A particle-in-cell/Monte Carlo simulation of a 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

Outline

- The 1D particle-in-cell/Monte Carlo collision simulation
    - The chlorine discharge
- Comparison with measurements
- Capacitively Coupled Chlorine Discharge at 13.56 MHz – Voltage Source
- Capacitively Coupled Chlorine Discharge at 27.12 MHz – Current Source
- Capacitively Coupled Chlorine Discharge – dual frequency 27.12 MHz and 2 MHz – Current Source
- Summary

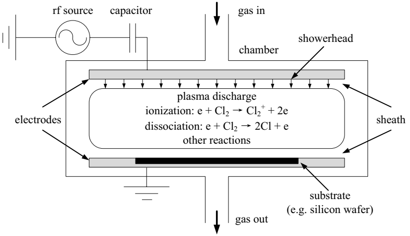
The 1D particle-in-cell/Monte Carlo collision simulation

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., *Plasma Sources Sci. Technol.*, **22** 035011 (2013)

The chlorine discharge



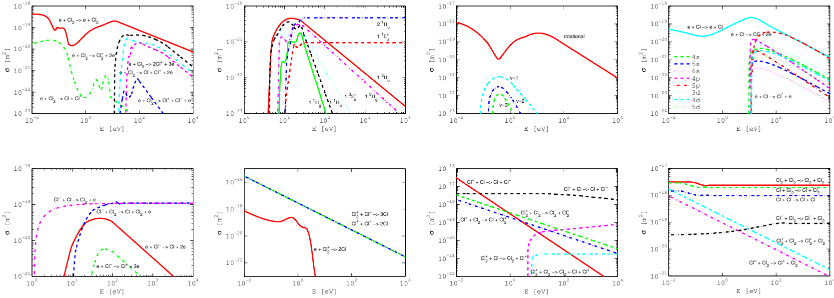
- We consider a discharge that consists of:
  - electrons
  - the ground state chlorine molecule $Cl_2(X\,^1\Sigma_g^+, v = 0)$,
  - the ground state chlorine atom Cl($3p^{5\,2}P$)
  - the negative chlorine ion Cl^-
  - the positive chlorine ions Cl^+ and Cl_2^+

The chlorine discharge

- In the chlorine discharge, the number of Cl atoms is much larger than the number of charged species
- Thus, we apply a global model[1] beforehand to calculate the fraction of Cl atoms under certain control parameters including the discharge pressure, absorbed power and the gap length between two electrodes
- The absorbed power found in the PIC/MCC simulation is used as an input parameter in the global model iteratively
- Both Cl_2 molecules and Cl atoms are treated as the initial background gas in the simulation

[1] Thorsteinsson and Gudmundsson, *Plasma Sources Sci. Technol.*, **19** 015001 (2010)

The chlorine discharge



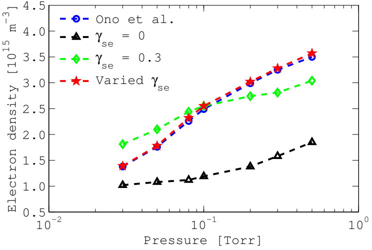
- The reaction set for the chlorine is comprehensive and includes 44 reactions

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

Comparison with experiments

Comparison with experiments

- Electron density versus discharge pressure (30 – 600 mTorr)
- Secondary electrons actually affect the electron density
- We allow the secondary electron emission coefficient, $\gamma_{\rm se}$, to vary from 0.15 to 0.45 in order to fit the simulation to the experimental values



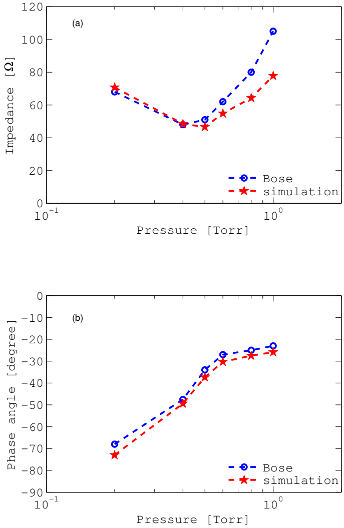
Ono et al., 1992, J. Vac. Sci. Technol. A, **10** 1071

Comparison with experiments

- Impedance and phase angle versus discharge pressure
- Secondary electrons have little influence
- The agreement with the measured data is excellent with only small discrepancy above 600 mTorr in the impedance

Bose, PhD Thesis, Swiss Federal Institute of Technology

Zurich, 1995



Capacitively Coupled Chlorine Discharge at 13.56 MHz

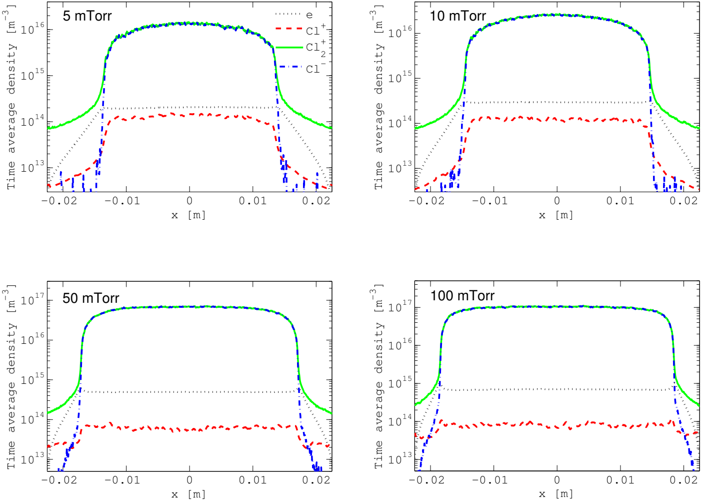
Capacitively Coupled Chlorine Discharge at 13.56 MHz

- We apply a voltage source with a single frequency

$$V(t) = V_{\mathrm{rf}} \sin(2\pi f t)$$

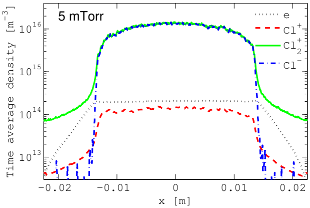
- The electrodes are circular with a diameter of 14.36 cm
- The gap between the electrodes is 4.5 cm
- We set V_{rf} = 222 V and f = 13.56 MHz
- The neutrals (Cl_2 and Cl) are treated as background gas at T_{g} = 300 K with a Maxwellian distribution
- The dissociation fraction is found using a global model
- The explored pressure range is 5 – 100 mTorr

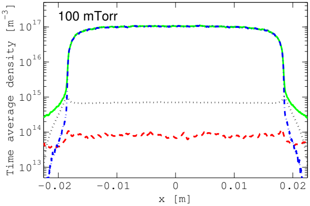
Capacitively Coupled Chlorine Discharge at 13.56 MHz



Capacitively Coupled Chlorine Discharge at 13.56 MHz

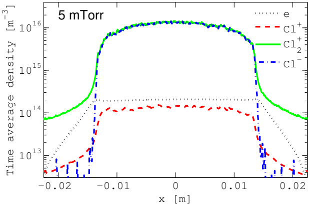
- At low pressures, the profile for Cl_2^+ ions is cosine-like or parabolic since Cl_2^+ ions are lost mainly due to diffusion to the walls
- As the pressure increases, the recombination between Cl_2^+ and Cl^- ions becomes the major loss mechanism for Cl_2^+ ions
- Thus, the density profile for Cl_2^+ and Cl^--ions becomes quite flat in the bulk region

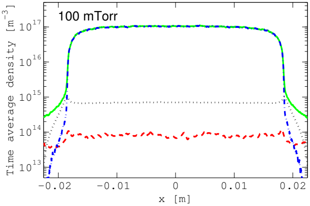




Capacitively Coupled Chlorine Discharge at 13.56 MHz

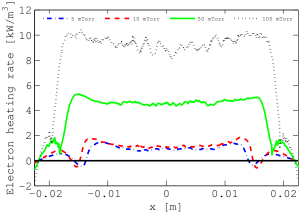
- The density profile for Cl^+-ions is very different from that for Cl_2^+-ions
- In the bulk region the density of Cl^+-ions is uniform at relatively low value
- In the sheath region the density of Cl^+-ions increases with increasing pressure – through non-resonant charge transfer

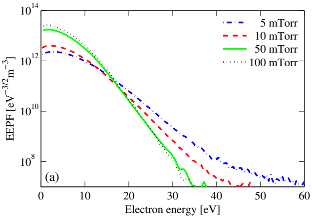




Capacitively Coupled Chlorine Discharge at 13.56 MHz

- At low pressures the power absorbed by the electrons is distributed in the bulk and sheath region through electron–neutral collisions and stochastic heating due to the oscillating sheath, respectively
- At high pressures the power absorbed by the electrons is mainly due to electron–neutral collisions in the bulk





Capacitively Coupled Chlorine Discharge at 27.12 MHz – Current Source

Capacitively Coupled Chlorine Discharge at 27.12 MHz

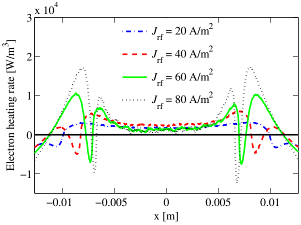
- We apply a current source with a single frequency

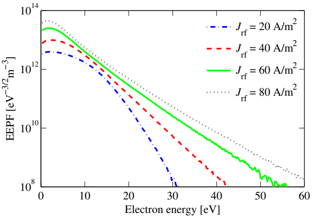
$$J(t) = J_{\mathrm{rf}} \sin(2\pi f t)$$

- The electrodes are circular with a diameter of 10.2 cm
- The gap between the electrodes is 2.54 cm
- We set J_{rf} = 20 – 80 A/m^2 and f = 27.12 MHz
- The neutrals (Cl_2 and Cl) are treated as background gas at T_{g} = 300 K with a Maxwellian distribution
- The dissociation fraction is found using a global model
- The pressure is 10 mTorr

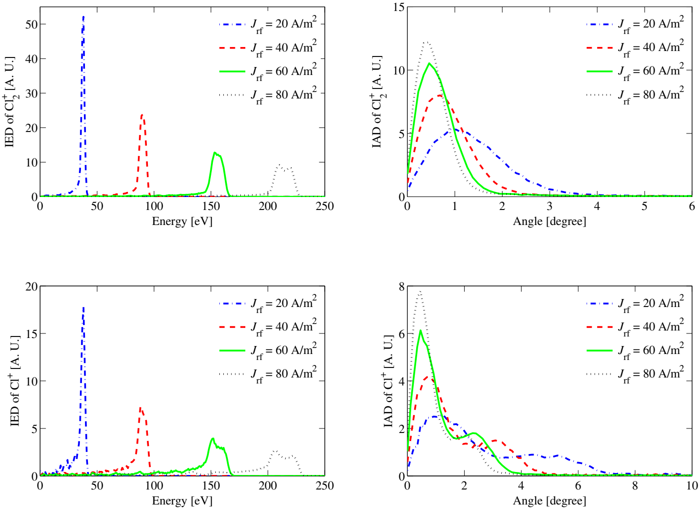
Capacitively Coupled Chlorine Discharge at 27.12 MHz

- Stochastic heating in the sheath becomes more prominent as the current increases
- The electron energy distribution function changes from Druyvesteyn to Maxwellian, and then to bi-Maxwellian as the current increases





Capacitively Coupled Chlorine Discharge at 27.12 MHz



Capacitively Coupled Chlorine Discharge – dual frequency 27.12 MHz and 2 MHz – Current Source

Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz

- We apply a current source that consists of two frequency components

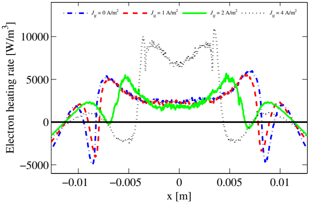
$$J(t) = J_{\mathrm{hf}} \sin(2\pi f_{\mathrm{hf}} t) + J_{\mathrm{lf}} \sin(2\pi f_{\mathrm{lf}} t)$$

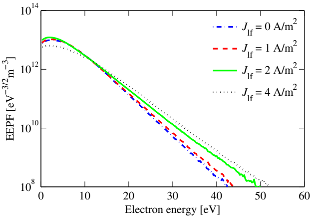
- The electrodes are circular with a diameter of 10.2 cm
- The gap between the electrodes is 2.54 cm
- We set J_{hf} = 40 A/m^2 and f = 27.12 MHz
- We set J_{lf} = 1 – 4 A/m^2 and f = 2 MHz
- The neutrals (Cl_2 and Cl) are treated as background gas at T_{g} = 300 K with a Maxwellian distribution
- The dissociation fraction is found using a global model
- The pressure is 10 mTorr

Huang and Gudmundsson, *Plasma Sources Sci. Technol.*, **23** 025015 (2014)

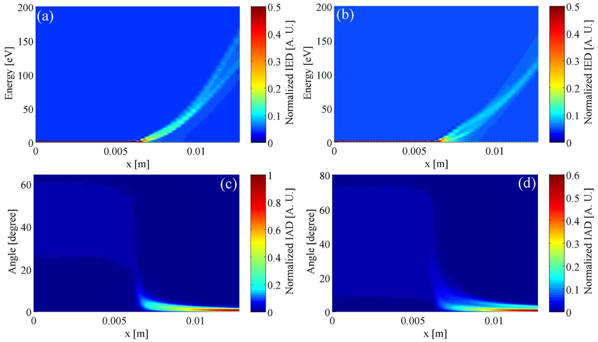
Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz

- As the low-frequency current increases, the heating in the bulk region first decreases slightly and then increases dramatically
- The number of low-energy electrons first increases and then decreases, while the number of the high-energy electrons increases steadily with increasing low frequency current





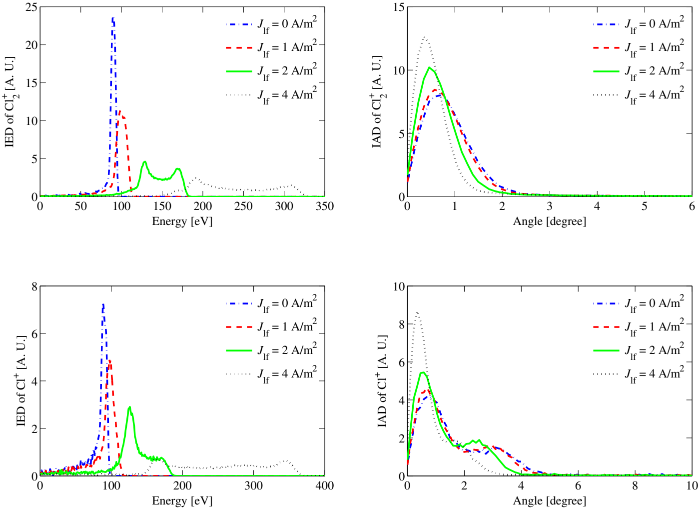
Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz



- As the ions reach the presheath–sheath boundary they are accelerated across the sheath towards the electrode
- The IEDs become wider and shift from single-peak to bimodal profile

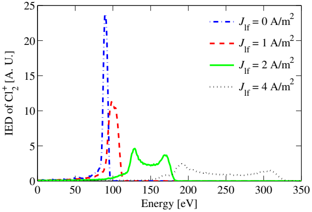
Huang and Gudmundsson, *IEEE Trans. Plasma Science*, accepted 2014

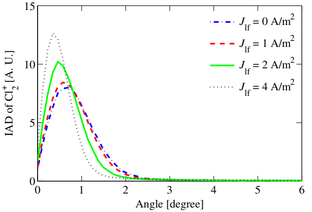
Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz



Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz

- The IED becomes wider and extends to the high-energy region with increasing low-frequency current
- The IAD is more concentrated in the small-angle region with increasing low-frequency current

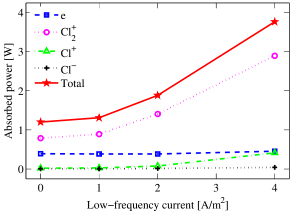


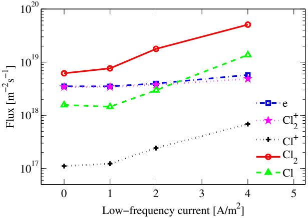


Huang and Gudmundsson, *Plasma Sources Sci. Technol.*, **23** 025015 (2014)

Capacitively Coupled Chlorine Discharge at 27.12 MHz + 2 MHz

- The average sheath potential drop increases with increased low frequency current and thus the absorbed power while the flux of charged particles remains roughly constant
- The flux of high energy (> 1 eV) neutrals and Cl^+ increases with increased low frequency current





Summary

- We demonstrated particle-in-cell/Monte Carlo collision simulation of a capcacitively coupled chlorine disharge
- Both chlorine atoms and Cl^+-ions are considered in the reaction set
- We explored voltage source driven discharge of single frequency and current source driven single and dual frequency discharges
- In a future work we will systematically explore the influence of the driving frequency and the driving current for both the high and low frequency source

References

The slides can be downloaded at

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

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