COMSOL CONFERENCE 2014 CAMBRIDGE

Two-dimensional Fluid Simulation of an RF Capacitively Coupled Ar/H_2 Discharge

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September 18, 2014

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Effect of small amount of H_2 added to Ar

Charge accumulation of the focus ring

DC-bias generated by the blocking capacitor

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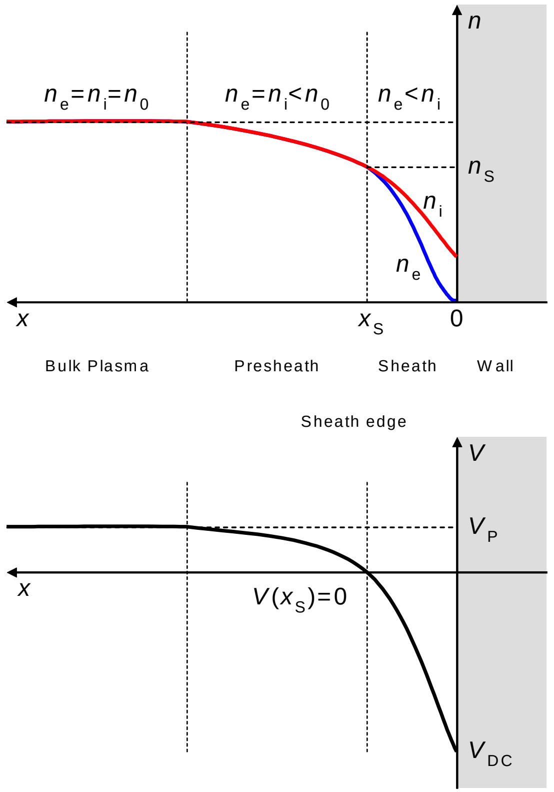
RF discharge and CCP plasma (1)

- 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

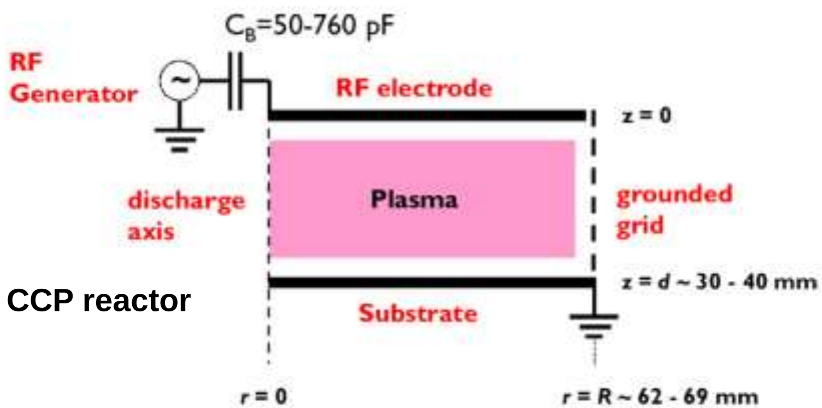
Interaction between plasma and wall

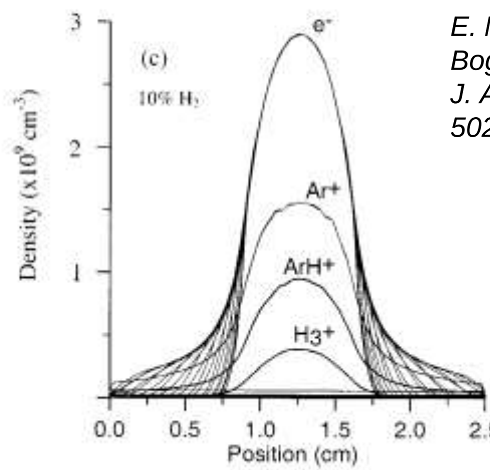


RF discharge and CCP plasma (2)

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

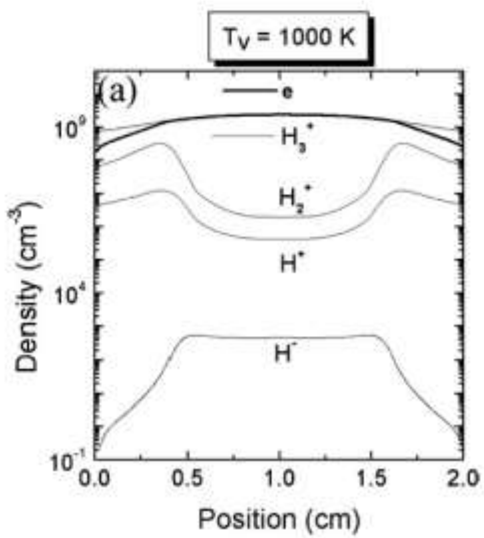
One−dimensional model



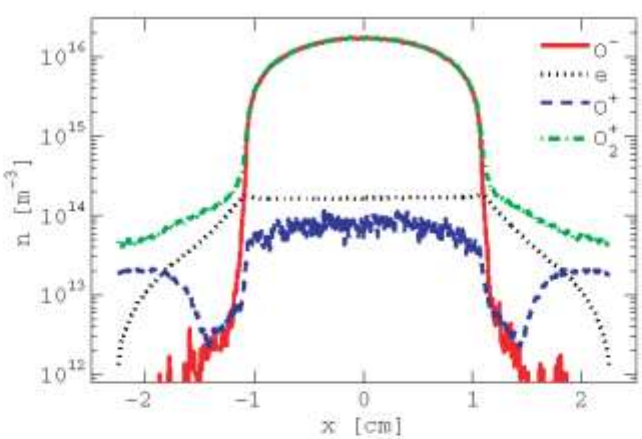


E. Neyts, M. Yan, A. Bogaerts, and R. Gijbels : J. Appl. Phys., ***93*** *(2003) 5025-5033*

L. L. Alves and L. Marques : Plasma Phys. Control. Fusion ***54*** *(2012) 124012 (8pp)*



B. Kalache, T. Novikova, et al.: J. Phys. D: Appl. Phys. ***37*** *(2004) 1765–1773*



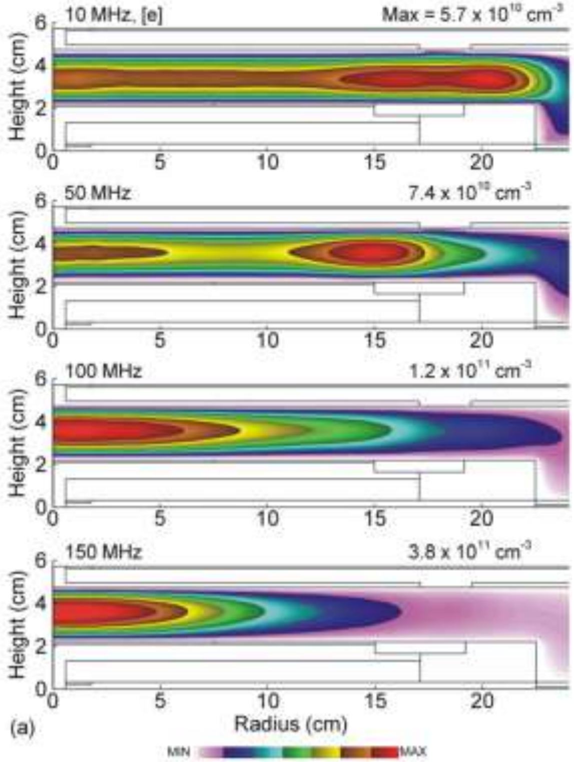
J. T. Gudmundsson, E. Kawamura and M. A. Lieberman : Plasma Sources Sci. Technol. ***22*** *(2013) 035011 (11pp)*

RF discharge and CCP plasma (3)

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

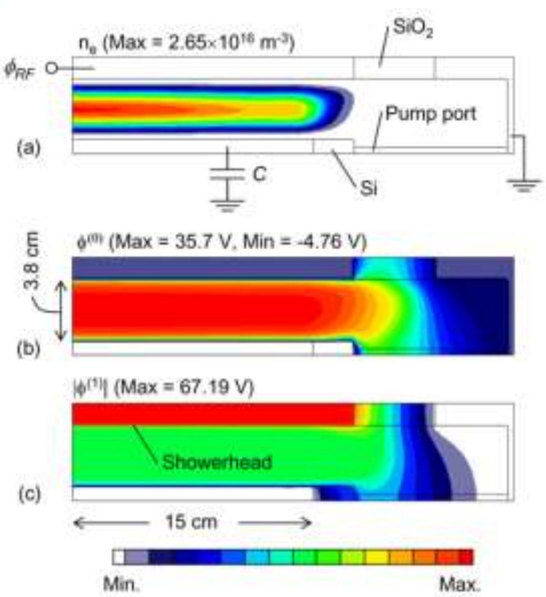
Two-dimensional model

High frequency



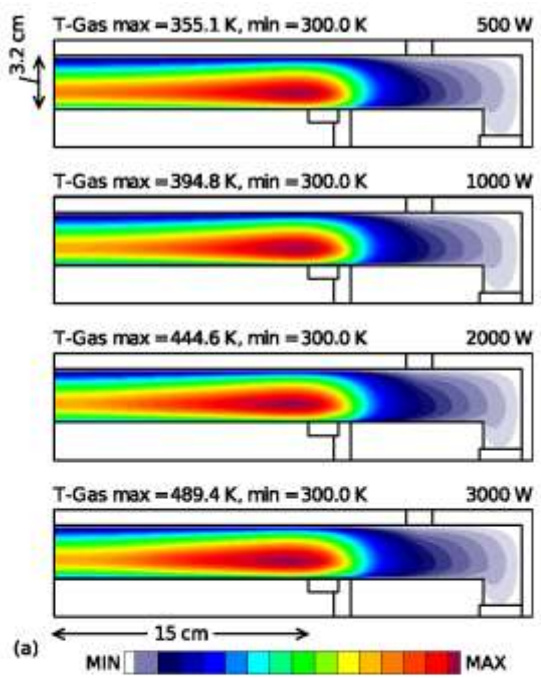
Y. Yang and M. J. Kushner : Plasma Sources Sci. Technol. ***19*** *(2010) 055011 (17pp)*

Very high frequency (180 MHz)



S. Rauf, K. Bera and K. Collins : Plasma Sources Sci. Technol. ***17*** *(2008) 035003 (9pp)*

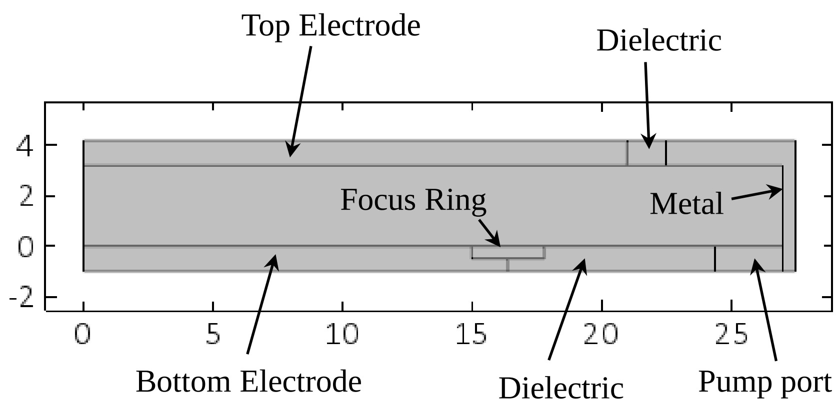
Gas heating



A. Agarwal, S. Rauf and K. Collins : Plasma Sources Sci. Technol. ***21*** *(2012) 055012 (12pp)*

The computational model (1)

Model geometry



Computational conditions:

- Gases: Ar/H_2 mixtures (pure Ar, 1%H_2)
- Species: e^-, Ar, H_2, Ar^+, H^+, H_2^+, H_3^+, ArH^+, Ar^*, H, H(2*p*), H(2*s*)
- 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: SiO_2

No.	Reaction
1	$Ar + e^- \rightarrow Ar + e^-$
2	$Ar + e^- \rightarrow Ar^* + e^-$
3	$Ar + e^- \rightarrow Ar^+ + 2e^-$
4	$Ar^* + e^- \rightarrow Ar^+ + 2e^-$
5	$Ar^* + Ar^* \rightarrow Ar^+ + Ar + e^-$
6	$Ar^* + Ar \rightarrow Ar + Ar$
7	$H_2 + e^- \rightarrow H_2 + e^-$
8	$H_2 + e^- \rightarrow H + H + e^-$
9	$H_2 + e^- \rightarrow H + H(2s) + e^-$
10	$H_2 + e^- \rightarrow H(2p) + H(2s) + e^-$
11	$H_2 + e^- \rightarrow H_2^+ + 2e^-$
12	$H_2 + e^- \rightarrow H + H^+ + 2e^-$
13	$H_2^+ + e^- \rightarrow H^+ + H + e^-$
14	$H_3^+ + e^- \rightarrow H_2 + H$
15	$H_2 + H_2^+ \rightarrow H_3^+ + H$
16	$H + e^- \rightarrow H + e^-$
17	$H + e^- \rightarrow H(2p) + e^-$
18	$H + e^- \rightarrow H(2s) + e^-$
19	$H(2s) + e^- \rightarrow H(2p) + e^-$
20	$H + e^- \rightarrow H^+ + 2e^-$
21	$H(2s) + e^- \rightarrow H^+ + 2e^-$
22	$H(2p) \rightarrow H + hv$
23	$Ar^* + H_2 \rightarrow Ar + H + H$
24	$Ar^+ + H_2 \rightarrow Ar + H_2^+$
25	$Ar^+ + H_2 \rightarrow H + ArH^+$
26	$ArH^+ + H_2 \rightarrow H_3^+ + Ar$
27	$ArH^+ + e^- \rightarrow Ar + H$
28	$Ar^* \rightarrow Ar$ (wall loss)
29	$H_2^+ \rightarrow H_2$ (wall loss)
30	H_3^+ ⍰→ $H + H_2$ (wall loss)
31	$H^+ \rightarrow H$ (wall loss)
32	H $1/2H_2$ (wall loss)
33	$H(2p) \rightarrow H$ (wall loss)
34	$H(2s) \rightarrow H$ (wall loss)

The computational model (2)

Drift-diffusion equations for electrons

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e$$

$$\Gamma_e = -n_e(\mu_e \mathbf{E}) - D_e \nabla n_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot \Gamma_\varepsilon + \mathbf{E} \cdot \Gamma_e = R_\varepsilon$$

$$\Gamma_\varepsilon = -n_\varepsilon(\mu_\varepsilon \mathbf{E}) - D_\varepsilon \nabla n_\varepsilon$$

Source term

$$\boldsymbol{R_e = \sum_{j=1}^{M} x_j k_j N_n n_e}$$

Source term

$$\boldsymbol{R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j}$$

Reaction rate $\boldsymbol{k_j = \gamma \int_0^\infty \varepsilon \sigma_j(\varepsilon) f(\varepsilon) d\varepsilon}$ $\boldsymbol{\gamma = (2q/m)^{1/2}}$

Cross sections for electron collisions

Boundary conditions:

$$-\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} v_{e,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n})$$

$$-\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} v_{e,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n})$$

The computational model (3)

Modified Maxwell-Stefan equation for ion and neutral species

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u}\cdot\nabla)w_k = \nabla\cdot\mathbf{j}_k + R_k$$

ここに

$$\mathbf{j}_k = \rho\omega_k\mathbf{V}_k \qquad \mathbf{V}_k = \sum_{j=1}^{Q}\widetilde{D}_{kj}\mathbf{d}_k - \frac{D_k{}^T}{\rho\omega_k}\nabla lnT$$

$$\mathbf{d}_k = \frac{1}{cRT}\left[\nabla p_k - \omega_k\nabla p - \rho_k\mathbf{g}_k + \omega_k\sum_{j=1}^{Q}\rho_j\mathbf{g}_j\right]$$

Boundary conditions: $-\mathbf{n}\cdot\mathbf{j}_k = M_\omega R_k + M_\omega c_k Z\mu_k(\mathbf{E}\cdot\mathbf{n})[Z_k\mu_k(\mathbf{E}\cdot\mathbf{n}) > 0]$

Poisson's equation

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

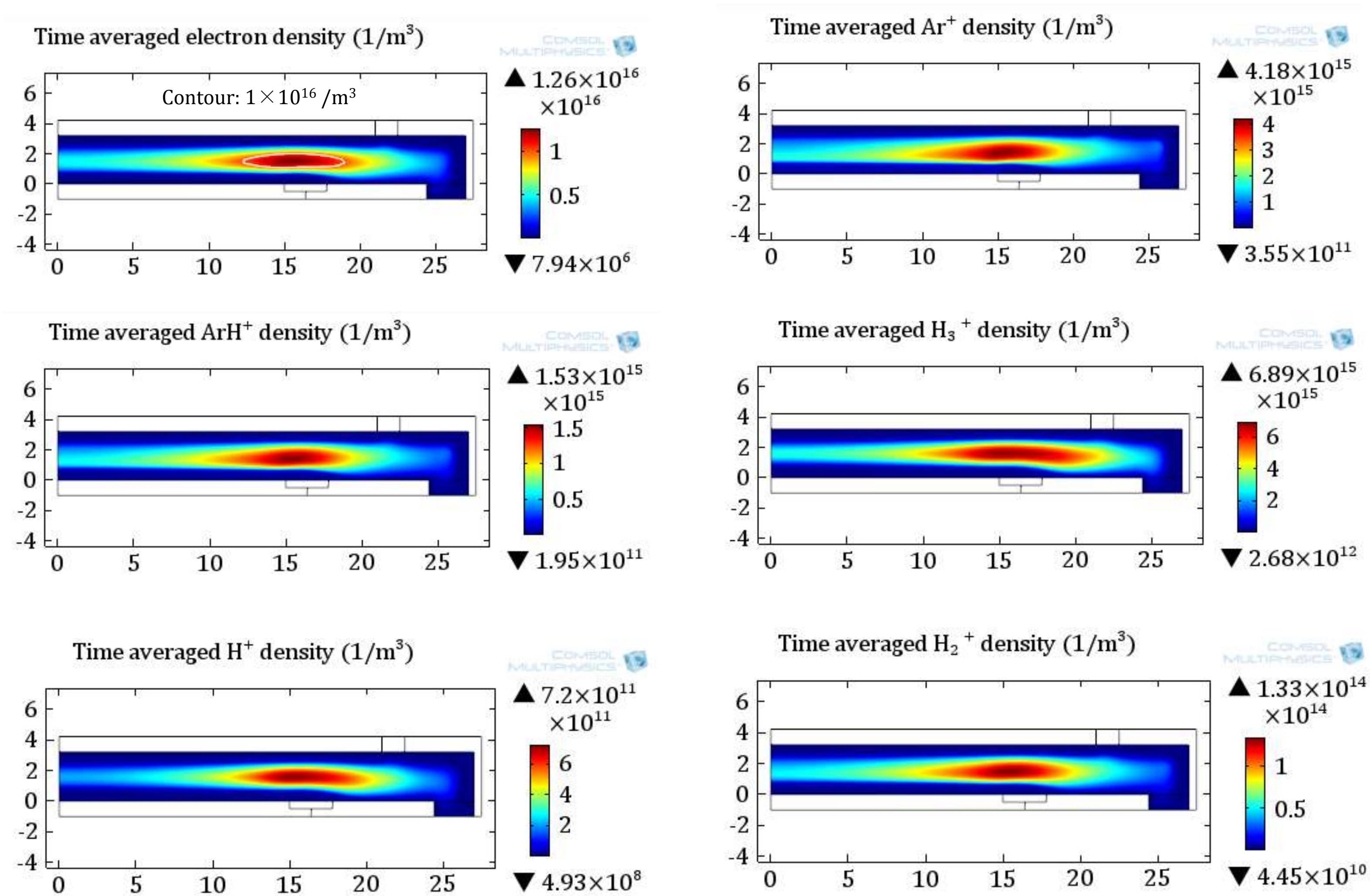
Charge accumulation on the dielectric surface:

$$\mathbf{n}\cdot(\mathbf{D}_1 - \mathbf{D}_2) = \rho_s \qquad \frac{d\rho_s}{dt} = \mathbf{n}\cdot\mathbf{J}_i + \mathbf{n}\cdot\mathbf{J}_e$$

Results (1)

CCP discharge structure in Ar/1%H_2 mixture

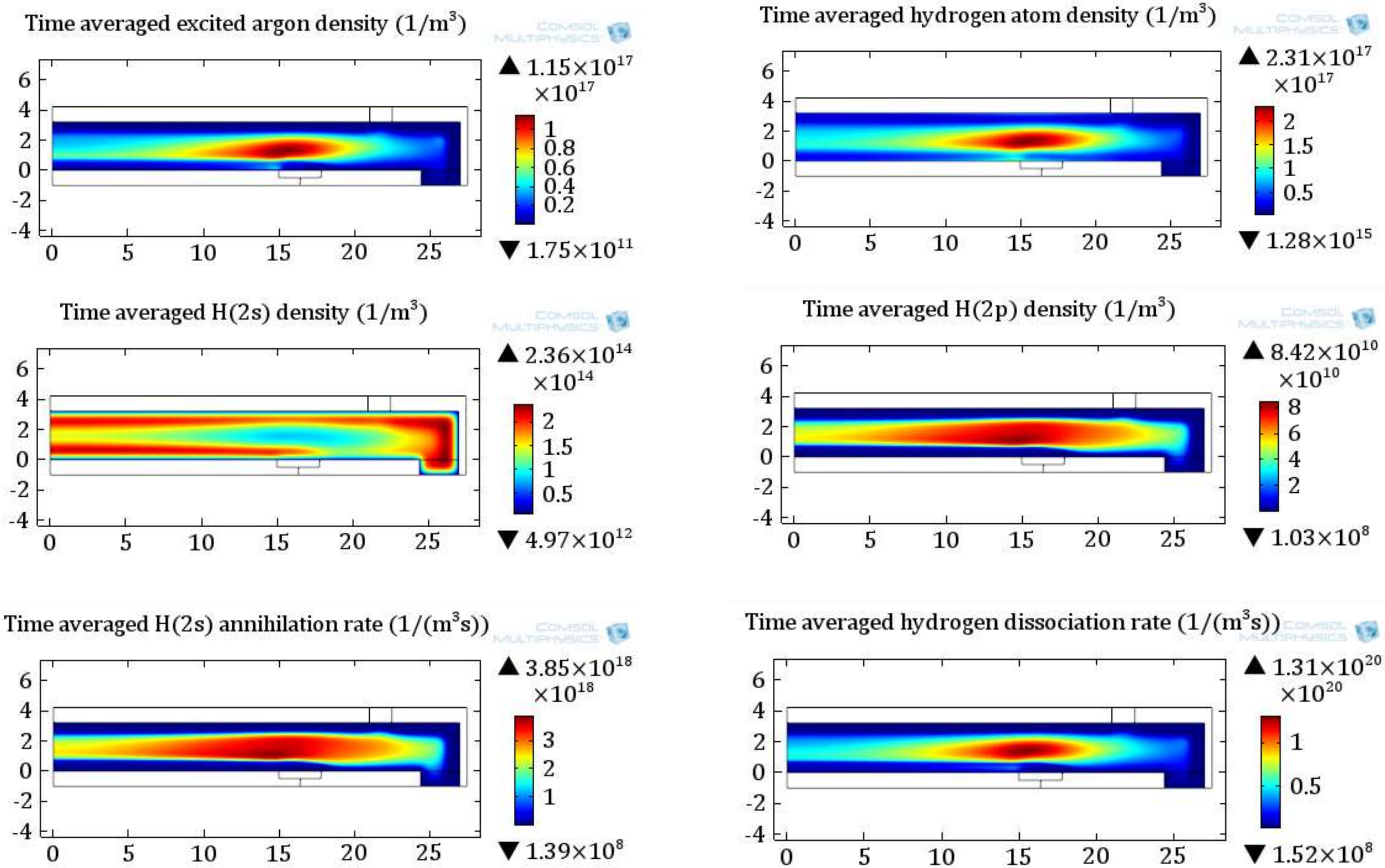
Electron and ion densities



Results (2)

CCP discharge structure in $Ar/1\%H_2$ mixture

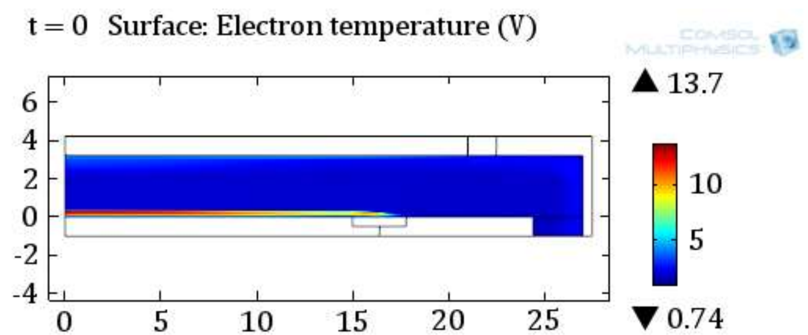
Neutral species densities

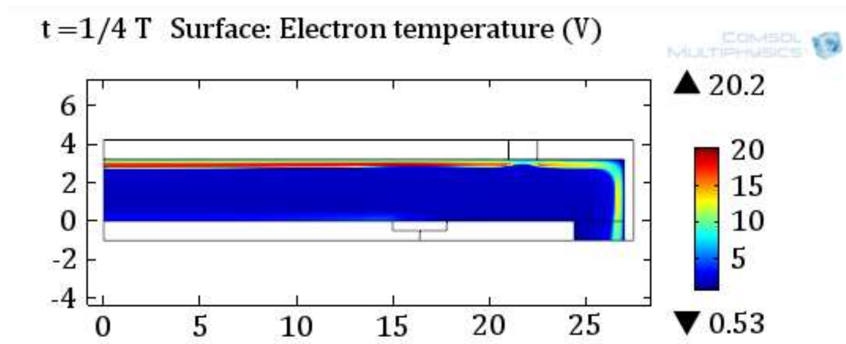


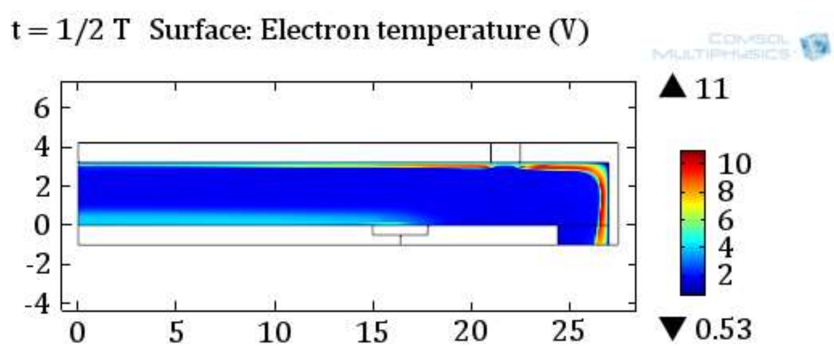
Results (3)

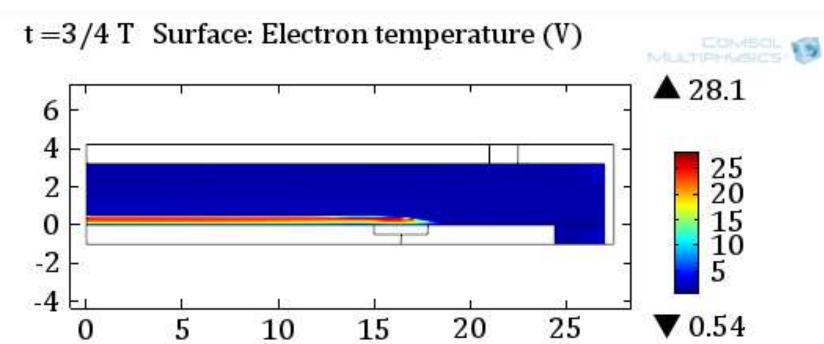
CCP discharge structure in $Ar/1\%H_2$ mixture

Electron temperature





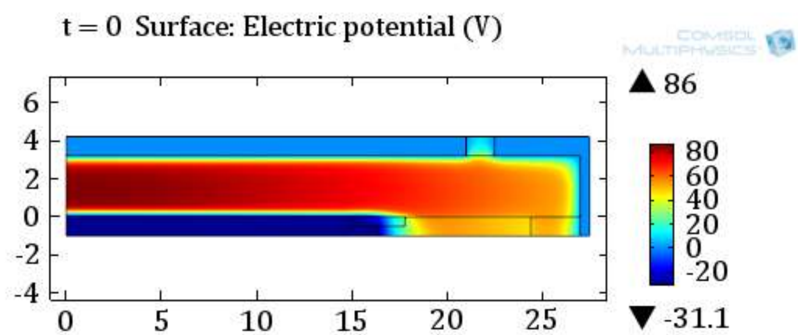


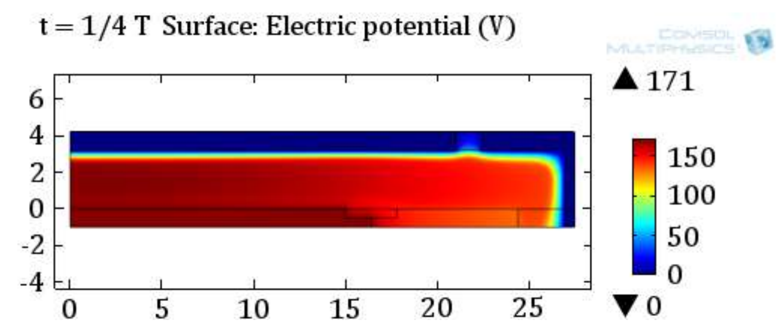


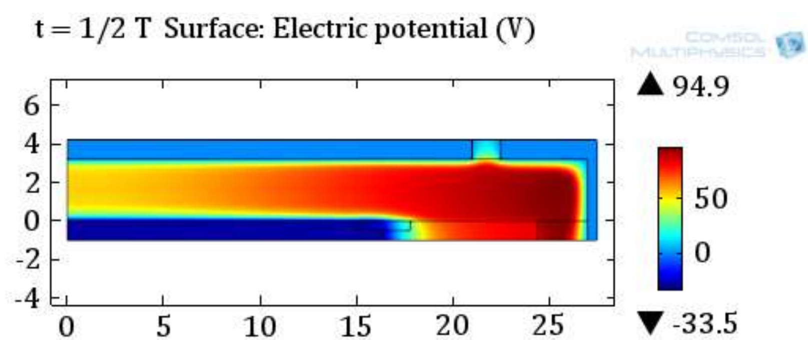
Results (4)

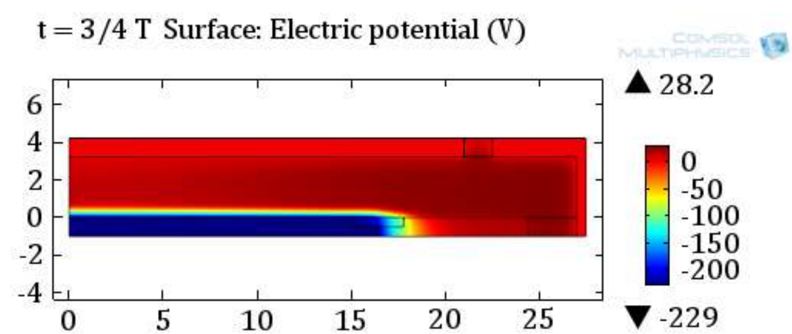
CCP discharge structure in $Ar/1\%H_2$ mixture

Electric potential





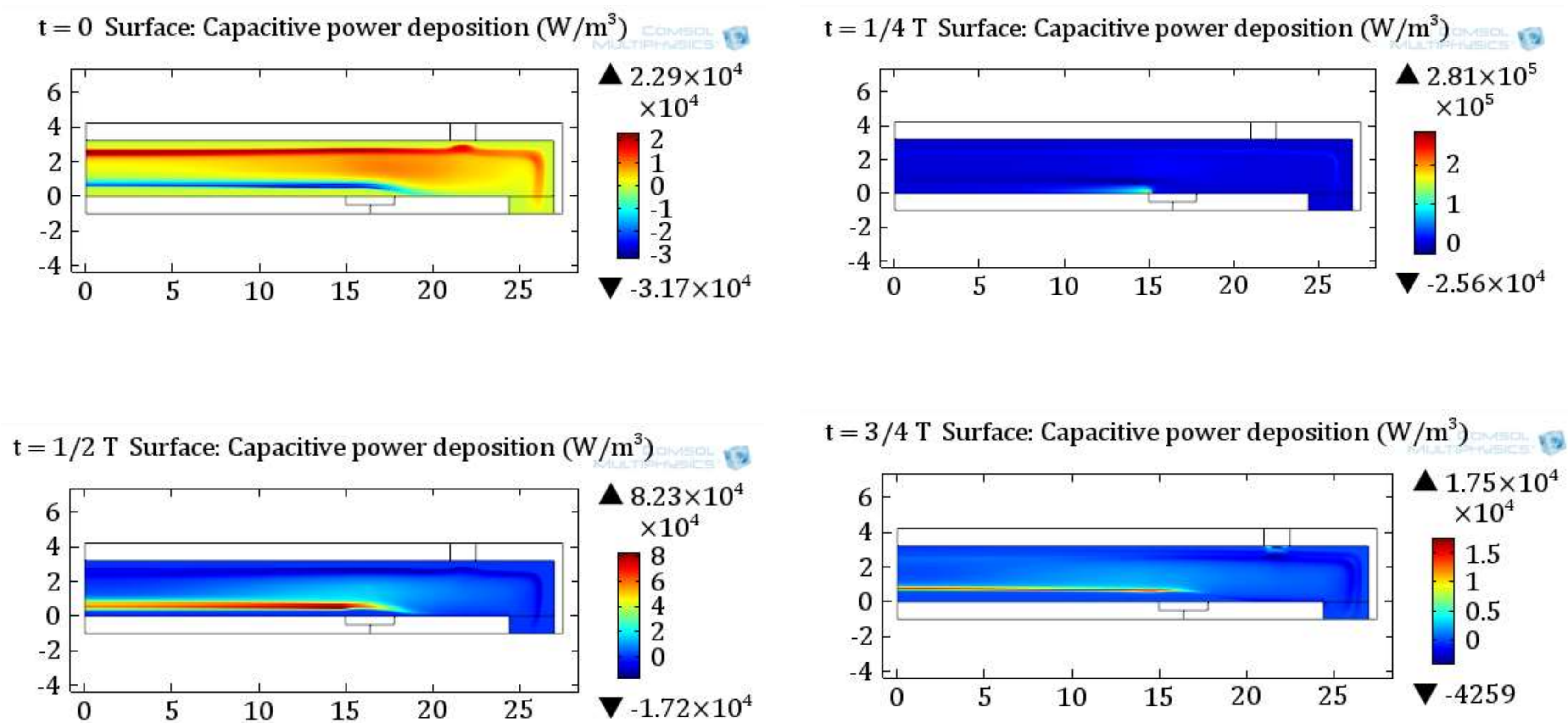




Results (5)

CCP discharge structure in Ar/1%H_2 mixture

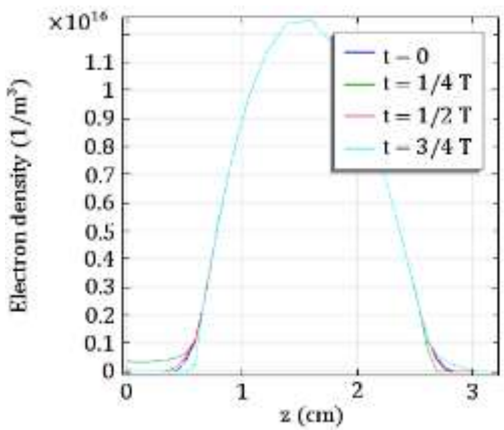
Power deposition



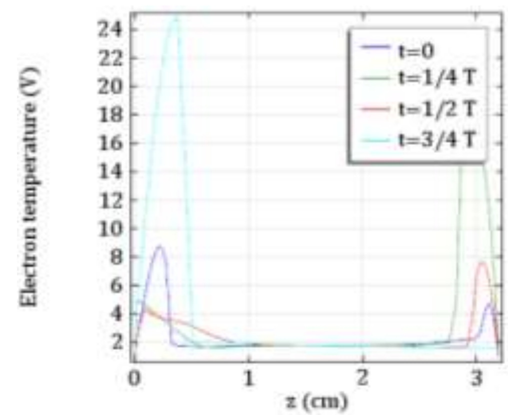
Results (6)

Discharge structure around the focus ring

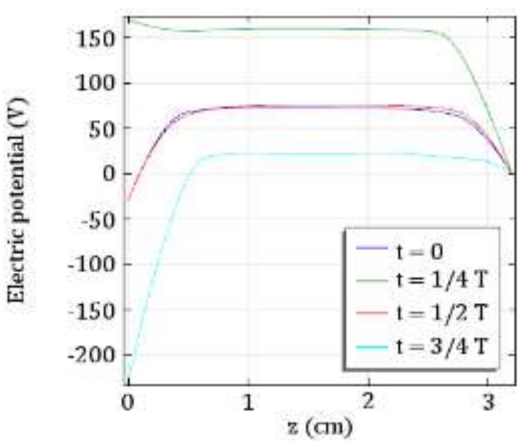
Electron density at r = 15 cm over the focus ring



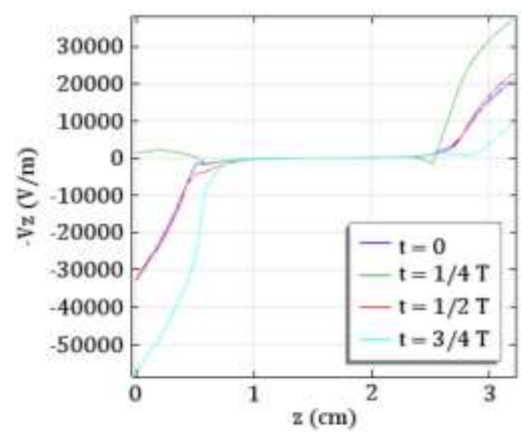
Electron temperature at r = 15 cm over the focus ring



Electric potential at r = 15 cm over the focus ring



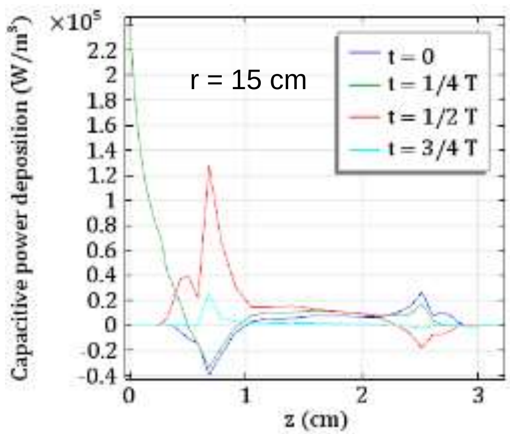
Electric field at r = 15 cm over the focus ring

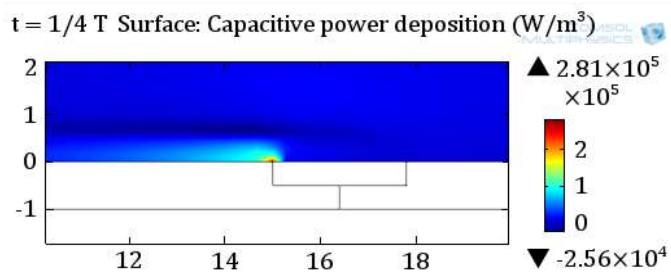


Results (7)

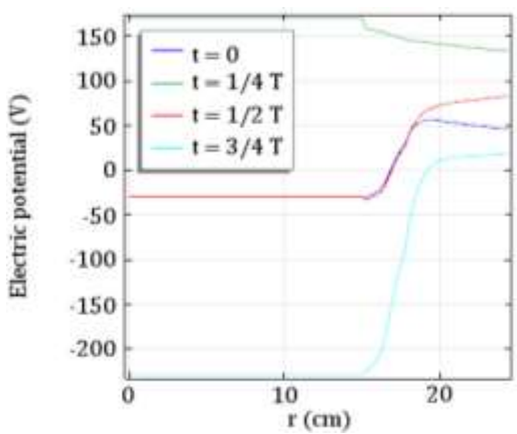
Effect of the focus ring and blocking capacitor

Power deposition around the focus ring

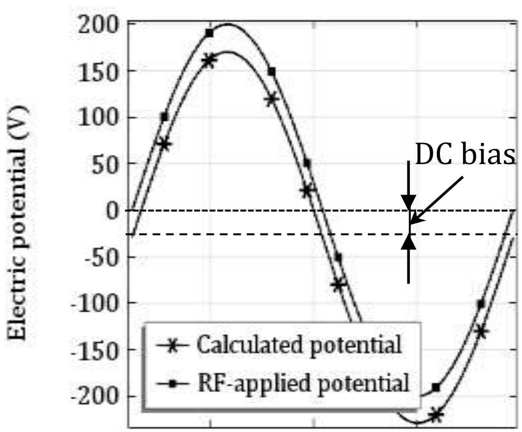




Electric potential along the surface of substrate and adjacent dielectrics

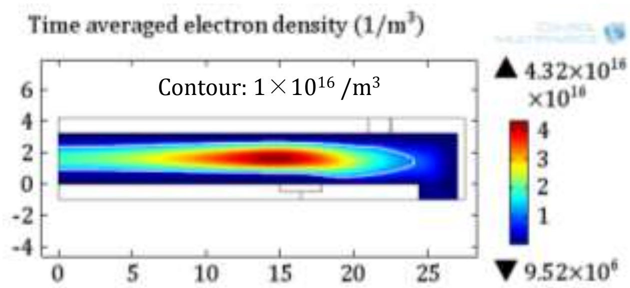


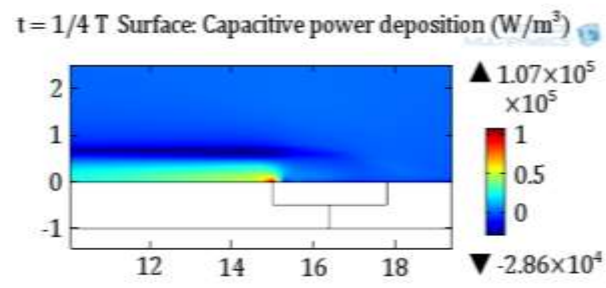
DC-bias generated by the blocking capacitor



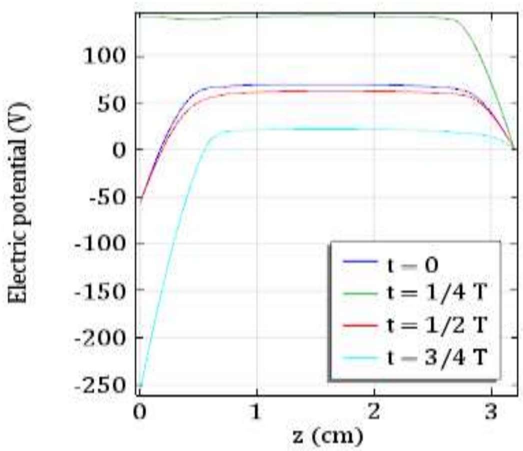
Results (8)

CCP discharge structure in pure Ar

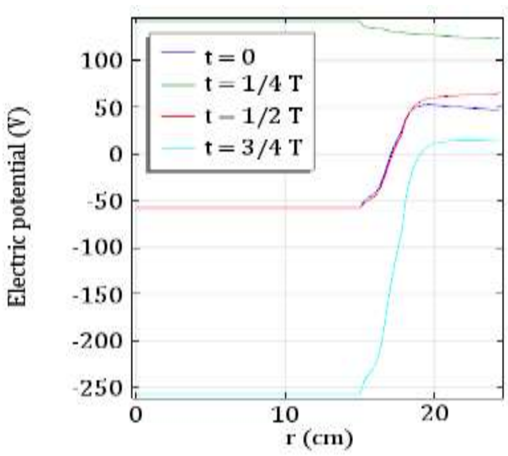




Electric potential at r = 15 cm over the focus ring



Electric potential along the surface of substrate and adjacent dielectrics

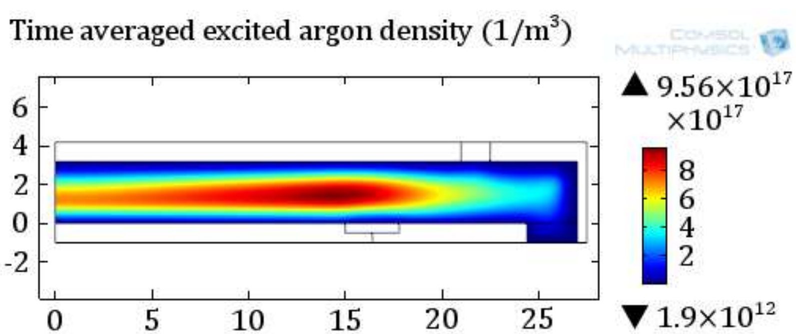


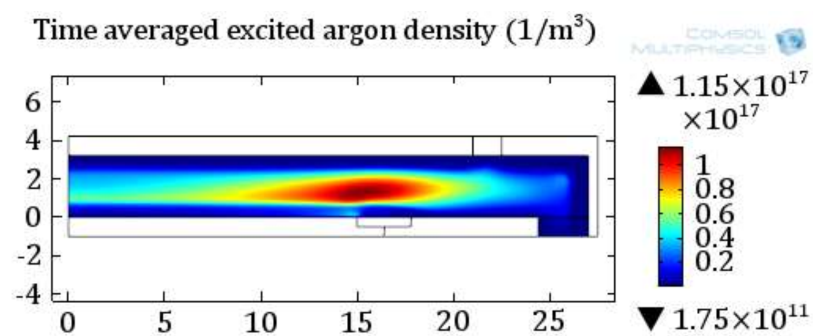
Results (9)

Comparison with the discharge in $Ar/1\%H_2$ and pure Ar

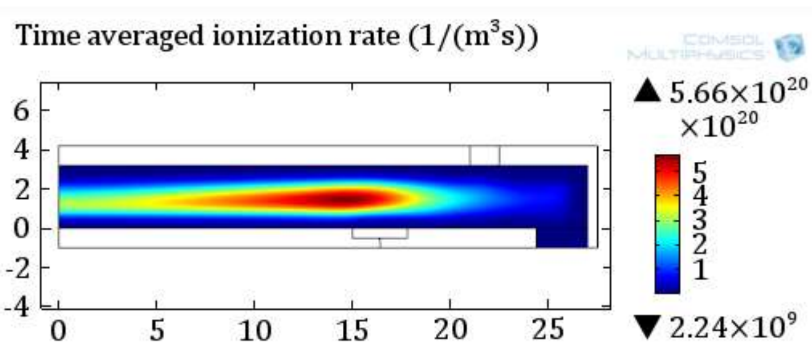
Pure Ar | $Ar/1\%H_2$

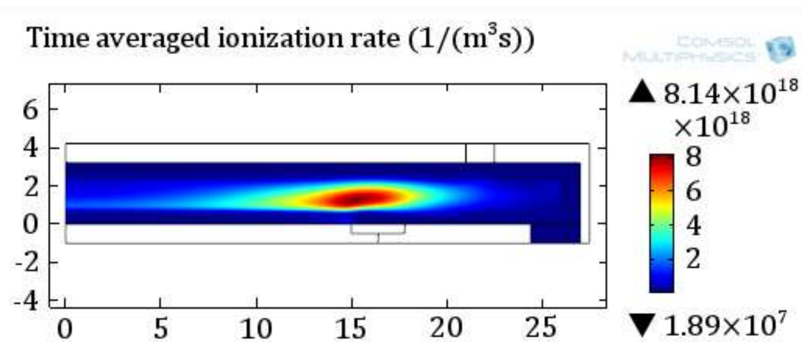
Excited argon density | Excited argon density





Pooling ionization rate $\quad Ar^* + Ar^* \rightarrow Ar^+ + Ar + e^-$ $\quad$ Pooling ionization rate





Conclusions

- This paper presents the simulation results of low-pressure capacitively coupled RF plasmas in Ar/H_2.
- The addition of small amount of H_2 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 H_2 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 ?