Experimental benchmarks and sensitivity analysis of PIC/MCC simulations of oxygen CCPs

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Low-pressure capacitively coupled radio frequency discharges operated in O_2 and driven by tailored voltage waveforms have been investigated experimentally and by means of kinetic simulations [1]. Pulse-type (peaks/valleys) and sawtooth-type voltage waveforms that consist of up to four consecutive harmonics of the fundamental frequency were used to study the amplitude asymmetry effect as well as the slope asymmetry effect at different fundamental frequencies (5, 10, and 15 MHz) and at different pressures (50–700 mTorr). Several discharge characteristics such as the DC self-bias, the total flux as well as the flux-energy distribution of O_2^+ ions, the discharge power, and the spatio-temporal excitation rates have been determined experimentally and are compared with the predictions of Particle-in-Cell/Monte Carlo Collisions (PIC/MCC) simulations [1]. The good agreement between the experimental and simulation data confirms that the discharge is described well by our model. This study also addresses electron power absorption mode transitions. As an example, figure 1 shows a transition from the hybrid α / drift-ambipolar mode to the α-mode that is induced by changing the number (*N*) of consecutive harmonics included in a valley-type driving voltage waveform. We have performed sensitivity analyses of the effect of various parameters including the rate of surface quenching of oxygen singlet delta metastable molecules, the magnitude of the isotropic part of the $O_2^+ + O_2$ charge-exchange cross section, and the magnitude of the cross section of the $O_2^+ + O^-$ mutual neutralization process.

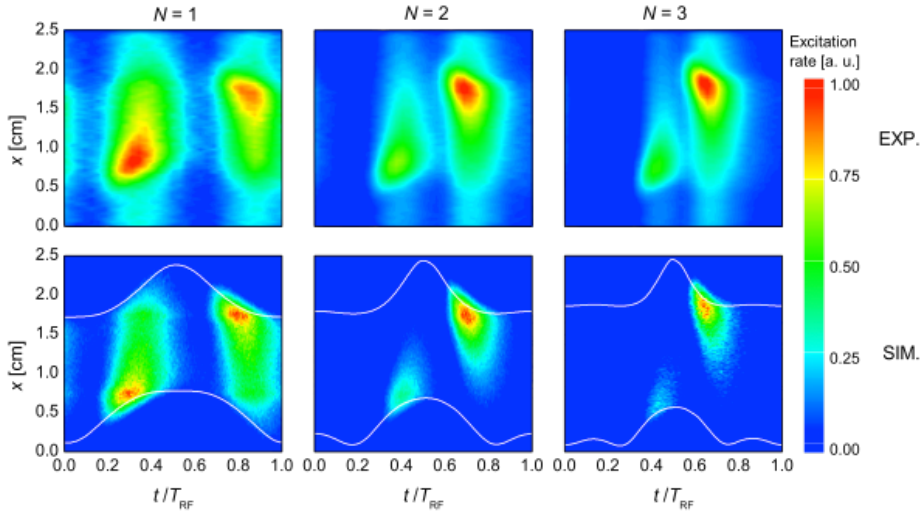

Figure 1. Experimental (from Phase-Resolved Optical Emission Spectroscopy) and PIC/MCC simulation results of the spatio-temporal distribution of the excitation rate in an oxygen CCP, for 150 mTorr pressure, 2.5 cm electrode gap, with valley-type excitation waveforms of 15 MHz base frequency and 400 V peak-to-peak voltage.

[1] A. Derzsi, *et al.*, *Plasma Sources Sci. Technol.* **25**,15004 (2016); **26**, 034002 (2017).