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Electron heating in electronegative capacitively coupled discharge of complex chemistry

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A brief overview is given on the development of a comprehensive reaction set for the oxygen discharge for particle-in-cell Monte Carlo collision (PIC/MCC) simulations. A particular attention is given to the creation and destruction of the negative ion O^- . Then the one-dimensional object-oriented PIC/MCC code `oopd1`, using this comprehensive reaction set, is applied to explore the charged particle density profiles, the electron heating mechanism and the electron energy probability function (EEPF) in a single frequency capacitively coupled oxygen discharge. We explore how including and excluding detachment by the singlet metastable molecules $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g)$ influences the electron heating mechanism and the discharge electronegativity. We demonstrate that the detachment processes have a significant influence on the discharge properties, in particular at the higher operating pressures (> 30 mTorr) [1,2]. We show that for low driving frequency and low pressure (5 and 10 mTorr), a combination of stochastic (α -mode) and drift ambipolar (DA) heating in the bulk plasma (the electronegative core) is observed and the DA-mode dominates the time averaged electron heating [3]. As the driving frequency or pressure are increased, the heating mode transitions into a pure α -mode, where electron heating in the sheath region dominates [3]. This transition coincides with a sharp decrease in electronegativity. Furthermore, we demonstrate that the electrodes surface quenching coefficient has a significant influence on the density of the singlet metastable $O_2(a^1\Delta_g)$ and thus the discharge electronegativity and electron heating mechanisms [4]. [1] J. T. Gudmundsson and M. A. Lieberman, *Plasma Sources Sci. Technol.* **24**, 035016 (2015) [2] J. T. Gudmundsson and B. Ventéjou, *J. Appl. Phys.* **118**, 153302 (2015) [3] J. T. Gudmundsson, D. I. Snorrason and H. Hannesdottir, *Plasma Sources Sci. Technol.* **27**, 025009 (2018) [4] A. Proto and J. T. Gudmundsson, *Plasma Sources Sci. Technol.* accepted for publication 2018