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Oxygen loss frequency and recombination probability in oxygen-containing plasmas

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In most plasma processes, surfaces interact with either the active discharge or its afterglow. Heterogeneous surface kinetics plays a role there, affecting both the plasma and surface properties. In particular, in oxygen-containing discharges the adsorption and recombination of atomic oxygen on reactor surfaces determine the gas composition, the availability of O for important volume reactions and eventually the flux of reactive oxygen species (ROS) towards target surfaces. In CO_2 conversion plasmas, atomic oxygen is extremely important as reactant either for dissociation ($CO_2 + O \rightarrow CO + O_2$) or for recombination ($CO + O + M \rightarrow CO_2 + M$). O is essentially produced by electron-impact dissociation ($CO_2 + e \rightarrow CO + O + e$) and, particularly at low pressures (below 50 Torr), it can be lost by recombination on the wall.

The effective rate of surface recombination is determined by a condition-dependent probability γ_O, that can be estimated from loss frequency measurements and is often used as fundamental input parameter in models. The loss frequencies of O atoms have been measured in the positive column of O_2 and CO_2 glow discharges in a Pyrex tube (borosilicate glass), for several pressures, currents and wall temperatures [1,2]. However, the procedure for deducing γ_O from the loss frequency is not straightforward, since the processes determining the net losses of O are not known *a priori*. In this work, the Lisbon Kinetics (LoKI-B+C) simulation tool [3] is employed in steady-state and current-modulated modes to assess the processes determining the loss frequency and the most accurate way to estimate γ_O. The procedure developed allows not only to derive optimal values of γ_O, but also to assess the validity of different hypotheses on the most relevant processes for the net losses of O [4].

Figure 1 shows the different γ_O that can be obtained from the same loss frequency measurements, according to different hypotheses, for the case of CO_2 plasma. The figure shows that γ_O depends on the different hypotheses. The optimal γ_{OPT} are obtained as the values that allow the loss frequency from modulated current simulations to fully match the experimentally-measured loss frequency. Unlike the case in oxygen plasma [4], the simulations in figure 1 show that in CO_2 γ_{OPT} is close to γ_O obtained from the simple assumption that the net losses of O are mostly determined by surface recombination processes and not by volume processes (hypothesis 5).

References:

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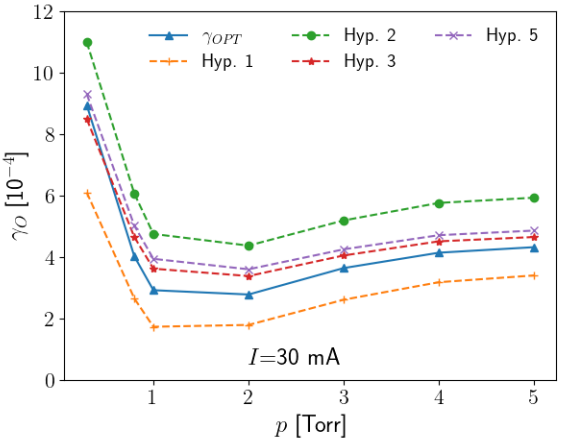

Figure 1: Atomic oxygen recombination probability in Pyrex in CO_2 plasma, as function of pressure, for 50ºC wall temperature and 30 mA current, for different hypotheses on the relevant processes for O loss.