On electron heating mode transitions in low pressure capacitively coupled oxygen discharge

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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)

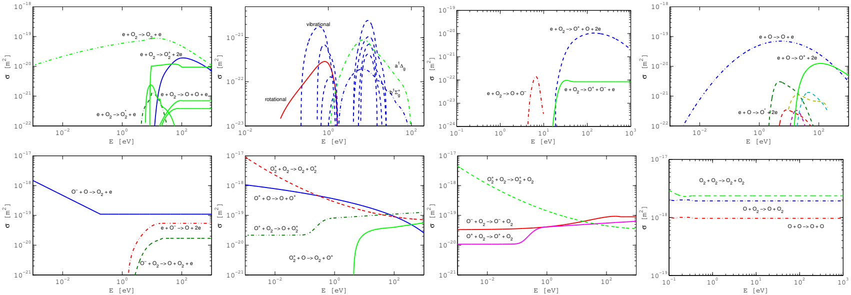
The oxygen discharge

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)

The oxygen discharge



- The reaction set for the oxygen is comprehensive and for this study includes up to 67 reactions

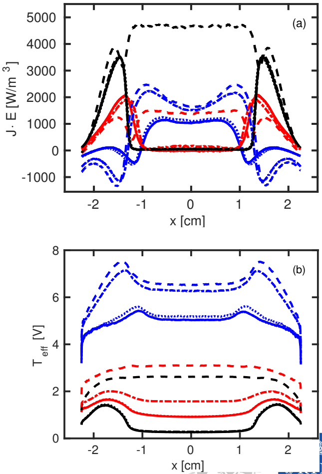
Gudmundsson et al., *Plasma Sources Sci. Technol.*, **22** 035011 (2013)

Gudmundsson and Lieberman, *Plasma Sources Sci. Technol.*, **24** 035016 (2015)

Hannesdottir and Gudmundsson, *Plasma Sources Sci. Technol.*, **25** 055002 (2016)

Oxygen CCP – pressure dependence

- The number of cold electrons increases and 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 heating in the 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) *Plasma Sources Sci. Technol.*

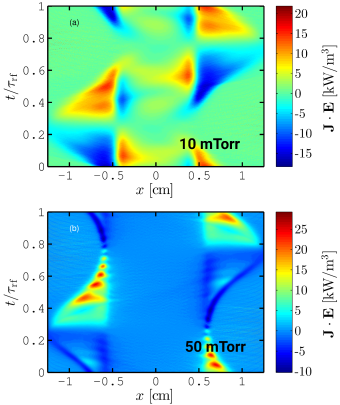
Capacitively Coupled Oxygen Discharge single frequency at 13.56 MHz

– pressure dependence –

including $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$ and $\gamma_{\rm see}(E)$

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 $\mathbf{J}_e \cdot \mathbf{E}$ 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



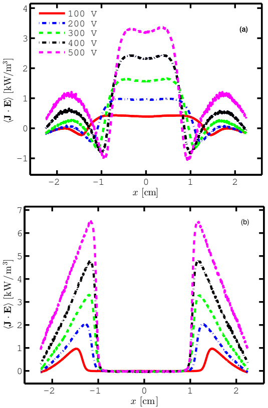
Gudmundsson and Snorrason (2017) JAP **122** 193302

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

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

Oxygen CCP – pressure dependence

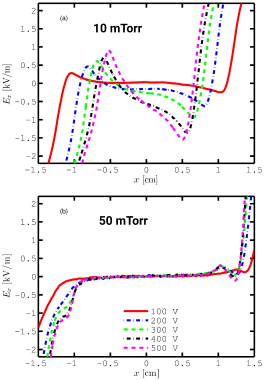
- The time averaged electron heating $\langle \mathbf{J}_\mathrm{e} \cdot \mathbf{E} \rangle$ at 10 and 50 mTorr
- At 10 mTorr there is significant electron heating within the electronegative core
- At 50 mTorr, the heating rate in the electronegative core is roughly zero, and electron heating is almost 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 $\alpha < 0.1$



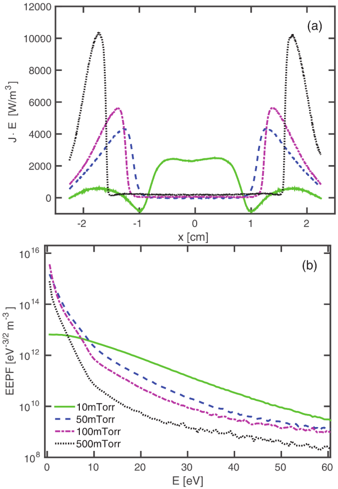
Gudmundsson and Snorrason (2017) JAP **122** 193302

Oxygen CCP – pressure dependence

- At low pressure the EEPF curves outwards, the population of low energy electrons is relatively low
- As the pressure is increased the number of low energy electrons increases and the number of higher energy electrons (> 10 eV) decreases
- Thus the EEPF curves outwards or becomes bi-Maxwellian as the pressure is increased

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

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

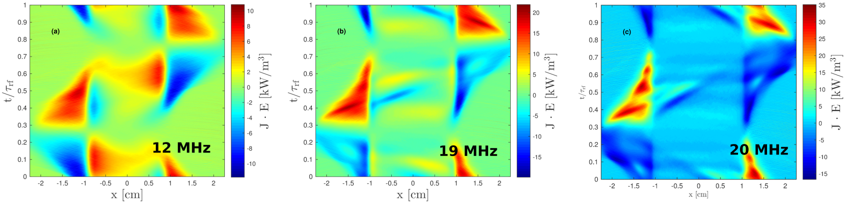


Capacitively Coupled Oxygen Discharge single frequency at 10 mTorr

– driving frequency dependence –

including $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$ and $\gamma_{\rm see}(E)$

Oxygen CCP – frequency dependence

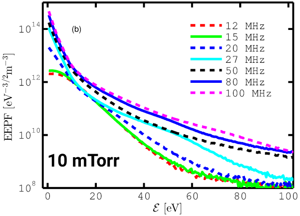


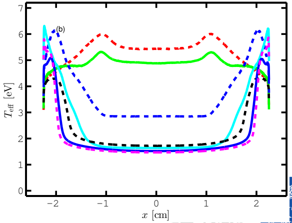
- At 12 MHz significant heating is observed in the plasma bulk but also in the sheath region
- At 19 MHz the heating and cooling in the sheath regions has increased, however there is contribution to the electron heating in the bulk region (note the change in scale)
- At 20 MHz there is almost no electron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

Oxygen CCP – frequency dependence

- At low driving frequency the EEPF is curves outwards, the population of low energy electrons is relatively low
- The EEPF curves outwards for driving frequency up to 15 MHz and has transitioned to bi-Maxwellian shape at 20 MHz
- Increasing the driving frequency enhances the high energy tail as the number of high energy electrons increases

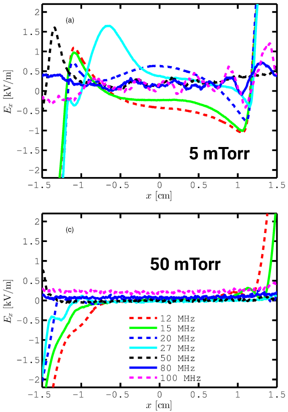
Gudmundsson et al. (2018) *Plasma Sources Sci. Technol.* **27** 025009





Oxygen CCP – frequency dependence

- The electric field profile at $t/\tau_{rf} = 0.5$ for discharges operated at 5 and 50 mTorr
- We see a significant electric field strength within the electronegative core at low driving frequency and low pressure
- The strong electric field within the plasma bulk (the electronegative core), at low pressure and low driving frequency, indicates a drift-ambipolar (DA) heating mode



Gudmundsson et al. (2018) PSST **27** 025009

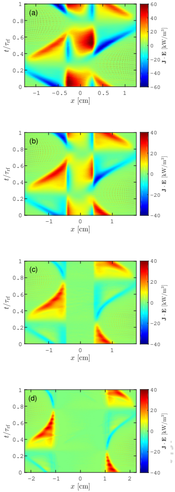
Capacitively Coupled Oxygen Discharge

– electrode spacing –

including $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$ and $\gamma_{\rm see}(E)$

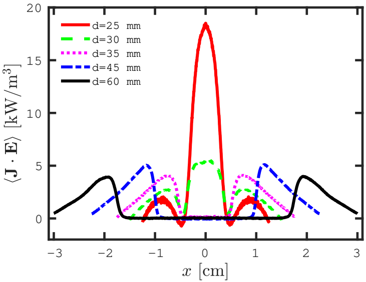
Oxygen CCP – electrode spacing

- 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

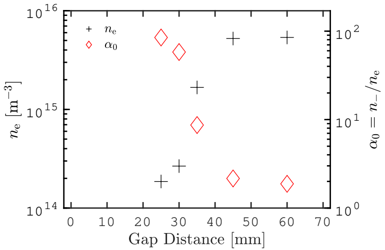
- The time averaged electron power absorption $\langle \mathbf{J}_\mathrm{e} \cdot \mathbf{E} \rangle$
- For 25 mm almost all the electron heating occurs in the plasma bulk (the electronegative core).
- As the electrode spacing is increased the electron heating in the bulk region decreases and the heating in the sheath regions increases



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

Oxygen CCP – electrode spacing

- 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)



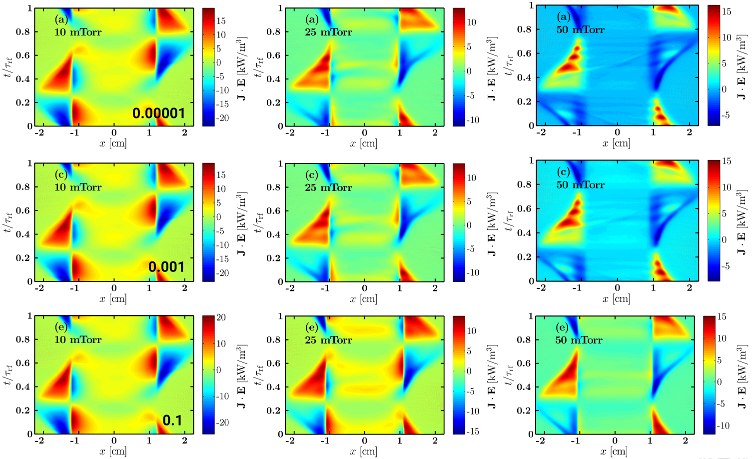
Gudmundsson and Proto (2019) PSST **28** 045012

Capacitively Coupled Oxygen Discharge

– surface quenching of $O_2(a^1\Delta_g)$ –

including $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$ and $\gamma_{\rm see}(E)$

Oxygen CCP – surface quenching of $O_2(a^1\Delta_g)$

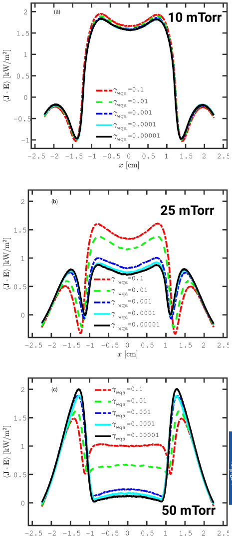


Proto and Gudmundsson (2018) *Plasma Sources Sci. Technol.* **27** 074002

Oxygen CCP – surface quenching of $O_2(a^1\Delta_g)$

- At 10 mTorr almost all the electron heating occurs in the plasma bulk (the electronegative core) and the electron heating profile is independent of the surface quenching coefficient
- At 50 mTorr only for the highest surface quenching coefficients 0.1 and 0.01 there is some electron heating observed in the bulk region
- Typical value is 0.007 for iron (Sharpless and Slanger, 1989)

Proto and Gudmundsson (2018) *Plasma Sources Sci. Technol.* **27** 074002



Summary

Summary

- We demonstrated particle-in-cell/Monte Carlo collision simulation of a capcacitively coupled disharge
- Including the detachment processes by the singlet metastable states has a strong influence on the effective electron temperature and electronegativity in the oxygen discharge
- At low pressure the discharge is operated in a combined drift-ambipolar (DA) and α-mode, and at higher pressure it is operated in the pure α-mode
- A heating mode transition is observed as the driving frequency, electrode gap spacing or surface quencing coefficient of the oxygen metastable $O_2(a^1\Delta_g)$ is varied

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Thank you for your attention

The slides can be downloaded at

`http://langmuir.raunvis.hi.is/~tumi/ranns.html`

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