w_k) + \rho (u \cdot \nabla) w_k = \nabla \cdot j_k + R_k
\]

\[
j_k = \rho \omega_k v_k\]

\[
v_k = \sum_{j=1}^{Q} \tilde{D}_{kj} d_k - \frac{D_{kT}}{\rho \omega_k} \nabla \ln T
\]

\[
d_k = \frac{1}{cRT} \left[ \nabla p_k - \omega_k \nabla p - \rho_k g_k + \omega_k \sum_{j=1}^{Q} \rho_j g_j \right]
\]

Boundary conditions: \(-n \cdot j_k = M_\omega R_k + M_\omega c_k Z \mu_k (E \cdot n) [Z_k \mu_k (E \cdot n) > 0]\)

**Poisson’s equation**

\[-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho \quad \rho = q \left( \sum_{k=1}^{N} Z_k n_k - n_e \right)\]

Charge accumulation on the dielectric surface:

\[
n \cdot (D_1 - D_2) = \rho_s \quad \frac{d\rho_s}{dt} = n \cdot J_i + n \cdot J_e
\]
Results (1)

CCP discharge structure in Ar/1%H$_2$ mixture

Electron and ion densities

- Time averaged electron density (1/m$^3$)
  - Contour: $1 \times 10^{16}$ /m$^3$
  - $1.26 \times 10^{16}$
  - $7.94 \times 10^{8}$

- Time averaged Ar$^+$ density (1/m$^3$)
  - $4.18 \times 10^{15}$
  - $3.55 \times 10^{11}$

- Time averaged ArH$^+$ density (1/m$^3$)
  - $1.53 \times 10^{15}$
  - $1.95 \times 10^{11}$

- Time averaged H$_3^+$ density (1/m$^3$)
  - $6.89 \times 10^{15}$
  - $2.68 \times 10^{12}$

- Time averaged H$^+$ density (1/m$^3$)
  - $7.2 \times 10^{11}$
  - $4.93 \times 10^{8}$

- Time averaged H$_2^+$ density (1/m$^3$)
  - $1.33 \times 10^{14}$
  - $4.45 \times 10^{10}$
Results (2)  CCP discharge structure in Ar/1%H₂ mixture

Neutral species densities

- Time averaged excited argon density (1/m³)
  - 1.15 x 10¹⁷
  - 1.75 x 10¹¹

- Time averaged H(2s) density (1/m³)
  - 2.36 x 10¹⁴
  - 4.97 x 10¹²

- Time averaged H(2p) density (1/m³)
  - 8.42 x 10¹⁰
  - 1.03 x 10⁸

- Time averaged H(2s) annihilation rate (1/(m³s))
  - 3.85 x 10¹⁸
  - 1.39 x 10⁶

- Time averaged hydrogen dissociation rate (1/(m³s))
  - 1.31 x 10²⁰
  - 1.52 x 10⁸
Results (3)

CCP discharge structure in Ar/1%H₂ mixture

Electron temperature

$t = 0$  Surface: Electron temperature (V)

$t = 1/4 \, T$  Surface: Electron temperature (V)

$t = 1/2 \, T$  Surface: Electron temperature (V)

$t = 3/4 \, T$  Surface: Electron temperature (V)
Results (4)

CCP discharge structure in Ar/1\%H_2 mixture

Electric potential

\[ \text{t} = 0 \] Surface: Electric potential (V)

\[ \text{t} = 1/4 \ T \] Surface: Electric potential (V)

\[ \text{t} = 1/2 \ T \] Surface: Electric potential (V)

\[ \text{t} = 3/4 \ T \] Surface: Electric potential (V)
Results (5)

CCP discharge structure in Ar/1%H$_2$ mixture

Power deposition

$t = 0$ Surface: Capacitive power deposition (W/m$^3$)

$t = 1/4$ T Surface: Capacitive power deposition (W/m$^3$)

$t = 1/2$ T Surface: Capacitive power deposition (W/m$^3$)

$t = 3/4$ T Surface: Capacitive power deposition (W/m$^3$)
Results (6)

Discharge structure around the focus ring

Electron density at $r = 15$ cm over the focus ring

Electric potential at $r = 15$ cm over the focus ring

Electron temperature at $r = 15$ cm over the focus ring

Electric field at $r = 15$ cm over the focus ring
Results (7)

Effect of the focus ring and blocking capacitor

Power deposition around the focus ring

Electric potential along the surface of substrate and adjacent dielectrics

DC-bias generated by the blocking capacitor
Results (8)

CCP discharge structure in pure Ar

Electric potential at $r = 15$ cm over the focus ring

Electric potential along the surface of substrate and adjacent dielectrics
Results (9)

Comparison with the discharge in Ar/1%H₂ and pure Ar

**Pure Ar**

**Excited argon density**

*Time averaged excited argon density (1/m²)*

**Poolion ionization rate**

Ar° + Ar° → Ar⁺ + Ar + e⁻

**Time averaged ionization rate (1/(m³s))**


**Ar/1%H₂**

**Excited argon density**

*Time averaged excited argon density (1/m²)*

**Poolion ionization rate**

**Time averaged ionization rate (1/(m³s))**
Conclusions

- This paper presents the simulation results of low-pressure capacitively coupled RF plasmas in Ar/H₂.

- The addition of small amount of H₂ to Ar causes the electron density markedly decrease. The high electron density region is formed above the focus ring. The effect of the self DC-bias of the blocking capacitor is presented.

- It is found that with the increase of the amount of H₂ added to Ar, the density of metastable argon atoms is dramatically decreased. The pooling ionization rate due to the collisions among these atoms reduces down to 1.5% of that of pure argon.

- It could be concluded that the control of gas composition, focus ring and blocking capacitor would be very beneficial in finding the design parameters of RF CCP plasma reactors.
Thank you for your attention!

Questions & Comments?