# Study of plasma-solid interaction in electronegative gases at medium pressures

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### 1. Introduction

Low-temperature reactive plasmas based on electronegative gas mixtures are often used in modern technologies. Negative ions in such plasmas affect the transport of charged species from the plasma to immersed substrates and in this way influence the physical and chemical processes both in the sheath and on the surface of substrates. Similar problems arise in the probe diagnostics of chemically active plasmas – [1], [2], [3].

Another problem important in the present industrial applications of plasma is the surface treatment of materials at higher pressures, including the atmospheric pressure plasma without a need of any vacuum equipment, e.g. [4], [5].

The understanding of processes taking place during plasma-solid interaction is desirable from the point of view of both probe diagnostics as well as plasma chemical technologies. The theoretical analysis of processes in electronegative plasma at medium and high pressures is difficult, because the theories derived for collisionless or slightly collisional plasmas lose their validity in these conditions and the structure of such plasmas is more complex than in conventional electropositive gases. In such conditions the computational approach, both fluid modelling [6] and various particle simulation techniques (e.g. [7], [8]), proved to be the best solution.

## 2. Models

We prepared a computer experiment devoted to the study of the role of negative ions in the formation of sheath surrounding substrates immersed into plasma and the influence of plasma pressure on this process. The technique of modelling used was the particle simulation in two modifications: standard self-consistent PIC-MC method (described e.g. in our previous paper [9]) and the non self-consistent modelling with the distribution of electric potential near the substrate given externally. The simulation was based on experimental data obtained in our laboratory in a DC glow discharge in the mixtures of oxygen with rare gases [10].

The simulation was performed in two spatial dimensions for various geometries of substrates or probes. Following questions were studied:

- the influence of plasma composition and pressure on the distribution of electric potential near the metal substrate,
- the spatial and time evolution of energy and angular velocity distributions of charged particles in the vicinity of the substrate,
- the influence of substrate geometry on the sheath region in the electronegative plasma in the dependence on plasma pressure.

The model was written in Fortran 95 programming language and processed by PC microcomputer. Typical number of charged particles in the self-consistent simulations was  $2 \times 10^6$ , while in the non self-consistent simulations it was significantly reduced.

#### 3. Results and discussion

In the contribution we studied the dependence of plasma-solid interaction on the plasma composition and pressure. In order to analyse the influence of negative ions, we introduced parameter c, the relative concentration of negative ions, ranging from 0 % for electropositive gases to 100 % for completely electronegative plasma. For the study of the pressure dependence we supposed that the cross-sections of interactions of charged particles with neutrals change linearly, while the concentrations behave according to experimental data [10].

In following figures obtained results of our computational study are summarized and some examples are demonstrated. The simulation was performed for several substrate/probe geometries – planar and cylindrical – with various radii.

• Distribution of electric potential – influence of pressure:

The spatial distribution of electric potential in the vicinity of metal substrates is demonstrated in Figs. 1 and 2. In Fig. 1 the sheath region for various concentrations of negative ions and two plasma pressures is shown. It can be seen that the thickness of the sheath increases with increasing concentration of negative ions and decreases with increasing pressure of plasma.

• Distribution of electric potential – influence of substrate geometry:

The influence of substrate geometry on the spatial distribution of electric potential in the vicinity of substrates is summarized in Fig. 2 for cylindrical substrates/probes of various radii (see also Fig. 1 for the planar substrate). The data in the figure were calculated at pressure 133 Pa. Other simulations proved that for cylindrical probes the dependence on the pressure is similar to the one shown in Fig. 1. From the comparison of obtained data it can be concluded that with decreasing curvature of the substrate the characteristics

resemble the data obtained for the planar configuration. The influence of negative ions has again the same tendency as shown in Fig. 1.

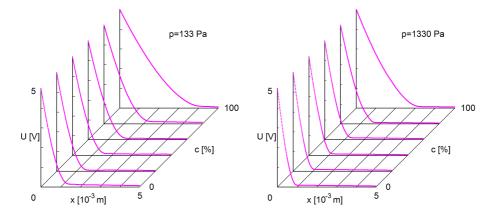


Figure 1: Potential distribution U(x) in the sheath region for various relative concentrations of negative ions c. Planar probe. Plasma pressure 133 (left) and 1330 Pa (right).

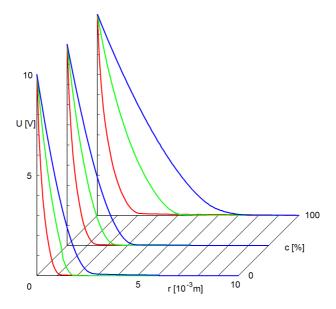


Figure 2: Potential distribution U(x) in the sheath for various relative concentrations of negative ions c. Cylindrical probes of radii  $2 \times 10^{-4}$  m (red),  $2 \times 10^{-3}$  m (green) and  $2 \times 10^{-2}$  m (blue).

## • Distributions of charged particles:

Besides the characterization of the sheath and presheath, the energy and angular distributions of charges particles as well as spatial distributions of individual charged species were studied in our computer experiment, too (for the derivation of distributions of electrons and both positive and negative ions the non self-consistent approach was better suited). It was found that while the substrate geometry influence the distributions of charged particles impinging substrate profoundly, the effect of the pressure (in studied limits 13 to 1330 Pa) is much less important. For details see our other contribution [11].

While the effect of substrate geometry can be simulated in two-dimensional particle model with no problem and the results correspond to the expectation, the modelling of plasma-solid interaction at higher pressures is difficult. The main problem is the intensification of scattering resulting in large time demands of particle codes and in the change of particle's movement, which rather resemble chaotic behaviour of electrons in solids. It was found that for these conditions both the standard PIC-MC method and the more advanced deterministic simulations are less advantageous compared to some other techniques.

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