A 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^+
- For comparison we define a limited reaction set that includes only, 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 earlier work using the XPDP1 code (Vahedi and Surendra, 1995)
- We assume the oxygen molecules are reflected from the electrodes and that the oxygen atoms recombine to form O_2 at the electrodes with a 50 % probability and are reflected with a 50 % probability

electron impact O_2

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

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	l
$O^- + O_2 \longrightarrow O + O_2 + e$	detachment by oxygen molecule	l
$O^- + O \longrightarrow O_2 + e$	detachment by oxygen atom	

recombination

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

charge exchange

$O_2^+ + O_2 \longrightarrow O_2 + O_2^+$	charge exchange	l
$O^+ + O_2 \longrightarrow O + O_2^+$	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^+	l

scattering

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

l reaction included in the limited reaction set

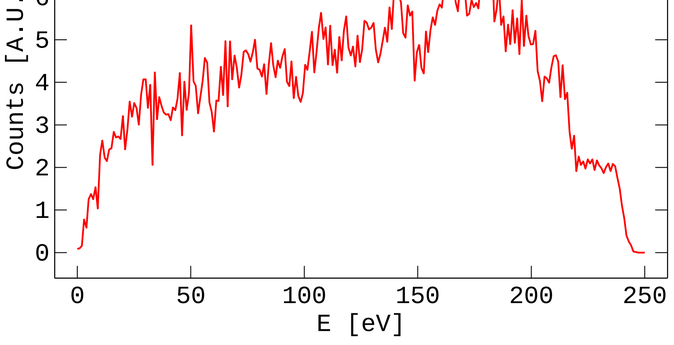

Figure 3: The ion energy distribution for the oxygen ion O^+ (a) at 2 mTorr and (b) 20 mTorr, calculated assuming a full reaction set.

- The ion energy distribution for the oxygen ion O^+ is broad and continuous
- A broad ion energy distribution for the oxygen ion O^+ has been observed experimentally by Janes and Huth (1992b) which suggested that it is due to mechanisms that are not dominated by charge-exchange collisions

Results and discussion

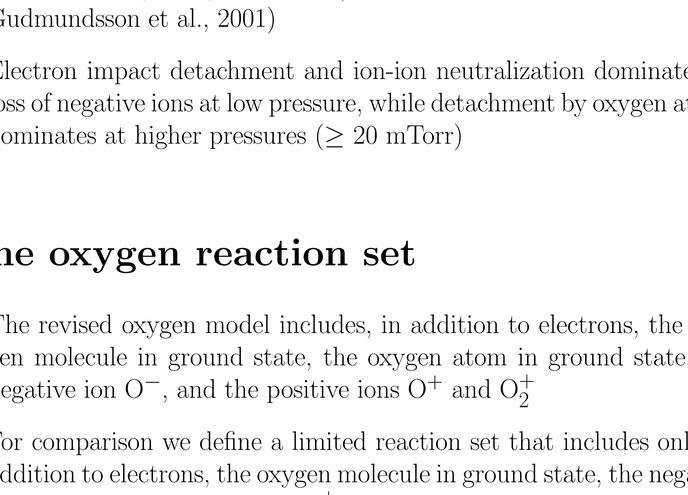

Figure 1: The electron energy probability function (EEPF) for an oxygen discharge at 2 mTorr. The EEPF is calculated assuming a full reaction set (red line) and a limited reaction set (blue line).

- We assume a parallel plate capacitively coupled oxygen discharge with with a gap separation of 5 cm and cross sectional area of 20 cm^2
- The discharge is driven by a 500 V voltage source at 13.56 MHz

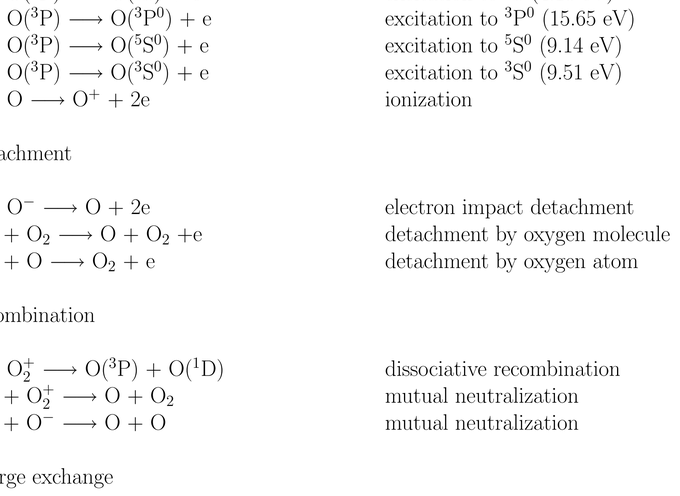

Figure 2: The ion energy distribution for the oxygen ion O_2^+ calculated assuming a full reaction set (red line) and limited reaction set (blue line) for oxygen discharge at 2 mTorr.

- The ion energy distribution for the oxygen ion O_2^+ at 20 mTorr shows distinct peaks that are caused by charge-exchange collisions in the sheath with targets mainly having thermal energies
- This is consistent with what has been observed experimentally (Janes and Huth, 1992a) and demonstrated by PIC-MC simulations (Babaeva et al., 2005)
- There are clear differences in the fine structure when comparing results from calculations assuming a full reaction set and a limited reaction set

Conclusions

- A new PIC-MC code, the oopd1, was applied to explore a capacitively coupled oxygen discharge
- The code was used to determine the electron energy distribution and the ion energy distribution for both O^+ and O_2^+-ions

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