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Study of sheath structure in electronegative gases at various pressures

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Abstract

The contribution is focused on the plasma-solid interaction in chemically active plasma. For detailed study of the processes in sheath region the computational approach was used and the computer experiment was based on the combination of two techniques – fluid modelling and non self-consistent particle modelling. The measurements performed in a dc glow discharge in mixtures of rare gases with oxygen were taken as input data for simulation. The influence of plasma composition and plasma pressure on the structure of the sheath and the presheath region has been analyzed.

1. Introduction

Low-temperature chemically active plasma based on electronegative gases is often used in modern technologies. Negative ions in such plasma affect the transport of charged species from the plasma to immersed substrates and in this way they influence the physical and chemical processes both in the sheath region and on the surface of substrates [1-3]. The surface treatment of materials at higher pressures, including the atmospheric pressure plasma, is another important problem in present plasma based or plasma chemical technologies [4,5].

The theoretical analysis of processes in electronegative plasma at medium and high pressures becomes difficult, since the theories derived for collisionless or slightly collisional plasmas lose their validity in these conditions. In such conditions the computational approach, both fluid modelling and particle simulations, proved to be the best solution.

Differences between common computational techniques are connected particularly with times of computation, accuracy and applicability scope. The most accurate self-consistent particle technique is not suitable for extensive analysis due to long computer running times. On the other hand, fluid description does not lead to detailed microscopic information about plasma processes. In the frame of this contribution, we have used the non self-consistent algorithm, where solving Poisson's equation is eliminated and external potential is used during the simulation instead [6,7]. In particular, we use electric potential resulting from the fluid model.

2. Computational description

All simulations were performed with data taken from O2/Ar plasma in the positive column of dc glow discharge. Only the most important species – electrons e^-, positive argon ions Ar^+ and negative oxygen ions O^- – were included into the model.

The combination of the fluid model and non self-consistent particle model was applied to plasma-solid interaction for variety of input parameters. The cylindrical geometry of immersed substrate was assumed. The main attention was devoted to the role of negative ions during the formation of sheath region in the vicinity of metal substrate or probe immersed into plasma.

2.1. Fluid model

Mathematical description of the fluid model is governed by moments of the Boltzmann equation. Continuity equation (1) and drift-diffusion approximation (2) for each species k of considered electronegative O2/Ar plasma and electron energy equation (3) were taken into account. The system of fluid equations was completed by Poisson's equation (4).

$$\frac{\partial n_\mathrm{k}}{\partial t} + \nabla \cdot \mathbf{J}_\mathrm{k} = R_\mathrm{k} \tag{1}$$

$$\mathbf{J}_\mathrm{k} = \pm \mu_\mathrm{k} n_\mathrm{k} \mathbf{E} - D_\mathrm{k} \nabla n_\mathrm{k} \tag{2}$$

$$\frac{\partial w_\mathrm{e}}{\partial t} + \nabla \cdot \left(-\frac{5}{3}\mu_\mathrm{e} w_\mathrm{e} \mathbf{E} - \frac{5}{3} D_\mathrm{e} \nabla w_\mathrm{e} \right) + e\mathbf{J}_\mathrm{e} \cdot \mathbf{E} + C_\mathrm{e,n} + \sum_j H_\mathrm{j} R_\mathrm{j} = 0 \tag{3}$$

$$\Delta \varphi = -\frac{e}{\varepsilon_0} \left(n_{\mathrm{Ar}^+} - n_{\mathrm{O}^-} - n_\mathrm{e} \right) \tag{4}$$

Quantities in equations (1-4) have their usual meaning – particle density n, particle flux $\mathbf{J}$, electric potential φ, electric intensity $\mathbf{E}$ and energy density w. D and μ are transport coefficients, R_k is particle source term, $C_\mathrm{e,n}$ is energy loss due to elastic electron-neutral collisions and the last term of equation (3) describes energy loss due to non-elastic collisions. Source terms and boundary conditions are described in [7,8].

The system of partial differential equations was solved by finite element method. Commercial package COMSOL Multiphysics 3.2 was used. Additional description of the fluid model is given in [8].

2.2. Particle model

Computational description of the interaction of electronegative plasma and a probe has already been introduced using the self-consistent particle approach with solving the Poisson's equation within the particle simulation [1]. Due to long computer running times of the self-consistent algorithms especially in more dimensions, the non self-consistent approach was used in this study. The algorithm combines the deterministic molecular dynamics simulation of motion of charged particles and the stochastic Monte Carlo treatment of collision processes between charged particles and neutral background. Collision processes included into the model are elastic scattering for each considered species, charge transfer for positive ions and excitation and ionization for electrons. Non self-consistent technique was applied to two-dimensional problem of plasma-solid interaction considering a cylindrical probe of infinite length immersed into plasma. Particular parameters of the model are summarized below.

3. Results

The attention was given to influence of plasma composition, plasma pressure and substrate geometry on the sheath structure. The results were carried out for various relative concentrations of negative ions in plasma, various values of the probe radius and two pressures 133 Pa and 1330 Pa.

In the first analysis we were interested in influence of pressure and plasma composition on the sheath structure. Parameters of the model were as follows: radius of cylindrical probe $R_p = 1 \times 10^{-4}$ m, probe voltage U_p = 10 V, size of the computational domain R = 0.01 m, number of charged particles $N = 2 \times 10^6$, electron temperature T_e = 23210 K, temperature of positive argon ions and negative oxygen ions T_i = 300 K, time step for molecular dynamics simulation of electrons $\triangle t_e = 1 \times 10^{-11}$ s, time step for molecular dynamics simulation of ions $\triangle t_i = 1 \times 10^{-8}$ s. The simulation was performed for various relative concentrations of negative ions and for two pressures p = 133 Pa and p = 1330 Pa. The potential distribution and charge species distribution in vicinity of the cylindrical probe is shown in Fig. 1.

The second scan shows dependence on probe radius. Parameters of the model were as follows: U_p = 10 V, R = 0.01 m, p = 133 Pa, $N = 2 \times 10^6$, T_e = 23210 K, T_i = 300 K, $\triangle t_e = 1 \times 10^{-11}$ s, $\triangle t_i = 1 \times 10^{-8}$ s. The simulation was performed for various radii of the cylindrical probe R_p with limiting case of planar probe and for two relative concentrations of negative ions 0 % and 50 %. Dependence of sheath structure and plasma quantities on the geometry of the immersed cylindrical probe is shown in Fig. 2.

4. Discussion and conclusions

According to computational simulation, expected logarithmic dependence of particle density on the distance from the cylindrical probe limits to linear dependence for probe of infinite radius (Fig. 2), which is in agreement both with results of experimental investigations and with the analytical solution of the diffusion equation.

The presence of negative ions in plasma influences not only the macroscopic parameters of the sheath as its thickness, but also the spatial distributions of the most important charged species in the sheath (Fig. 1,2). Considering the positive bias of the probe, only electrons are the main component of the sheath at low and medium relative concentrations of negative ions. The negative ions start to penetrate into the sheath at very large ion concentrations.

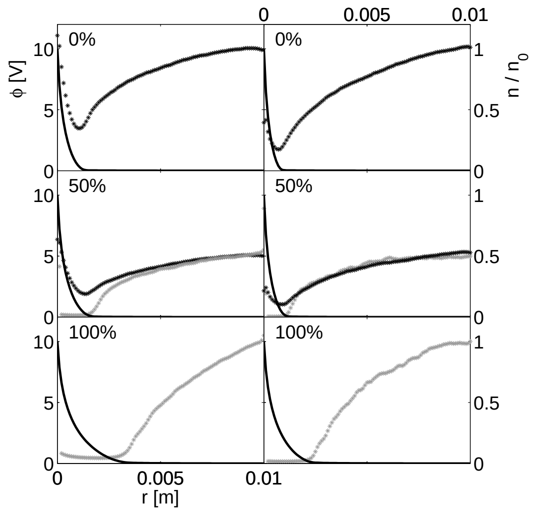

Figure 1: Normalized concentrations of electrons (black) and negative ions (grey) on right y axis and potential distribution on left y axis as functions of the distance from the substrate r. Cylindrical geometry. Left – pressure 133 Pa, right – pressure 1330 Pa. Parameter – relative concentration of negative ions. Density of undisturbed plasma is $n_0 = 1 \times 10^{15}\ m^{-3}$ for 133 Pa and $n_0 = 3.16 \times 10^{15}\ m^{-3}$ for 1330 Pa.

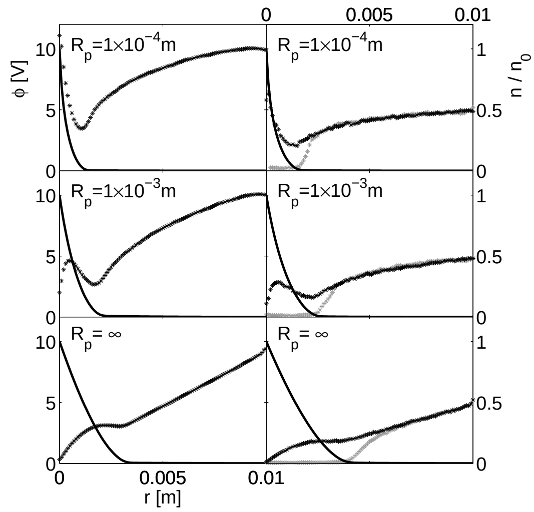

Figure 2: Normalized concentrations of electrons (black) and negative ions (grey) on right y axis and potential distribution on left y axis as functions of the distance from the substrate r. Cylindrical geometry. Left – relative concentration of negative ions 0%, right – relative concentration of negative ions 50%. Parameter – radius of the probe.

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References

[1] R. Hrach et al., Thin Solid Films **459**, 137 (2004)

[2] R. Hrach, V. Hrachová and M. Vicher, Vacuum **76**, 425 (2004)

[3] J. I. Fernández Palop et al., J. Phys. D: Appl. Phys. **29**, 2832 (1996)

[4] C. Leys, Contrib. Plasma Phys. **44**, 542 (2004)

[5] J. I. Fernández Palop et al., J. Phys. D: Appl. Phys. **38**, 868 (2005)

[6] D. Trunec, P. Španěl and D. Smith, Contrib. Plasma Phys. **42**, 91 (2002)

[7] E. Havlíčková, P. Bartoš and R. Hrach, J. of Phys. Conf. Series **63**, 012019 (2007)

[8] P. Bartoš and R. Hrach, Czech. J. Phys. **56**, B638 (2006)