Electron power absorption in low pressure capacitively coupled discharges of complex chemistry

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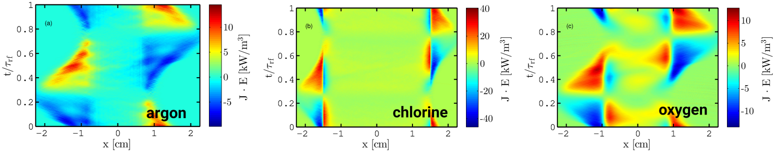
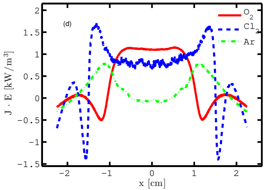
Introduction

- The capacitively coupled discharge is sustained by applying radio-frequency (rf) voltage or current between electrodes and a neutral gas at low pressure is injected between the electrodes
- A high-voltage sheath forms between the plasma bulk and the electrodes
- The two main electron power absorption mechanisms in these discharges are
  - Ohmic (or collisional) heating in the bulk and sheath regions
  - momentum transfer due to the moving sheaths which leads to stochastic (pressure or collisionless) heating
- We explore this for three different chemistries
  - electropositive argon discharge
  - weakly electronegative oxygen discharge
  - highly electronegative chlorine discharge.

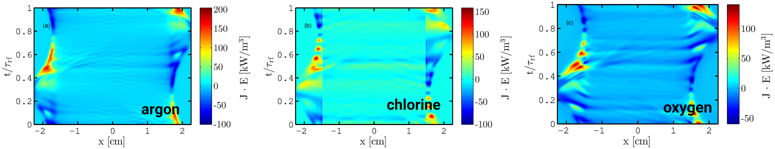
Introduction



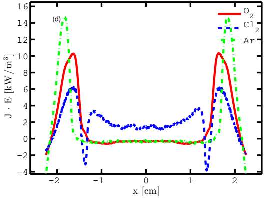


- The electron power absorption
  - p = 10 mTorr
  - f = 13.56 MHz
  - gap = 45 mm
  - γ_{see} = 0.0
- For argon the discharge is operated in α-mode
- Chlorine and oxygen discharges operate in hybrid α- and drift ambipolar (DA)-mode

Introduction



- The electron power absorption
  - p = 10 mTorr
  - f = 27.12 MHz
  - gap = 45 mm
  - γ_{see} = 0.0
- The argon and oxygen discharges are operated in α-mode
- The chlorine discharge operated in hybrid α- and drift ambipolar (DA)-mode



The oxygen discharge

Introduction

- Oxygen forms a weakly electronegative discharge
- The oxygen chemistry is rather involved, in particular due to the presence of **metastable molecular and atomic** oxygen and their role in dissociative attachment and detachment processes
- We use the 1d3v `oopd1` (objective oriented plasma device for one dimension) **particle-in-cell Monte Carlo collision** code to simulate the discharge

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

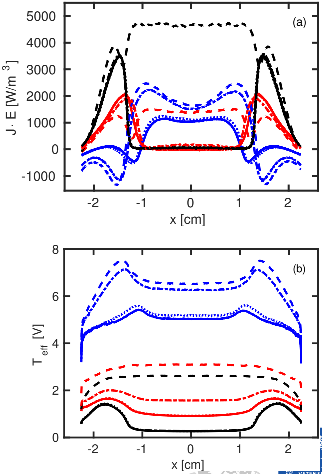
The oxygen discharge

- We consider a discharge that consists of:
  - electrons
  - the ground state oxygen molecule $O_2(X^3\Sigma_g^-)$
  - the metastable oxygen molecule $O_2(a^1\Delta_g)$
  - the metastable oxygen molecule $O_2(b^1\Sigma_g)$
  - the ground state oxygen atom $O(^3P)$
  - the metastable oxygen atom $O(^1D)$
  - the negative oxygen ion O^-
  - the positive oxygen ions O^+ and O_2^+
- The discharge model includes energy dependent secondary electron emission yield
- We apply a global model[1] beforehand to calculate the partial pressure of the various neutrals

[1] Thorsteinsson and Gudmundsson, *Plasma Sources Sci. Technol.*, **19** 055008 (2010)

Oxygen CCP – pressure dependence

- The negative ion density decreases as the metastables $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g)$ are added to the discharge model
- The electron power absorption in the plasma bulk drops to zero at the higher pressures
- The effective electron temperature profile changes significantly when detachment by singlet metastables is added to the reaction set
- **10 mTorr**, **50 mTorr** and **200 mTorr**

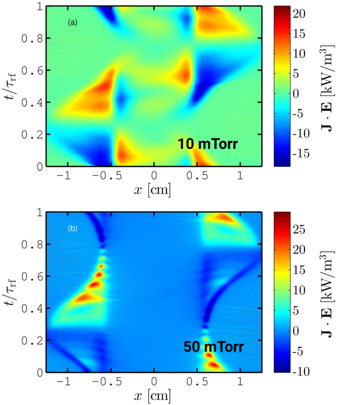


Gudmundsson and Hannesdottir, AIP Conf. Proc. **1811** 120001 (2017)

Gudmundsson and Lieberman (2015) PSST **24** 035016

Oxygen CCP – pressure dependence

- A parallel plate capacitively coupled oxygen discharge at driving frequency of 13.56 MHz for gap separation of 45 mm
- The spatio-temporal electron heating $\mathbf{J}_\mathrm{e} \cdot \mathbf{E}$ at 10 and 50 mTorr
- At 10 mTorr there is a significant electron heating within the electronegative core
- At 50 mTorr the electron heating occurs almost solely in the sheath region



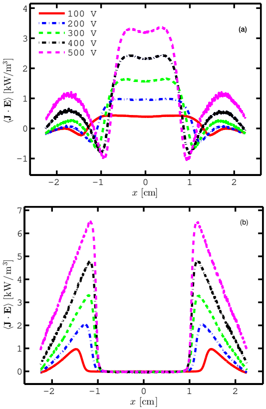
Gudmundsson and Snorrason (2017) JAP **122** 193302

Hannesdottir and Gudmundsson (2016) PSST, **25** 055002

Gudmundsson and Ventéjou (2015) JAP **118** 153302

Oxygen CCP – pressure dependence

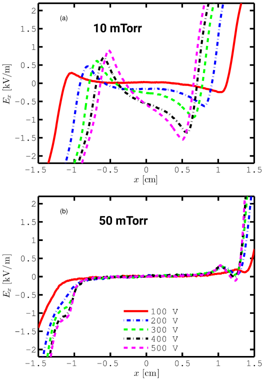
- The time averaged electron heating $\langle \mathbf{J}_e \cdot \mathbf{E} \rangle$ at 10 and 50 mTorr
- At 10 mTorr there is significant electron heating within the electronegative core
- At 50 mTorr, the heating rate in the electronegative core is roughly zero, and electron heating is almost entirely located in the sheath regions



Gudmundsson and Snorrason (2017) JAP **122** 193302

Oxygen CCP – pressure dependence

- The axial electric field at $t/\tau_{\mathrm{rf}} = 0.5$ for both 10 and 50 mTorr
- At 10 mTorr there is a significant electric field strength within the electronegative core while at 50 mTorr it is zero
- This strong electric field within the plasma bulk (the electronegative core) indicates a drift-ambipolar (DA) heating mode
- The electronegativity is significantly higher when operating at 10 mTorr $\alpha > 20$ than when operating at 50 mTorr $\alpha < 0.1$



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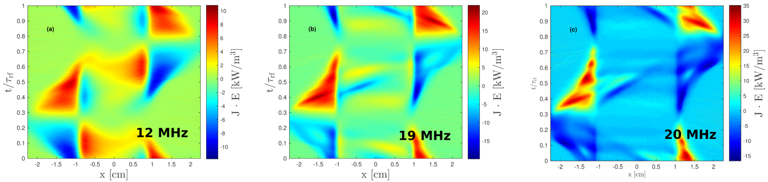
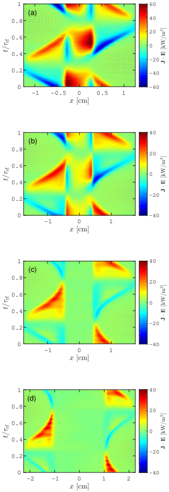
Oxygen CCP – frequency dependence



- At 12 MHz significant heating is observed in the plasma bulk but also in the sheath region
- At 19 MHz the heating and cooling in the sheath regions has increased, however there is contribution to the electron heating in the bulk region (note the change in scale)
- At 20 MHz there is almost no electron heating in the plasma bulk

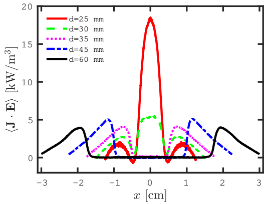
Oxygen CCP – electrode spacing

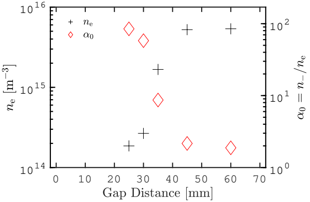
- A parallel plate capacitively coupled oxygen discharge at 50 mTorr driven by a 400 V voltage source at 13.56 MHz as the gap separation is varied
- At small electrode spacing a combination of stochastic (α-mode) and drift ambipolar (DA) heating in the bulk plasma (the electronegative core) is observed
- The DA-mode dominates the time averaged electron heating
- As the electrode spacing is increased, the heating mode transitions into a pure α-mode



Oxygen CCP – electrode spacing

- The time averaged electron power absorption $\langle \mathbf{J}_\mathrm{e} \cdot \mathbf{E} \rangle$
- The electron density in the discharge center (left *y* axis) and the electronegativity in the discharge center (right *y* axis) as a function of the gap separation
- The heating mode transition coincides with a sharp decrease in electronegativity
- This agrees with recent experimental findings of You et al. (2019)





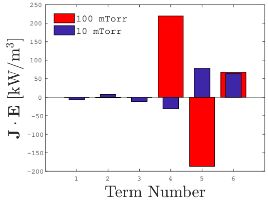
Gudmundsson and Proto (2019) PSST **28** 045012

Oxygen CCP – Bolzmann term analysis

- To explore the electron power absorption processes we apply Boltzmann term analysis Schulze et al. (2018) PSST **27** 055010

$$E = \underbrace{\underbrace{-\frac{m_e}{e}\frac{\partial u_e}{\partial t}}_{\text{I}} + \underbrace{\frac{m_e}{e}\frac{u_e^2}{n_e}\frac{\partial n_e}{\partial x}}_{\text{II}} + \underbrace{\frac{m_e}{e}\frac{u_e}{n_e}\frac{\partial n_e}{\partial t}}_{\text{III}}}_{\text{inertia}} \underbrace{- \underbrace{\frac{T_e}{n_e}\frac{\partial n_e}{\partial x}}_{\text{IV}} - \underbrace{\frac{\partial T_e}{\partial x}}_{\text{V}}}_{\text{pressure}} \underbrace{- \underbrace{\frac{m_e u_e \nu_c}{e}}_{\text{VI}}}_{\text{Ohmic}}$$

- The pressure terms are important
- The Terms IV (ambipoar) and V (electron temperature gradient) flip signs and are sharply smaller in the absolute value at 10 mTorr
- The Ohmic term's magnitude (Term VI) is similar at both pressure



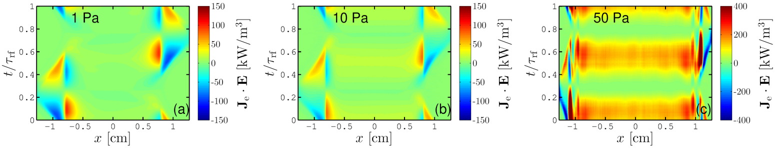
Proto and Gudmundsson (2020) JAP **128** 113302

The chlorine discharge

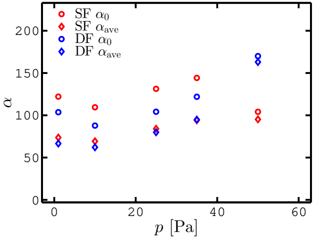
Chlorine CCP

- 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
- 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 $Cl(3p^5\,^2P)$
  - the negative chlorine ion Cl^-
  - the positive chlorine ions Cl^+ and Cl_2^+

Chlorine CCP

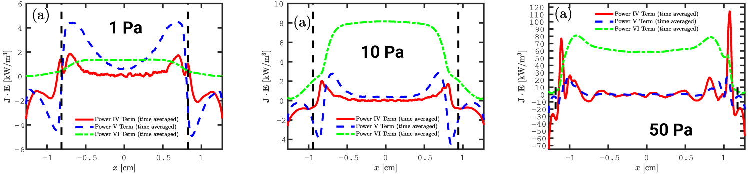


- There is significant electron power absorption (red and yellow areas) and smaller power loss (dark blue areas) evident within the plasma bulk
- This indicates that the electron power absorption occurs predominantly through DA electron power absorption

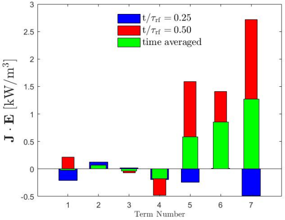


Skarphedinsson and Gudmundsson (2020) PSST **29** 084004

Chlorine CCP



- The Ohmic term has the largest contribution to electron power absorption at 1Pa
- All the terms contribute to the electron power absorption
- The time averaged terms IV (ambipolar) and V (electron temperature gradient) have opposite signs



Summary

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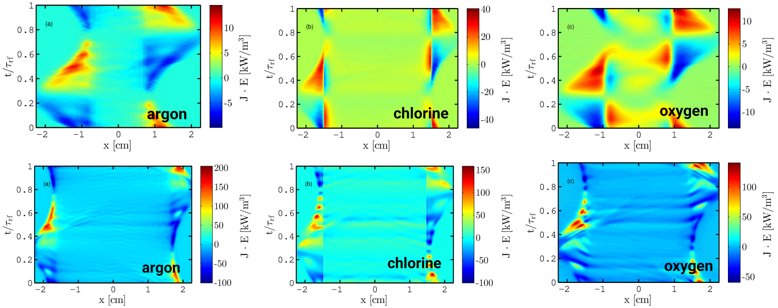
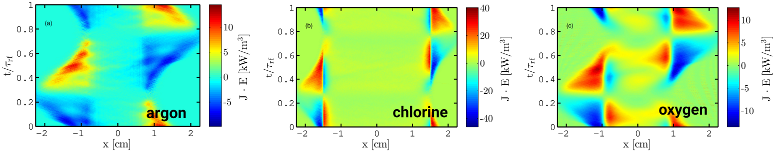


- Capcacitively coupled argon, oxygen and chlorine discharges were studied by particle-in-cell/Monte Carlo collision simulations

Summary



- In a chlorine discharge DA electron power absorption dominates and becomes increasingly more Ohmic with increased pressure
- Including the detachment processes by the singlet metastable states has a strong influence on the electronegativity in the oxygen discharge
- A heating mode transition, from hybrid drift-ambipolar (DA) and α-mode to pure α-mode, is observed as the pressure, driving frequency, or electrode gap spacing are increased, or the quenching coefficient of the oxygen metastable $O_2(a^1\Delta_g)$ is varied

Acknowledgements

Thank you for your attention

The slides can be downloaded at
`http://langmuir.raunvis.hi.is/~tumi/ranns.html`

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