The effect of pressure and driving frequency on electron heating in a capacitively coupled oxygen discharge

J. T. Gudmundsson^{1,2}, D. I. Snorrason¹, and H. Hannesdottir¹

¹Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

² Department of Space and Plasma Physics, KTH–Royal Institute of Technology, Stockholm SE-100 44, Sweden





Abstract

The oopd1 particle-in-cell Monte Carlo collision (PIC/MCC) code is used to simulate a capacitively coupled discharge in oxygen. At low driving frequency and low pressure (5 and 10 mTorr) a combination of stochastic (α -mode) and drift ambipolar (DA) heating in the bulk plasma (the electronegative core) is observed and the DA-mode dominates the time averaged electron heating. As the driving frequency or pressure are increased the heating mode transitions into a pure α -mode, where sheath heating dominates.

Introduction

The oxygen discharge is of vital importance in various materials processing applications such as ashing of photoresist, etching of polymer films and oxidation and deposition of thin film oxides.

Oxygen is a weakly electronegative gas and the presence of negative ions has a strong influence on the kinetics and dynamics of the oxygen discharge.

The oxygen chemistry is rather involved, in particular due to the presence of metastable molecular and atomic oxygen and detachment processes.

Description of the simulation

The oxygen model includes, in addition to electrons, the oxygen molecule in the ground state, the oxygen atom in the ground state, the negative ion O^- , the positive ions O^+ and O_2^+ , and the metastable states $O(^1D)$, $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g)$. The reaction set and cross sections included in the oopd1 code are discussed in the earlier work [1, 2, 3].

For this study we assume the discharge to be operated at a single frequency in the range 12 - 100 MHz.

The simulation grid is uniform and consists of 1000 cells. The electron time step varies with driving frequency from 4.17×10^{-11} s at 12 MHz, 1×10^{-11} s at 50 MHz, to 5×10^{-12} s at 100 MHz according to the stability criterion. The simulation is run for 5500 rf cycles for each case.

Results and discussion

Figure 1 shows the spatio-temporal behavior of the electron power absorption $\mathbf{J}_e \cdot \mathbf{E}$, where \mathbf{J}_e and \mathbf{E} are the spatially and temporally varying electron current density and electric field, respectively.

The most significant heating is observed in the sheath region, during sheath expansion, and the most significant cooling is observed during the sheath collapse.

A significant energy gain (red and yellow areas) and small energy loss (dark blue areas) are evident in the plasma bulk region at 12 - 19 MHz as seen in Figures 1 (a) – (d).

At 20 MHz the electron heating rate in the sheath region has increased and there is almost no electron heating in the plasma bulk as seen in Figure 1 (e). At higher driving frequencies the electron heating is observed only in the sheath region.

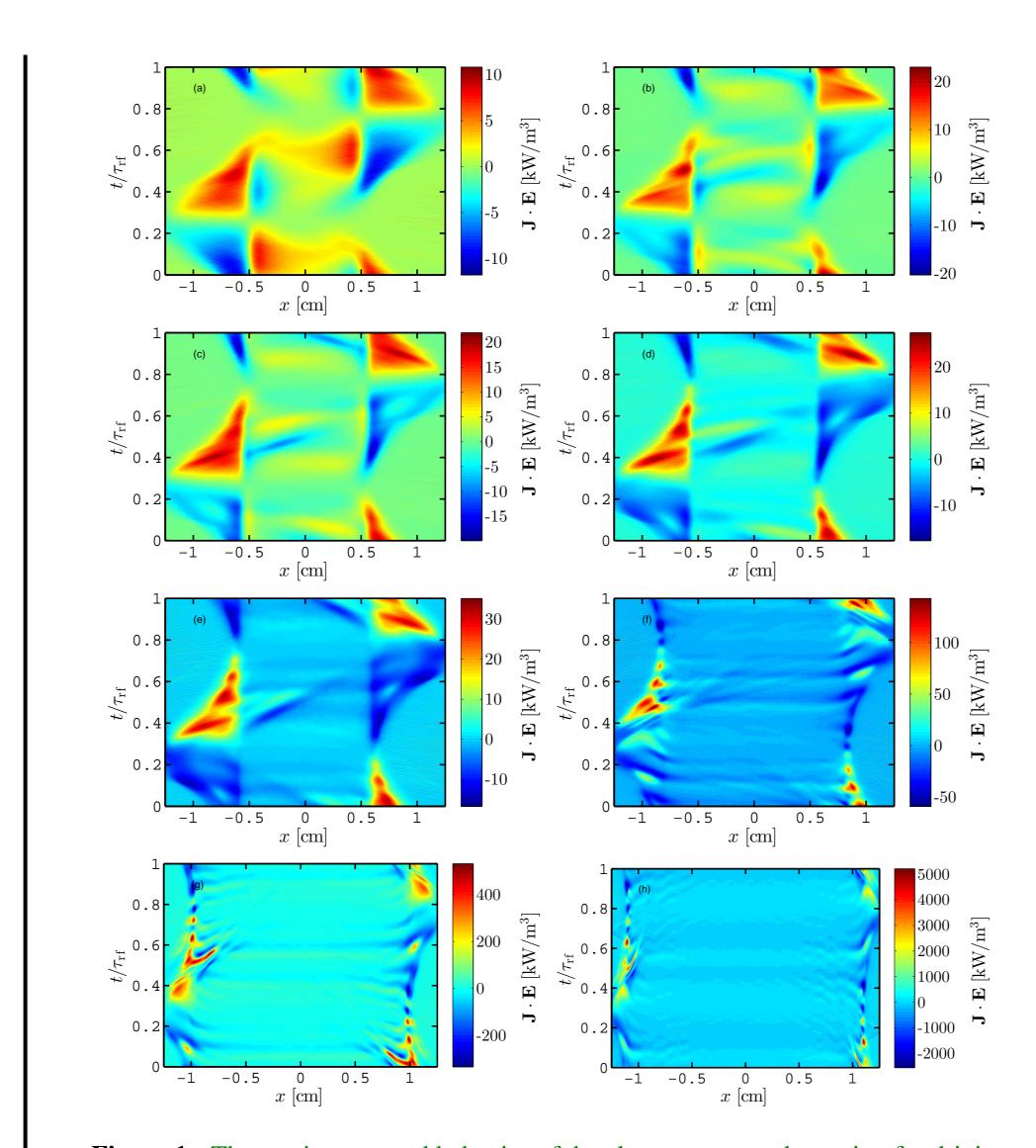


Figure 1: The spatio-temporal behavior of the electron power absorption for driving frequency (a) 12 MHz, (b) 18 MHz, (c) 19 MHz, (d) 19.5 MHz, (c) 20 MHz, (d) 27.12 MHz, (e) 50 MHz, and (f) 100 MHz, for a parallel plate capacitively coupled oxygen discharge at 10 mTorr with a gap separation of 4.5 cm driven by a 222 V voltage source.

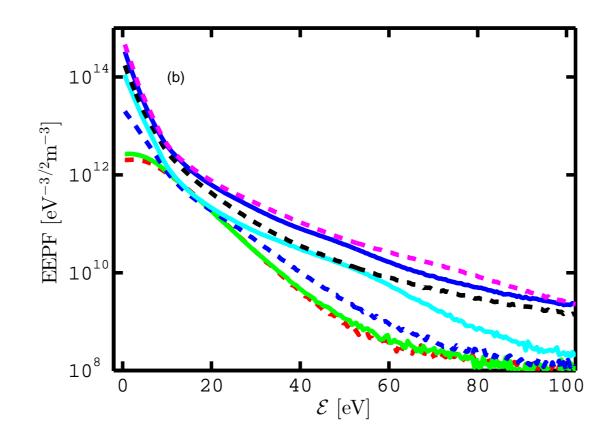


Figure 2: The electron energy probability function (EEPF) in the center of a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm driven by a 222 V voltage source at 13.56 MHz.

At low pressure and low driving frequency the EEPF is concave.

As the driving frequency is increased the number of low energy electrons increases and the number of higher energy electrons (> 10 eV) decreases. At high driving frequency the EEPF develops a convex shape or becomes bi-Maxwellian as seen in figure 2.

The spatio-temporal plots of the effective electron temperature are shown in Figure 3. The effective electron temperature is given as $T_{\rm eff} = (2/3)\langle \mathcal{E} \rangle$ where $\langle \mathcal{E} \rangle$ is the average electron energy.

We note that the effective electron temperature is high within the plasma bulk for driving frequency up to 19.5 MHz (Figures 3 (a) – (d)). This high effective electron temperature coincides with high electron power absorption within the bulk as seen in Figures 1 (a) – (d).

At 27.12 MHz (see Figure 3 (f)) the effective electron temperature has dropped below 1 eV within the plasma bulk and high effective electron temperature is only observed at the expanding sheath edge. For driving frequency of 27.12 MHz and above the electron heating demontrates a pure α -mode.

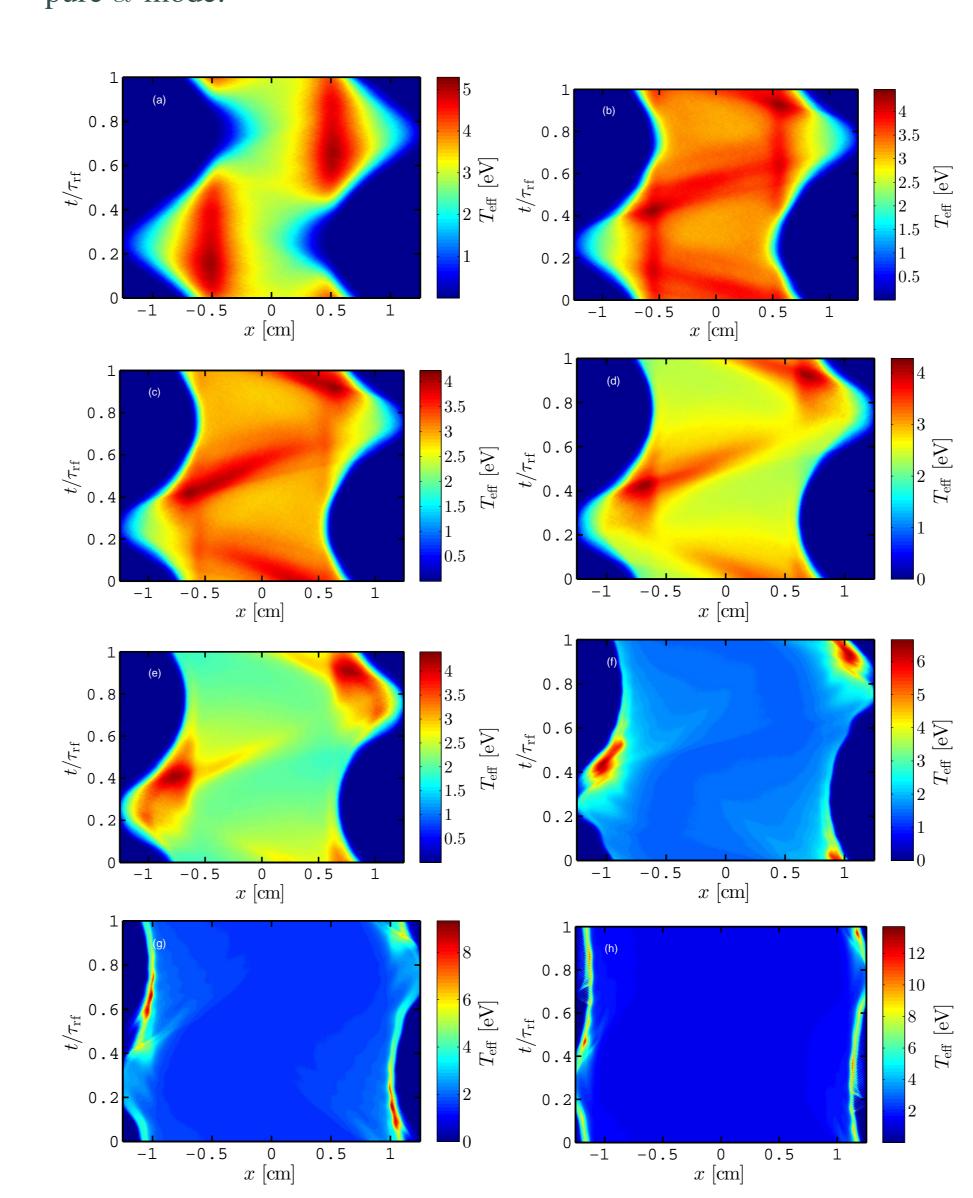


Figure 3: The spatio-temporal behavior of the effective electron temperature for driving frequency (a) 12 MHz, (b) 18 MHz, (c) 19 MHz, (d) 19.5 MHz, (e) 20 MHz, (f) 27.12 MHz, (g) 50 MHz, and (h) 100 MHz, for a parallel plate capacitively coupled oxygen discharge at 10 mTorr with a gap separation of 4.5 cm driven by a 222 V voltage source.

Figure 4 shows the center electronegativity $\alpha_0 = n_{-0}/n_{\rm e0}$, where n_{-0} is the center negative ion density and $n_{\rm e0}$ is the center electron density versus the driving frequency. We see that at 5 and 10 mTorr the electronegativity decreases with increasing driving frequency.

We also demonstrate that the electron heating within the plasma bulk coincides with high electric field within the plasma bulk and high elec-

tronegativity of the discharge and thus conclude it is drift-ambipolar (DA) heating [4].

When the discharge is operated at 5 and 10 mTorr and low driving frequency, the electron heating consists of stochastic heating in the sheath region and DA-heating within the electronegative core.

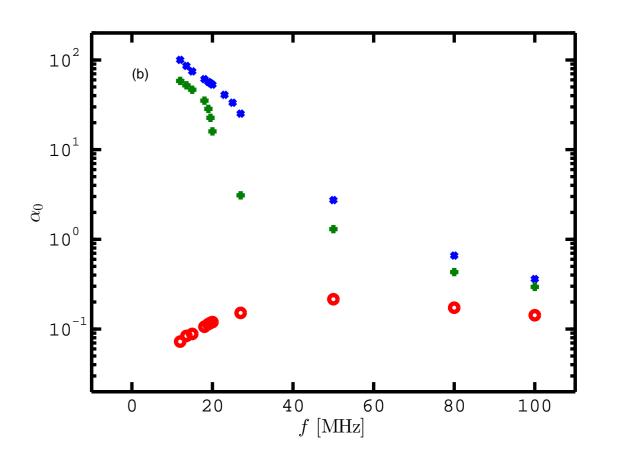


Figure 4: The center electronegativity as a function of the driving frequency for a parallel plate capacitively coupled oxygen discharge with a gap separation of 4.5 cm driven by a 222 V voltage source.

Conclusions

- At low driving frequency and low pressure (5 and 10 mTorr) a combination of stochastic (α -mode) and drift ambipolar (DA) heating in the bulk plasma (the electronegative core) is observed and the DA-mode dominates the time averaged electron heating.
- As the driving frequency or pressure are increased the heating mode transitions into a pure α -mode, where electron heating in the sheath region dominates. At low pressure (5 and 10 mTorr) this transition coincides with a sharp decrease in electronegativity.

References

- [1] J T Gudmundsson, E Kawamura, and M A Lieberman. A benchmark study of a capacitively coupled oxygen discharge of the oopd1 particle-in-cell Monte Carlo code. *Plasma Sources Science and Technology*, 22(3) 035011, 2013.
- [2] J T Gudmundsson and M A Lieberman. On the role of metastables in capacitively coupled oxygen discharges. *Plasma Sources Science and Technology*, 24(3) 035016, 2015.
- [3] H. Hannesdottir and J. T. Gudmundsson. The role of the metastable $O_2(b^{-1}\Sigma_g^+)$ and energy-dependent secondary electron emission yields in capacitively coupled oxygen discharges. *Plasma Sources Science and Technology*, 25(5):055002, 2016.
- [4] J. Schulze, A. Derzsi, K. Dittmann, T. Hemke, J. Meichsner, and Z. Donkó. Ionization by Drift and Ambipolar Electric Fields in Electronegative Capacitive Radio Frequency Plasmas. *Physical Review Letters*, 107(27) 275001, 2011.