

# Electron power absorption in radio frequency driven capacitively coupled chlorine discharge

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# Introduction

- Chlorine is an electronegative diatomic gas that is widely used in plasma etching of both semiconductors and metals, in particular poly-silicon gate and aluminum interconnects
- Chlorine atoms are believed to be the primary reactant in plasma etching
- The chlorine molecule has
  - a low dissociation energy (2.5 eV)
  - a near-zero threshold energy for dissociative attachment
- All electronic excitations of the molecule appear to be dissociative, and no metastable molecular states are of importance



# The 1D particle-in-cell/Monte Carlo collision simulation



# The *oopd1 1d-3v PIC/MCC code*

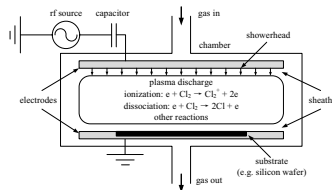
- We use the *oopd1* (objective oriented plasma device for one dimension) code to simulate the discharge
- The *oopd1* code was originally developed at the Plasma Theory and Simulation Group at UC Berkeley
- It has 1 dimension in space and 3 velocity components for particles (1d-3v)
- The *oopd1* code is supposed to replace the widely used *xpdx1* series (*xpdp1*, *xpdc1* and *xpds1*)
- It is developed to simulate various types of plasmas, including processing discharges, accelerators and beams
  - Modular structure
  - Includes relativistic kinematics
  - Particles can have different weights

Gudmundsson et al. (2013) *Plasma Sources Sci. Technol.*, **22**(3) 035011

Wen et al. (2021) *Plasma Sources Sci. Technol.*, **30** accepted



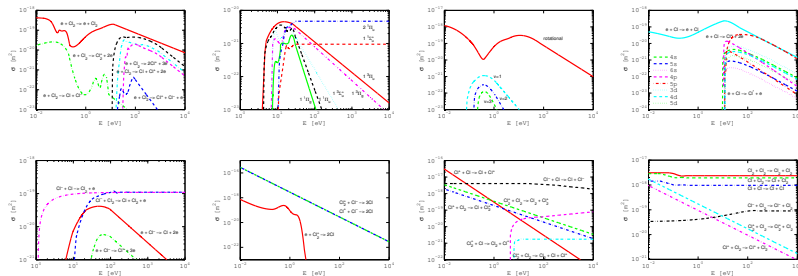
# The chlorine discharge



- We consider a discharge that consists of:
  - electrons
  - the ground state chlorine molecule  $\text{Cl}_2(X^1\Sigma_g^+, v=0)$ ,
  - the ground state chlorine atom  $\text{Cl}(3p^5^2P)$
  - the negative chlorine ion  $\text{Cl}^-$
  - the positive chlorine ions  $\text{Cl}^+$  and  $\text{Cl}_2^+$
- We apply a global model<sup>1</sup> beforehand to calculate the fraction of Cl atoms

<sup>1</sup> Thorsteinsson and Gudmundsson (2010) *Plasma Sources Sci. Technol.*, **19**(1) 015001

# The chlorine discharge



- The reaction set for the chlorine is comprehensive and includes 44 reactions

Huang and Gudmundsson (2013) *Plasma Sources Sci. Technol.*, **22**(5) 055020



# Electron power absorption

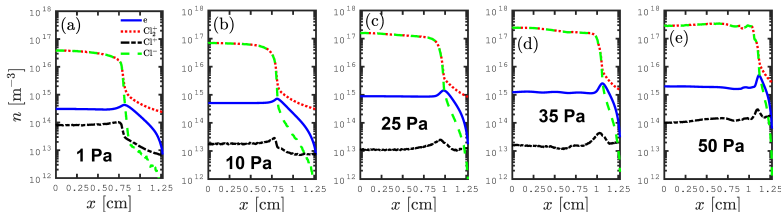
Voltage source operated at a single frequency

$$V(t) = V_{\text{rf}} \sin(2\pi ft)$$

gap = 2.54 cm,  $V_{\text{rf}} = 222$  V and  $f = 13.56$  MHz



# Electron power absorption



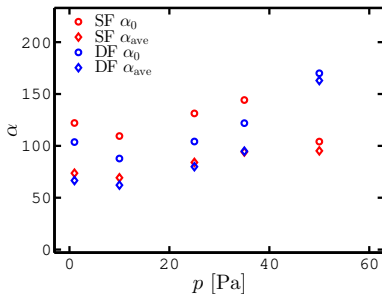
Proto and Gudmundsson (2021) PSST **30**(6) 065009

- The time averaged charged particle density profiles of a parallel plate capacitively coupled chlorine discharge
- At low pressures, the profile for Cl<sub>2</sub><sup>+</sup> ions is cosine-like or parabolic since Cl<sub>2</sub><sup>+</sup> ions are lost mainly due to diffusion to the walls
- As the pressure increases, the recombination between Cl<sub>2</sub><sup>+</sup> and Cl<sup>-</sup> ions becomes the major loss mechanism for Cl<sub>2</sub><sup>+</sup> ions and the density profile for Cl<sub>2</sub><sup>+</sup> and Cl<sup>-</sup> ions becomes flat in the bulk region



# Electron power absorption

- The electronegativity in the discharge center is very high and increases with increased operating pressure
- Negative ion creation proceeds via electron impact dissociative attachment whose cross-sections are high
- Drift-ambipolar (DA) power absorption is expected within the electronegative core



Skarphedinsson and Gudmundsson (2020) PSST **29**(8) 084004

Schulze et al. (2011) PRL **107**(27) 275001



# *Electron power absorption*

- To determine the electron power absorption mechanisms we apply Boltzman term analysis

Surendra and Dalvie (1993) PRE **48**(5) 3914 and Schulze et al. (2018) **27**(5) 055010

- The electric field within the electronegative core constitutes contributions through various different phenomena
- The electric field is composed of six terms

$$E = - \underbrace{\frac{m_e}{e} \frac{\partial u_e}{\partial t}}_I + \underbrace{\frac{m_e}{e} \frac{u_e^2}{n_e} \frac{\partial n_e}{\partial x}}_{II} + \underbrace{\frac{m_e}{e} \frac{u_e}{n_e} \frac{\partial n_e}{\partial t}}_{III} - \underbrace{\frac{T_e}{n_e} \frac{\partial n_e}{\partial x}}_{IV} - \underbrace{\frac{\partial T_e}{\partial x}}_V - \underbrace{\frac{m_e u_e \nu_c}{e}}_{VI}, \quad (1)$$



# Electron power absorption

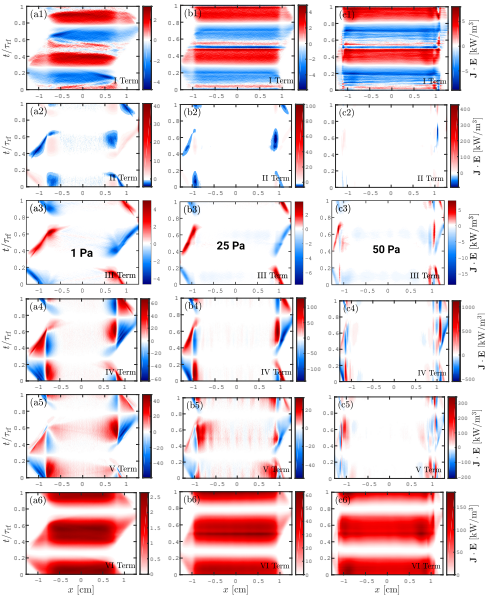
- The electron absorbed power can be determined as follows

$$\begin{aligned} J_e \cdot E = & \underbrace{m_e u_e n_e \frac{\partial u_e}{\partial t}}_{\text{I}} - \underbrace{m_e u_e^3 \frac{\partial n_e}{\partial x}}_{\text{II}} - \underbrace{m_e u_e^2 \frac{\partial n_e}{\partial t}}_{\text{III}} \\ & + \underbrace{e u_e T_e \frac{\partial n_e}{\partial x}}_{\text{IV}} + \underbrace{e n_e u_e \frac{\partial T_e}{\partial x}}_{\text{V}} + \underbrace{m_e n_e \nu_c u_e^2}_{\text{VI}} \end{aligned} \quad (2)$$

- Terms I and III – power absorption due to electron inertia
- Term II – the electron density gradient
- Term IV – ambipolar field – electron density gradient
- Term V – the electron temperature gradient
  - Terms IV and V are pressure or collisionless heating
- Term VI – electron neutral collisions or Ohmic heating



# Electron power absorption



- The spatio temporal behavior of the various terms that constitute the electron power absorption

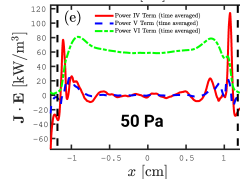
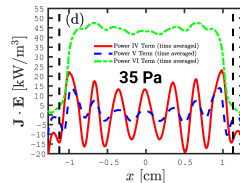
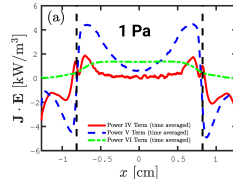
- Terms I and III – electron inertia
- Term I – electron density gradient
- Terms IV and V – pressure (collisionless) heating
- Term VI – Ohmic heating

Proto and Gudmundsson (2021) PSST 30(6) 065009

# Electron power absorption

- The time averaged electron power absorption profile of
  - term IV (red line)
  - term V (blue dashed line)
  - term VI (green dot dashed line)
- At 1 Pa the pressure terms and the Ohmic term contribute to the electron power absorption
- At higher pressures Ohmic power absorption dominates
- At 35 Pa striations are observed

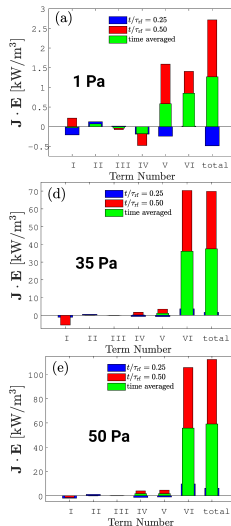
Proto and Gudmundsson (2021) PSST **30**(6) 065009



# Electron power absorption

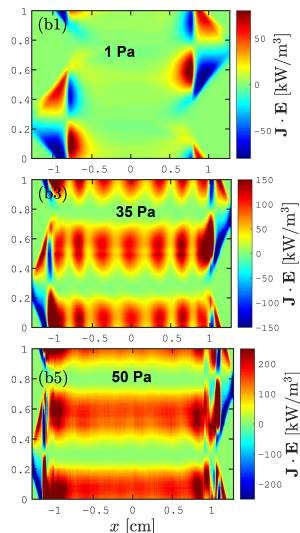
- The space averaged electron power absorption profile terms
  - $t/\tau_{rf} = 0.25$  blue bar
  - $t/\tau_{rf} = 0.50$  red bar
  - time averaged green bar
- At 1 Pa the pressure terms and the Ohmic term contribute to the electron power absorption
- At higher pressures Ohmic power absorption dominates

Proto and Gudmundsson (2021) PSST **30**(6) 065009



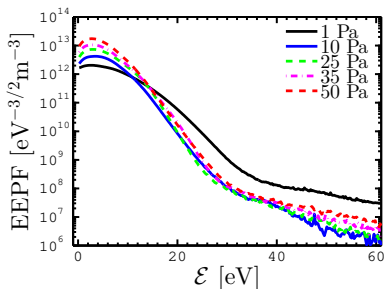
# Electron power absorption

- The spatio temporal behavior of the total electron power absorption  $\mathbf{J}_e \cdot \mathbf{E}$  over the full gap length for a capacitively coupled chlorine discharge
- At 1 Pa there is clear sign of drift ambipolar heating (DA-mode) and stochastic heating ( $\alpha$ -mode)
- At 35 and 50 Pa there are indications of striations in addition to drift ambipolar heating (DA-mode) and stochastic heating ( $\alpha$ -mode)



# *Electron power absorption*

- The electron energy probability function (EEPF) in the discharge center is Druyvesteyn like at all pressures
- This is expected when there is significant Ohmic heating in the plasma bulk





# Tailored voltage waveforms

Dual frequency voltage source

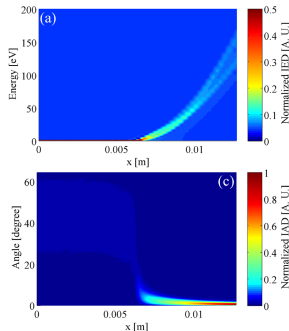
$$V(t) = \frac{V_0}{2} \sin(2\pi ft) + \frac{V_0}{2} \sin(4\pi ft + \theta)$$

gap = 2.54 cm,  $V_0 = 222$  V and  $f = 13.56$  MHz



# Tailored voltage waveforms

- By applying voltage at two or more frequencies, a fundamental frequency and its harmonics the ion bombarding energy can be controlled
- By adjusting the phase angle  $\theta$  between the fundamental and the second harmonic a dc self-bias voltage can be generated
- This gives separate control of the ion flux and ion energy in a capacitively coupled discharge
- Electrically asymmetric discharge is formed in otherwise a geometrically symmetric reactor

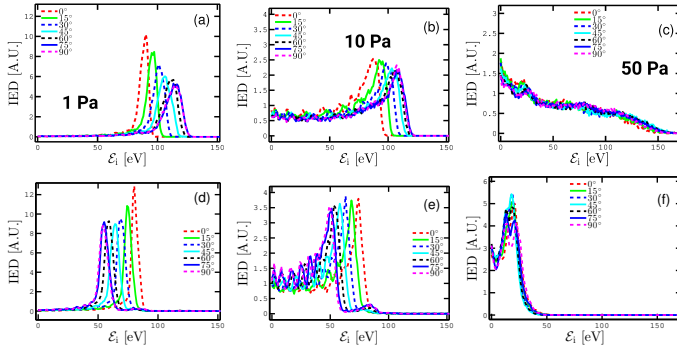


Huang and Gudmundsson (2014)

TPS 42(10) 2854



# Tailored voltage waveforms

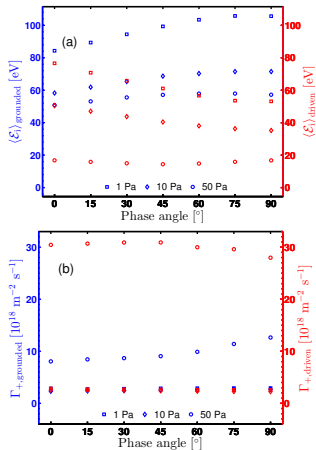


Skarphedinsson and Gudmundsson (2020) PSST **29**(8) 084004

- The IED for  $\text{Cl}_2^+$  ions bombarding the electrodes while varying the phase angle, between the fundamental and the second harmonic
- The grounded (upper row) and the driven (lower row) electrode

# Tailored voltage waveforms

- The mean ion energy bombarding both the electrodes is shown versus the phase angle  $\theta$
- At 1 and 10 Pa the mean ion energy on the grounded electrode increases by a factor of roughly 1.2 as the phase angle is increased from 0 to 90° – a narrow control range
- At 50 Pa the mean ion energy does not depend on the phase angle



# Summary



# Summary

- The chlorine discharge exhibits high electronegativity
- At the lowest pressure (1 Pa) the electron power absorption is due to both the pressure and the Ohmic terms and at higher pressure Ohmic terms dominate (drift-ambipolar (DA) mode)
- The electron power absorption increases in amplitude and the power absorption by the ions decreases with increased pressure
- The mean ion bombarding energy can be tuned nearly independently of the ion flux at 1 and 10 Pa through the electrical asymmetry effect, but the available control range is rather limited – At the highest pressure (50 Pa) it cannot be controlled



# References

The slides can be downloaded at

<http://langmuir.raunvis.hi.is/~tumi/plasma.html>

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