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Recombination and detachment in oxygen discharges: The role of metastables

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Introduction

- We report on a volume averaged global model calculation of a low pressure oxygen discharge
- The reaction rate coefficients have been revised from earlier work (Gudmundsson et al., 2001; Guðmundsson, 2004)
- The model includes thirteen species
  - electrons assumed to have a Maxwellian energy distribution in the range 1 – 7 eV
  - molecular oxygen in ground state $O_2(^3\Sigma_g^-)$, and the metastables $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g^+)$ and $O_2(A^3\Sigma_u^+, A'^3\Delta_u, c^1\Sigma_u^-)$
  - atomic oxygen in ground state $O(^3P)$, metastable atomic oxygen $O(^1D)$ and ozone O_3
  - the positive ions O^+ and O_2^+
  - the negative ions O^-, O_2^- and O_3^-

Ion-ion recombination

- For mutual neutralization of O^+ by O^-

$$O^- + O^+ \longrightarrow O + O$$

  we propose

$$4.0 \times 10^{-14}\,(300/T_i)^{0.43} \qquad m^3/s$$

- For mutual neutralization of O_2^+ by O^-

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

  and

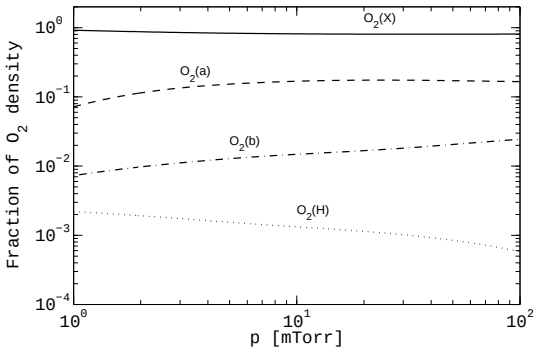
$$O^- + O_2^+ \longrightarrow 3O$$

  we propose

$$2.6 \times 10^{-14}\,(300/T_i)^{0.43} \qquad m^3/s$$

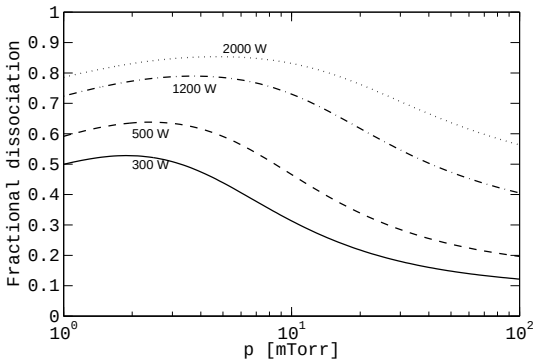
  for each reaction
- These replace values of 2.7×10^{-13} m^3/s and 1.0×10^{-13} m^3/s (Kossyi et al., 1992; Eliasson and Kogelshatz, 1986) commonly used (Gudmundsson and Lieberman, 2004)

Metastable O_2



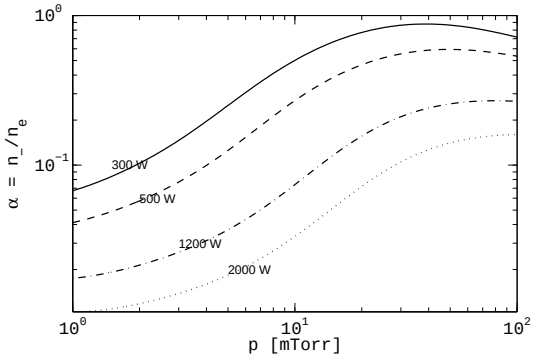
- The density of the metastable singlet delta state $O_2(a^1\Delta_g)$ is roughly 10 – 15 % of the total O_2 density in the pressure range of interest
- The density of the $O_2(b^1\Sigma_g^+)$ is roughly 1 – 2 % of the total O_2 density
- The density of the Herzberg states is negligible

Dissociation



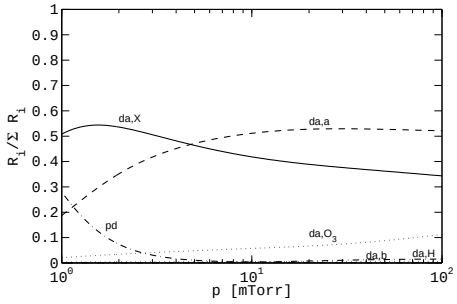
- The fractional dissociation increases with increased applied power and decreases with increased neutral gas pressure
- The wall recombination coefficient for atomic oxygen is 0.5 and for the metastable singlet delta state $O_2(a^1\Delta_g)$ it is 0.007

Negative ions



- Oxygen discharges are weakly electronegative
- The electronegativity increases with decreasing applied power and increasing pressure
- The dominant negative ion is O^- and the density of O_2^- and O_3^- ions is significantly smaller

Creation of O^-



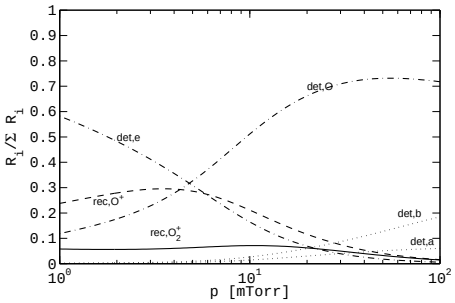
- Reaction rates for O^- creation at 500 W
- Creation of O^- is mainly through dissociative electron attachment to the oxygen molecule in ground state and the singlet delta state

$$e + O_2(X) \longrightarrow O^- + O$$

and

$$e + O_2(a) \longrightarrow O^- + O$$

Destruction of O^-



- At low pressure (< 3 mTorr) electron impact detachment dominates

$$e + O^- \longrightarrow O(^3P) + 2e$$

- At higher pressure (> 20 mTorr) associative detachment by oxygen atom dominates

$$O(^3P) + O^- \longrightarrow O_2 + e$$

- At low pressures (< 10 mTorr) ion-ion recombination accounts for roughly $30 - 40$ % of the total O^- loss

Summary

- New rate coefficients for ion-ion recombination are proposed
- Creation of O^- is mainly through dissociative electron attachment to the oxygen molecule in ground state and the singlet delta state
- Electron impact detachment dominates destruction of O^- at low pressure
- Associative detachment dominates destruction of O^- at high pressure
- The metastable $O_2(a^1\Delta_g)$ is important in the creation of O^- but not in the O^- loss

Acknowledgments

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