Simulation of a capacitively coupled oxygen discharge using the oopd1 particle-in-cell Monte Carlo code

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Introduction

- The oopd1 particle-in-cell Monte Carlo (PIC-MC) code is used to simulate a capacitively coupled discharge in oxygen
- oopd1 is a one-dimensional object-oriented PIC-MC code in which the model system has one spatial dimension and three velocity components
- It contains models for planar, cylindrical, and spherical geometries and replaces the xpdx1 series
- 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
- The oxygen chemistry is rather involved, in particular due to the presence of metastable molecular oxygen
- Global model studies indicate that at low pressure ($\leq$ 10 mTorr) and in particular at higher absorbed power the discharge is highly dissociated and oxygen atoms dominate the discharge and the O^+-ion is the dominating charged particle (Gudmundsson and Lieberman, 1998; Gudmundsson et al., 2001)
- Electron impact detachment and ion-ion neutralization dominate the loss of negative ions at low pressure, while detachment by oxygen atoms dominates at higher pressures ($\geq$ 20 mTorr)

The oxygen reaction set

- The revised oxygen model includes, in addition to electrons, the oxygen molecule in ground state, the oxygen atom in ground state, the negative ion O^-, and the positive ions O^+ and O_2^+
- We make a comparison of the new oopd1 code to the well known xpdp1 code which has a limited reaction set that includes, in addition to electrons, the oxygen molecule in ground state, the negative ion O^-, and the positive ion O_2^+
- The cross sections for the collisions among the oxygen species have been significantly revised from the xpdp1 code (Vahedi and Surendra, 1995)

Results and discussion

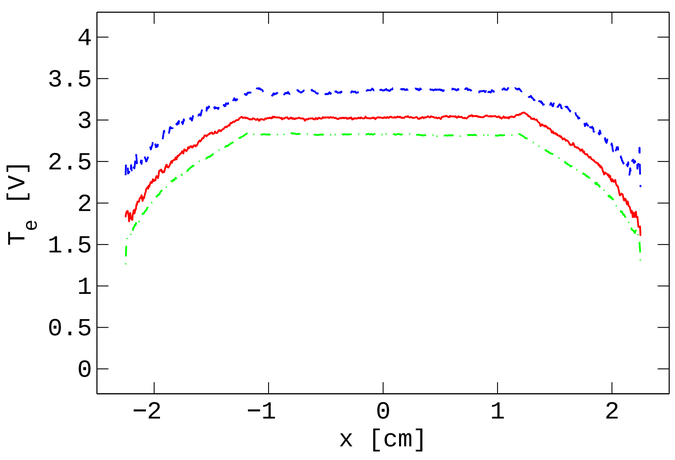

Figure 1: The electron temperature profile for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm by a 222 V voltage source at 13.56 MHz.

- We assume a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm
- The discharge is driven by a 222 V voltage source at 13.56 MHz
- These are the same parameters as explored in Lichtenberg et al. (1994) using the xpdp1 code which then was driven by an rf current source of 0.4 A
- We explore three cases
  - Case 1: xpdp1
  - Case 2: oopd1 using the xpdp1 cross section set
  - Case 3: oopd1 using the full revised oopd1 cross section set

electron impact O_2

$e + O_2 \longrightarrow O_2 + e$	elastic scattering	x
$e + O_2(r=0) \longrightarrow e + O_2(r>0)$	rotational excitation	x
$e + O_2(v=0) \longrightarrow e + O_2(v>0)$	vibrational excitation	x
$e + O_2 \longrightarrow e + O_2(a^1\Delta_g)$	metastable excitation (0.98 V)	x
$e + O_2 \longrightarrow e + O_2(b^1\Sigma_g^+)$	metastable excitation (1.63 V)	x
$e + O_2 \longrightarrow e + O_2(A^3\Sigma_u^+, A'^3\Delta_u, c^1\Sigma_u^-)$	metastable excitation (4.05 V)	x
$e + O_2 \longrightarrow O(^3P) + O(^3P) + e$	dissociation (6.12 V)	x
$e + O_2 \longrightarrow O(^3P) + O(^1D) + e$	dissociation (8.4 V)	x
$e + O_2 \longrightarrow O(^1D) + O(^1D) + e$	dissociation (9.97 V)	x
$e + O_2 \longrightarrow O_2^+ + 2e$	electron impact ionization	x
$e + O_2 \longrightarrow e + O + O(3p^3P)$	dissociative excitation (14.7 V)	x
$e + O_2 \longrightarrow O + O^-$	dissociative attachment	x
$e + O_2 \longrightarrow O^+ + O^- + e$	polar dissociation	
$e + O_2 \longrightarrow O^+ + O + 2e$	dissociative ionization	

electron impact O

$e + O \longrightarrow O + e$	elastic scattering	
$e + O(^3P) \longrightarrow O(^1D) + e$	excitation to ^1D (1.96 eV)	
$e + O(^3P) \longrightarrow O(^1S) + e$	excitation to ^1S (4.18 eV)	
$e + O(^3P) \longrightarrow O(^3P^0) + e$	excitation to $^3P^0$ (15.65 eV)	
$e + O(^3P) \longrightarrow O(^5S^0) + e$	excitation to $^5S^0$ (9.14 eV)	
$e + O(^3P) \longrightarrow O(^3S^0) + e$	excitation to $^3S^0$ (9.51 eV)	
$e + O \longrightarrow O^+ + 2e$	ionization	

detachment

$e + O^- \longrightarrow O + 2e$	electron impact detachment	x
$O^- + O_2 \longrightarrow O + O_2 + e$	detachment by oxygen molecule	x
$O^- + O \longrightarrow O_2 + e$	detachment by oxygen atom	

recombination

$e + O_2^+ \longrightarrow O(^3P) + O(^1D)$	dissociative recombination	x
$O^- + O_2^+ \longrightarrow O + O_2$	mutual neutralization	x
$O^+ + O^- \longrightarrow O + O$	mutual neutralization	

charge exchange

$O_2^+ + O_2 \longrightarrow O_2 + O_2^+$	charge exchange	x
$O^+ + O_2 \longrightarrow O + O_2^+$	charge exchange	
$O^+ + O \longrightarrow O + O^+$	charge exchange	
$O_2^+ + O \longrightarrow O_2 + O^+$	charge exchange	
$O_2^+ + O_2 \longrightarrow O^+ + O + O_2$	fragmentation by energetic O_2^+	

scattering

$O^- + O_2 \longrightarrow O^- + O_2$	scattering	x
$O + O_2 \longrightarrow O + O_2$	scattering	x
$O_2^+ + O_2 \longrightarrow O_2^+ + O_2$	scattering	x
$O^+ + O_2 \longrightarrow O^+ + O_2$	scattering	
$O_2 + O_2 \longrightarrow O_2 + O_2$	scattering	
$O + O \longrightarrow O + O$	scattering	

x reaction included in the limited reaction set of xpdp1

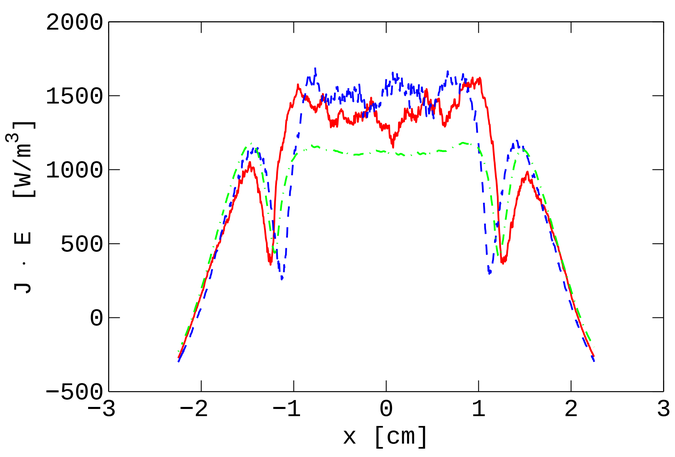

Figure 2: The electron heating rate for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm by a 222 V voltage source at 13.56 MHz.

- There are some differences between the xpdp1 and oopd1 that include:
  - oopd1 and xpdp1 use different algorithms for the scattering of the incident and ejected electrons, e.g. oopd1 uses a relativistic algorithm for electron impact ionization while xpdp1 uses a non-relativistic algorithm
  - The xpdp1 uses the non-isotropic differential cross section as described by Vahedi and Surendra (1995) and Surendra et al. (1990) while the oopd1 uses the isotropic differential cross sections for electron scattering given by Okhrimovskyy et al. (2002)

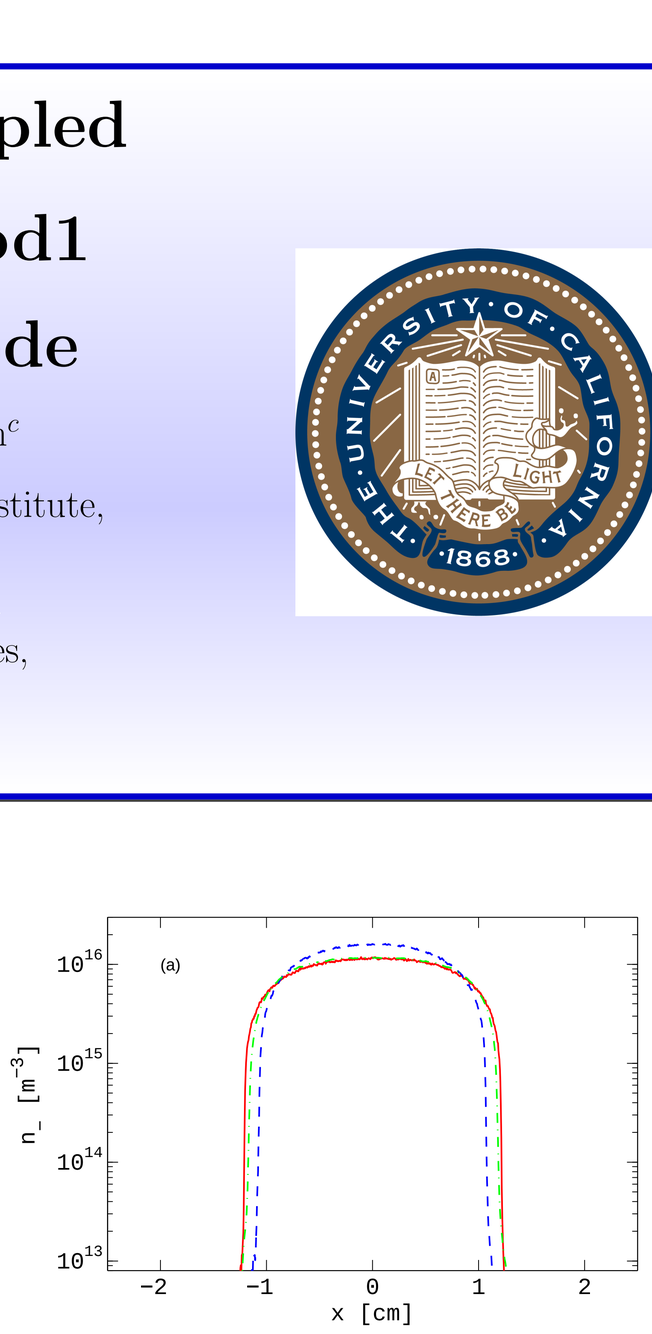

Figure 3: The (a) O^--ion density profile, (b) O_2^+-ion density profile, and (c) electron density profile for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm by a 222 V voltage source at 13.56 MHz.

Conclusions

- A new PIC-MC code, the oopd1, was compared to the well established xpdp1 and demonstrated for simulation of capacitively coupled rf discharges in oxygen
- The code includes significantly revised cross section database for collisional processes in oxygen, as well as the addition of O atoms and O^+-ions and the relevant reactions and cross sections

Acknowledgments

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