STUDY OF THE NON-MAXWELLIAN ELECTRON ENERGY DISTRIBUTION FUNC-TION IN AN RF OXYGEN DISCHARGE

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ABSTRACT

A planar one-dimensional particle-in-cell simulation with Monte Carlo Collisions (PIC/MCC) has been used to study a 13.56 MHz weakly dissociated oxygen discharge. In this case molecular oxygen is the dominant neutral species and O_2^+ the dominant positive ion species. Ion and electron density profiles have been obtained at pressures of 50 mTorr and 1 Torr. It was showed that as pressure increases the density profiles become flatter compared to the low-pressure case, where the profiles have a large sheath. The electron energy distribution functions (eedf) are non-Maxwellians, which is typical for electronegative gases. In order to explain this effect electron heating rates have been obtained for low and high pressure cases.

INTRODUCTION

Discharges with O_2 are typically used for industrial materials processing and most of processing plasmas are produced by both capacitively and inductively coupled RF discharges. A macroscopic analytic model for a electronegative plasma has been developed by Lichtenberg, Vahedi and Lieberman [1] in order to study the density profiles and electron energy distribution functions (eedf). They are non-maxwellians, which is typical for capacitively coupled rf discharges. Besides, the electronegative molecules easily attach free electrons from the plasma, decreasing the electron density and consequently affecting the eedf.

In this work, a planar one-dimensional particle-in-cell simulation with a Monte Carlo Collision Model, PIC-MCC [2] has been used to study a capacitive oxygen discharge. The profiles of the charged species, electrons, O^{-} and O_{2}^{+} have been obtained for low (50m Torr) and high pressure (1 Torr) cases. An analyze of the heating mechanism has been done in order to explain the non-maxwellian eedf's. A thorough description of the PIC technique can be found in Birdsall and Langdon [3].

COLLISION TYPES

The reactions considered in the oxygen model are:

- (1) $e + O_2 \rightarrow e + O_2$ (momentum transfer)
- (2) $e + O_2 \rightarrow e + O_2(r)$ (rotational excitation)

(3)-(6) $e + O_2 \rightarrow e + O_2(v=n,n=1,4)$ (vibrational excitation)

(7) $e + O_2 \rightarrow e + O_2 (a^1 \Delta_G)$ (metastable excitation - 0.98 eV)

(8) $e + O_2 \rightarrow e + O_2(b^1 \Sigma_G^+)$ (metastable excitation - 1.63 eV)

(9) $e + O_2 \rightarrow O + O^-$ (dissociative attachment-4.2 eV)

(10) $e + O_2 \rightarrow e + O_2 (c^1 \Sigma_U, A^3 \Sigma_u^+)$ (metastable excitation - 4.5 eV)

(11)
$$e + O_2 \rightarrow e + O(3P) + O(3P)$$
 (dissociation - 6.0 eV)

$$(12) e + O_2 \rightarrow e + O(3P) + O(1D)$$
 (dissociation - 8.4 eV)

(13) $e + O_2 \rightarrow e + O(1D) + O(1D)$ (dissociation - 10.0 eV)

(14) $e + O_2 \rightarrow e + O_2^+ + e$ (ionization - 12.06 eV)

(15) $e + O_2 \rightarrow e + O + O^*(3p^3P)$ (dissociative excitation-14.7 eV)

(16) $e + O_2^+ \rightarrow O + O$ (dissociative recombination)

(17) $e + O^- \rightarrow e + O + e^-$ (electron impact detachment)

(18) $O^- + O_2^+ \rightarrow O + O_2$ (mutual neutralization)

(19) $O^- + O_2 \rightarrow O + O_2 + e$ (detachment)

(20) $O^- + O_2 \rightarrow O_- + O_2$ (elastic scattering)

(21) $O_2^+ + O_2 \rightarrow O_2 + O_2^+$ (charge transfer)

(22) $O + O_2 \rightarrow O + O_2$ (scattering)

It is assumed that the molecular oxygen density (the neutral species) remains constant and uniform in space. All the other species are followed as particle species. The electrons in this model collide with three species two of which are particle species, O_2^+ and O^- . Note that the reactions included in this model do not include ionization of atomic oxygen. Thus, this model is valid only

for modeling weakly dissociated oxygen discharges, where O_2^+ is the dominant positive ion species. Besides, in low conventional capacitive rf discharges where the electron density is low ($n_e \approx 10^9 \text{ cm}^{-3}$) low fraction dissociation assumption is justified [4].

The details of PIC-MCC scheme for simulating an rf oxygen discharge was made by Vahedi and Surendra [5]. Detailed description of the MCC model including the reactions (1) up to (22) and the cross sections references can be found there.

In order to study the heating processes, particle density and the eedf's as pressure function in an rf oxygen plasma, a 50 mTorr, 500 mTorr and 1 Torr discharge with applied voltage of 200 V has been considered. The external circuit elements are R=L=0 and C=1F. The electrode spacing are L=5.0 cm, the electrode area A=0.2 cm and initial densities for electrons, O_2^+ , O^- are $0.4 \times 10^{16} \text{m}^{-3}$, $1.0 \times 10^{16} \text{m}^{-3}$, $0.6 \times 10^{16} \text{m}^{-3}$, respectively. The simulations were run until the equilibrium for electrons and ions have been reached.

RESULTS AND DISCUSSION

Figure 1(a) shows eedf's for 50 mTorr, 500 mTorr and 1 Torr. For all cases eedf is non-maxwellian. This behavior can be explained as the combined effect of stochastic electron heating of the fast electrons and ohmic heating of the slow electrons.

The low energy electrons are created through inelastic collisions, such as impact ionization by the high-energy electrons. Some of the low energy electrons are trapped in the bulk; others diffuse out towards the plasma-sheath interface. There, they are stochastically heated by oscillating sheaths and to return to the high-energy electron group. These are either lost to the walls or lost by inelastic collision as discussed before. Thus, the eedf seems to be a bi-maxwellian distribution. As observed in Fig. 1(a), the eedf is slightly convex at high pressure (1 Torr) and concave at low pressure (50 mTorr). The change of the eedf is due to a transition in the electron heatingmode from stochastically dominated heating at low pressures to ohmically dominated heating at high pressures. The same convex-concave eedf was measured by Godyak et al. [6] and simulated by Vahedi et al [7] in an rf argon discharge.

Figure 1(b) shows electron heating rates obtained from simulations for 50 mTorr, 500 mTorr and 1 Torr of pressure. They are peaked in electron heating rate near the plasma sheath boundaries for 1 Torr. These peaks are due to stochastic heating of the fast electrons in the driven sheaths. On the other hand the ohmic heating of the slow electrons occurs in the bulk plasma. For low pressures the ohmic heating is almost zero as can be seen in this figure.

Figure 2 shows electrons, O_2^+ and O^- densities for 50 mTorr and 1 Torr. For 50 mTorr there is a central elec-

tronegative region where $n_{\rm e}$ is greater than $n_{\rm e}$. Besides, due to small potential variations the electron density is essentially constant.

When the potential variations become larger one has an electroposive region near the sheaths where $n_e \approx n_+$. One can see that for p=1 Torr the sheath decreases and the profiles change slightly becoming a little peaked near the plasma sheaths due to the fast electrons near this region.



Figure 1: Electron energy distribution function at pressures of 50 mTorr (solid line), 500 mTorr (dashed line) and 1 Torr (dotted line) and electron heating rate for 50 mTorr (solid line), 500 mTorr (dashed line) and 1 Torr (dotted line.)

A planar one-dimensional particle-in-cell simulation with Monte Carlo collision package has been used to study a 13.56 MHz weakly dissociated oxygen discharge. It was shown that the electron energy distribution function is non-maxwellian.

The electron heating rates were obtained as pressure function. They are peaked near the plasma sheath boundaries as pressure increases. The density profiles were also obtained showing slight peaks near the sheath for 1 Torr.



Figure 2: Electron (dashed line), O_2^+ (dotted line) and O^- (solid line) densities, for (a) 50 mTorr and (b) 1 Torr.

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