The sheath structure in the multicomponent plasma-solid interaction at low and medium pressures

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1. Introduction

Low-temperature reactive plasmas are often used in modern technologies. Negative ions in such plasmas influence the transport of charged species from the plasma to immersed solids, both substrates in plasma-assisted technologies and probes in plasma diagnostics [1]-[3]. A detailed description of processes taking place during the plasma-solid interaction is rather difficult. It was proved that a combination of experimental and computational approaches is the best suited for the given task, especially at higher pressures and/or in chemically active plasmas [4]-[6].

2. Experimental

The discharges in various gases have been intensively studied over a very long period. In our laboratory in Prague the measurements were performed in the positive column of a DC glow discharge in oxygen, both pure and in the mixtures with rare gases. Various diagnostics, including optical, microwave and probe diagnostics, were used for the study of plasma properties. Some older results can be found in [7].

Main parameters of our experiments were the total gas pressure, the composition of the mixtures and the discharge current - see e.g. Fig. 1. The obtained experimental data were used as a basis for our computational study.

Fig. 1: Electron densities in positive column of DC glow discharge in argon and oxygen. Discharge current 10 to 30 mA.
3. Computer simulation

Two techniques of computational physics were used in the study. A macroscopic kinetic approach was chosen for the analysis of processes in the oxygen/argon plasma. The kinetic scheme consisted of more than one hundred reactions between neutral, charged and excited species in the oxygen, argon and their mixtures. The time dependencies of concentrations of these species were calculated for various discharge parameters. These concentrations were used as input data for the second model. The properties of an electronegative and multicomponent plasma near the surfaces of the immersed materials were studied by the self-consistent particle modelling, the PIC-MCC technique. The sheath structure was analyzed in dependence on the plasma pressure, the plasma composition and a surface geometry. The simulations were performed both in static and dynamic regimes where different masses of the individual charged particles influence both their concentrations in the sheath and their fluxes to the substrates. The potential distributions in the sheath and presheath were calculated and the concentrations of all kinds of the charged species were determined.

4. Results - electronegative plasma

For a characterization of the processes in plasma two levels of description were used. The qualitative study of plasma was performed under a simplified assumption of electronegative plasma consisting of electrons and one type of both positive and negative ions. The sheath properties were studied in dependence on the plasma pressure and composition and the probe geometry. The simulations were performed both in the static and dynamic regimes (Figs. 2-4).

Fig. 2: Potential distribution \( U(r) \) in the sheath for various relative concentrations of negative ions \( c \). Cylindrical probes of radii \( 2 \times 10^{-4} \) m (red), \( 2 \times 10^{-3} \) m (green) and \( 2 \times 10^{-2} \) m (blue).

Fig. 3: Concentrations of cardinal negatively charged species in the sheath (in the distance 5 mm from cylindrical probe) vs. plasma electronegativity \( c \). Probe radius: \( 1 \times 10^{-4} \) m (dashed), \( 1 \times 10^{-3} \) m (full line); voltage bias +10 volts.
5. Results - multicomponent plasma

For the detailed plasma characterization the so-called multicomponent plasma consisting of more types of positive and negative species was used. The concentrations of the most important species in the oxygen plasma were obtained by the macroscopic kinetic approach [8]. These concentrations derived in dependence on discharge parameters were used as input data for the following particle simulation. The species used in the particle simulations were:

- negatively charged: electrons, \( \text{O}^- \), \( \text{O}_2^- \) and \( \text{O}_3^- \),
- positively charged: \( \text{O}^+ \), \( \text{O}_2^+ \), \( \text{O}_4^+ \) and \( \text{Ar}^+ \).

Examples of the results derived can be found in Fig. 5 (static case) and 6 (plasma dynamics).

Fig. 5: Concentrations of charged species in multicomponent \( \text{O}_2/\text{Ar} \) plasma (plasma composition \( \text{Ar}:\text{O}_2 = 50:50 \)). Cylindrical probe (radius \( 1 \times 10^{-4} \) m), voltage bias +10 volts. Pressure: left - 150 Pa, right - 600 Pa.
Fig. 6: Current densities collected by the cylindrical probe (radius $1 \times 10^{-4}$ m). Parameters: pressure 133 Pa, plasma composition Ar:O$_2$ = 20:80, left - rectangular voltage steps, right - sinusoidal voltage, frequency 1 MHz. Magnitude: 1× (electrons), 500× (O$_2^+$, Ar$^+$), 1000× (O$^-$, O$^+$)

The dynamical simulations are especially important as the masses of the individual charged particles influence their concentrations in the sheath and their fluxes to the substrates.

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