Fluid modeling of a ccrf discharge in oxygen

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Theoretical studies of capacitively coupled radio frequency discharge plasmas in a reactor with plane electrodes are presented. Main features of the spatiotemporal fluid model are given and results for discharge at pressures between 50 and 100 Pa, applied voltages from 0.2 to 1 kV at a frequency of 13.56 MHz are reported. A remarkable electronegativity of the plasma was found for the conditions considered.

Capacitively coupled radio frequency (ccrf) oxygen plasmas are widely used for surface treatment applications. The most important applications are etching, sputter-deposition, growth of SiO2 films and photo-resist or polymer films removal. One specific topic of interest of oxygen discharges concerns the different species occurring in the plasma. Negative ions exist in oxygen containing plasmas and have an impact on the charge carrier transport, plasma sheath condition and production of electrons due to detachment processes. Furthermore, metastable oxygen molecules can reach a large particle density and, thus, can become important for the production of electrons and negative ions in attachment processes.

In the present contribution, results of fluid modeling of ccrf oxygen plasmas are reported. The studies have been performed for the plasma reactor configuration described in [1] for pressures \( p \) between 50 and 100 Pa. Although an asymmetric discharge situation exists in that experiment, in a first step a symmetric situation with given applied voltage \( V(t) = V_0 \sin(2\pi ft) \) has been investigated, where voltage amplitudes \( V_0 \) between 0.2 and 1 kV have been used and the frequency is \( f = 1/T = 13.56 \) MHz.

A schematic diagram of the discharge arrangement between plane-parallel electrodes (9 cm in diameter in the experiment, gap \( d = 2.5 \) cm) considered in the modeling is shown in figure 1.

Assuming radial symmetry of the discharge plasma, a time-dependent, spatially one-dimensional description has been employed to characterize the axial behaviour of the plasma between the electrodes. In the framework of the fluid model, the coupled system of balance equations of 17 heavy particle species, the electron component and the electron energy density as well as of Poisson’s equation has been solved. The fluxes of particles and electron energy are treated in drift-diffusion approximation, where the consistent diffusion coefficient and mobility for the electron energy transport have been used [2]. The detailed reaction kinetic model takes into account about 180 reactions including elastic electron collisions, electron impact excitation, deexcitation, dissociation, ionization, detachment and recombination, electron attachment, collisional quenching and negative ion detachment in heavy particle collisions, charge exchange reactions, ion-ion recombination and radiative processes.

Figure 2 illustrates the periodic evolution of the density and mean energy of the electrons for a pressure of 50 Pa and voltage amplitude of 0.2 kV by means of the instants \( t/T = 0, 1/4, 1/2 \) and \( 3/4 \) of the period. The electron density and mean energy show a large modulation with the applied voltage variation. A maximum of the electron density is found in front of the momentary anode followed by local minimum, while the density remains almost constant in the discharge centre. At the same time the mean electron energy possesses a maximum inside the momentary cathode region and is flat in the plasma bulk. A comparison with the line-integrated electron density measured in the discharge centre at
similar discharge conditions [3] shows that the corresponding calculated electron density integrated over the electrode diameter is of the same order of magnitude as the experimental result.

Figure 2: Periodic behaviour of electron density and mean energy at $p = 50$ Pa and $V_0 = 200$ V.

Figure 3 shows the density of the $\text{O}_2^+$, $\text{O}^+$, $\text{O}^-$ and $\text{O}_2^-$ ions as well as the electron density at $t/T = 0$ of the periodic state at 50 Pa for $V_0 = 0.2$ and 1 kV, respectively. Due to their large mass, the positive and negative ions respond mainly to the period-averaged field. Consequently, their densities remain almost constant in the discharge volume with an almost symmetric spatial profile, and small modulations occur only close to the boundaries. $\text{O}_2^+$ is the dominant positive ion, while the density of $\text{O}^+$ (and $\text{O}_2^+$) is always more than two orders of magnitude smaller than that of $\text{O}_2^+$ in the discharge centre. At lower voltage $\text{O}_2^-$ is the dominant negative ion, followed by $\text{O}^-$. When increasing the voltage amplitude, $\text{O}^-$ becomes the dominant negative ion and the electronegativity decreases from about 30 at 0.2 kV to 7 at 1 kV. At the same time, the densities of the positive and negative ions exhibit maxima in front of the electrodes, indicating that the dominant generation processes of these charge carriers peak close to the electrode.

Figure 3: Charged particles densities at $p = 50$ Pa for $V_0 = 0.2$ kV (left) and $V_0 = 1$ kV (right).

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References