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O-atoms downstream an Ar-O_2 surface-wave microwave discharge

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Chemically active oxygen atoms have been found to play a crucial role in numerous plasma applications, such as plasma based medical sterilization [1, 2, 3], synthesis of metal-oxide nanowires [4], oxide films deposition [5], functionalization of polymers [6, 7], removal of organic impurities [8], selective etching of composites [9], passivation of metals [10] and surface activation [11]. In several applications a synergetic effect between the O-atoms and ions (such as Ar^+), metastables or UV radiation (from Ar(4s) or NO(A,B)) has been observed. O-atoms are abundantly present in plasmas generated in O_2, however, even higher atomic oxygen to molecular oxygen density ratios can be obtained in gas mixtures such as N_2-O_2 or Ar-O_2. The aim of this work is to investigate by modelling the production of O-atoms in a flowing Ar-O_2 microwave discharge and follow their evolution in the afterglow.

The system under study is similar to the one used by Mafra *et al.* [7] in their experimental investigations. It is composed of a surface-wave microwave discharge generated by a surfatron [12, 13] at a field frequency of 2450 MHz in a 5 mm inner diameter tube, connected to an afterglow tube of 1.4 cm inner diameter.

The densities of the species in the discharge are calculated using a zero dimensional self-consistent kinetic model, which is based on the solutions of the electron Boltzmann equation for the microwave field, coupled to a system of rate-balance equations for the neutral and charged heavy species. A detailed description of model is given in Ref. [14], where the gas phase and surface reactions governing the chemical kinetics of the species Ar($^1S_0$, $^3P_2$, $^3P_1$, $^3P_0$, $^1P_1$), $O_2(X\ ^3\Sigma_g^-$,v), $O_2(a\ ^1\Delta_g$, $b\ ^1\Sigma_g^+$), O(^{3}P, ^{1}D), O_3, Ar^+, Ar_2^+, O_2^+, O^+ and O^- are also listed. Since we are interested only in the flowing afterglow of the discharge, the calculations for the discharge need to be conducted only for the value of the critical electron density for surface-wave propagation, in this case 3.74×10^{11} cm^{-3}, which occurs at the end of the plasma column and determines the density of species leaving the discharge zone. The evolution of the species along the early-afterglow downstream from the discharge is followed with a time-dependent system of species rate-balance equations. The same chemical-kinetics scheme is used as in the discharge region, although the electron impact excitation/ionization processes are omitted, due to the very low electron energies.

Herein we present results for the conditions used by Mafra *et al.* [7] in the case of polymer treatment. Fig. 1 (a) and (b) show the [O(^{3}P)] density and the dissociation degree ([O]/2[O_2]$_0$) along the early-afterglow at 4 mbar for different initial mixture compositions. The results show that the dissociation degree increases considerably with the Ar percentage, a dissociation degree as high as 37% being achieved in mixtures with 95%Ar. Notice that, while the O_2 density in the mixture decreases by a factor of 20 from pure O_2 to an Ar-5%O_2 mixture, the [O(^{3}P)] density decreases only by a factor of 8. In addition, the [O] density decreases essentially at the same rate along the afterglow, independently of the mixture composition.

Fig. 1 (c) depicts the density of O(^{3}P) atoms in an Ar-10%O_2 mixture at different pressures. Contrary to the measured data by Mafra *et al.* (with 10% of error indicated) our calculations do not show any saturation of the density in the 6-12 mbar pressures range. Accordingly, even though the calculated dissociation rates vary practically in the same range as the measured ones, 7-12% (at 14 ms afterglow time, see Fig. 1 (d)) to compare with 5-14% (Fig. 3 in [7]), respectively, they

exhibit different trends. In our calculations the dissociation degree is highest at 1 mbar and shows a minimum at 4 mbar, while experimentally a monotone decrease has been observed with pressure. Work is in progress to clarify this issue.

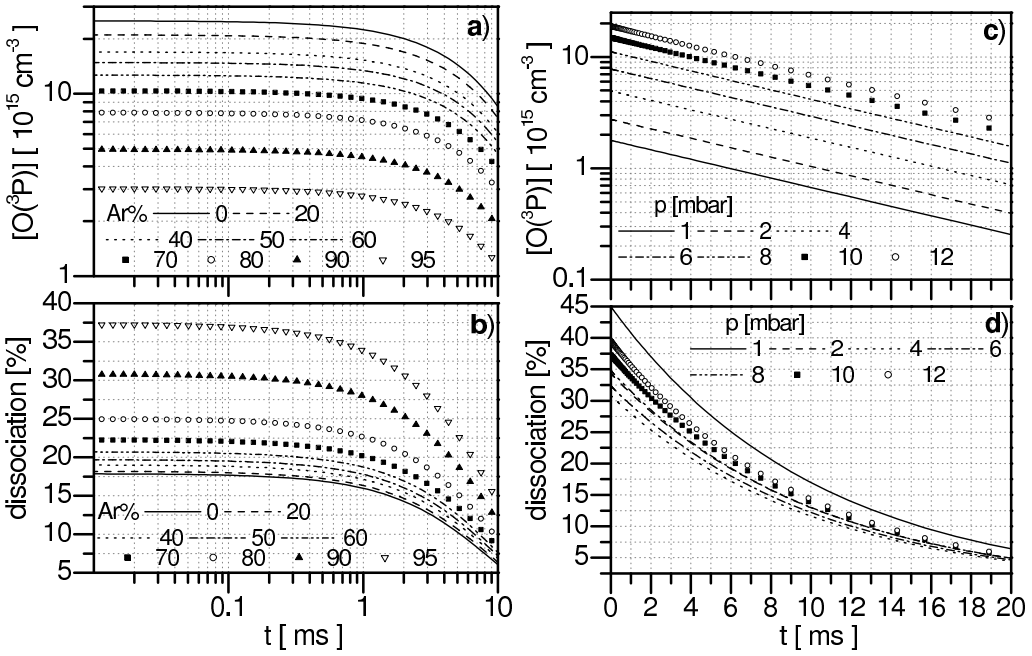

Fig. 1: O-atoms density and dissociation degree along the afterglow: (*i*) at 4 mbar for different initial mixture composition (a) and (b), respectively, and (*ii*) for Ar-10%O_2 mixture composition at different pressure values (c) and (d), respectively.

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