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## Parametric computational study of sheaths in multicomponent Ar/O<sub>2</sub> plasma

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# Parametric computational study of sheaths in multicomponent Ar/O<sub>2</sub> plasma

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**Abstract.** Our study is devoted to sheath structures emerging in Ar/O<sub>2</sub> plasma. By means of two dimensional PIC/MCC computer model two configurations were investigated – sheath structure in the vicinity of a cylindrical Langmuir probe for two different biases and changes of the sheath structure when a cylindrical probe passes into a semi-planar probe. It was shown that O<sup>+</sup> ions play important role in shielding out negative bias of a solid immersed in Ar/O<sub>2</sub> plasma and edge effects of a semi-planar probe on its sheath structure were evaluated.

## 1. Introduction

Plasma that contains more species of both negative and positive ions [1–3], so called multicomponent plasma, is widely used in many industrial applications nowadays, particularly in plasma-assisted technologies (i. e. thin film deposition, plasma etching, etc.). Multicomponent plasma is often a mixture of reactive gases that is chemically active and composed of mutually interacting charged and neutral particles that are out of the thermodynamic equilibrium. Thus, it is very demanding to describe it theoretically and therefore it is often taken advantage of computer modelling approach in multicomponent plasma research [4, 5].

Our contribution is devoted to investigation of sheath structures that are formed in the surroundings of solids immersed in Ar/O<sub>2</sub> plasma. The results were obtained by 2D PIC/MCC computer model, which is described in Section 2. Section 3 contains results of the computer simulation of a biased cylindrical Langmuir probe immersed in Ar/O<sub>2</sub> plasma. Further, results of a parametric study that captures a transition from a cylindrical to a planar solid substrate are also presented here.

## 2. Modelling technique

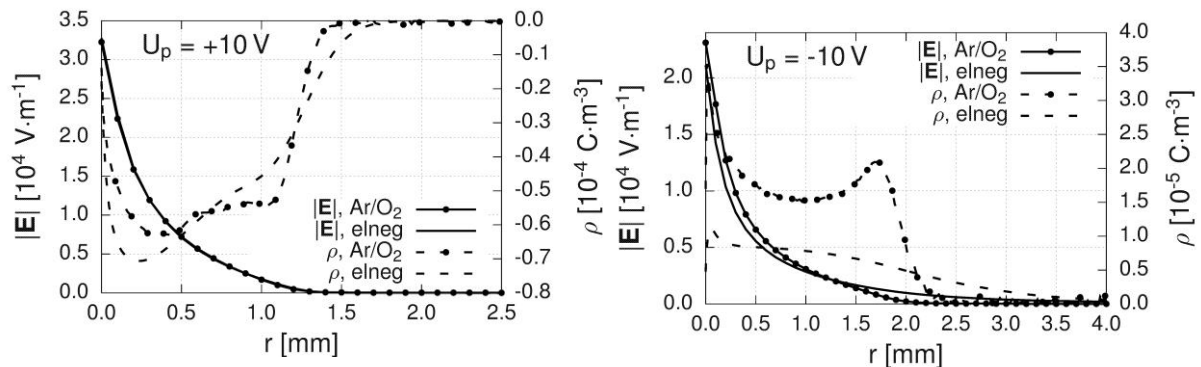
The sheath structures in the present contribution were modelled by means of two-dimensional PIC/MCC computer model that was already used to explore sheath structures in purely electronegative plasma [6]. The results of the chemical kinetics model published in [7] were adopted and used as an input for our simulation. The kinetic model takes into account more than 100 reactions between neutral, charged and excited species in Ar/O<sub>2</sub> plasma that are described by rate constants and consequently, continuity equations for all species in the ensemble are solved to obtain their number densities. Only the most important charged particles were considered in the PIC simulation: e<sup>-</sup>, O<sup>-</sup>, Ar<sup>+</sup>, O<sup>+</sup>, O<sub>2</sub><sup>+</sup>. Neutral particles that were taken into account: Ar, O, O<sub>2</sub>. Scattering processes were

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treated by modified null collision method [8]. The most important interactions between charged and neutral particles that were included in the PIC simulation:  $[e^-, \text{Ar}]$  – elastic scatter, excitation (11.5 eV), ionization (15.8 eV);  $[e^-, \text{O}]$  – elastic scatter, excitation (1.97 eV, 4.19 eV), ionization (13.62 eV);  $[e^-, \text{O}_2]$  – elastic scatter, ionization (12.06 eV);  $[\text{Ar}^+, \text{Ar}]$  – elastic scatter, charge transfer;  $[\text{Ar}^+, \text{O}]$ ,  $[\text{Ar}^+, \text{O}_2]$ ,  $[\text{O}^-, \text{O}]$ ,  $[\text{O}^+, \text{O}]$ ,  $[\text{O}_2^+, \text{Ar}]$ ,  $[\text{O}_2^+, \text{O}_2]$  – charge transfer;  $[\text{O}^-, \text{O}_2]$  – elastic scatter. Parameters of investigated Ar/O<sub>2</sub> discharge:  $E/N = 60$  Td, pressure 133 Pa, initial Ar to O<sub>2</sub> concentration ratio 50:50. The computational domain had dimensions  $(4.0 \times 4.0) \cdot 10^{-2}$  m in all investigated configurations and the computational mesh of  $400 \times 400$  cells was used to solve Poisson's equation.

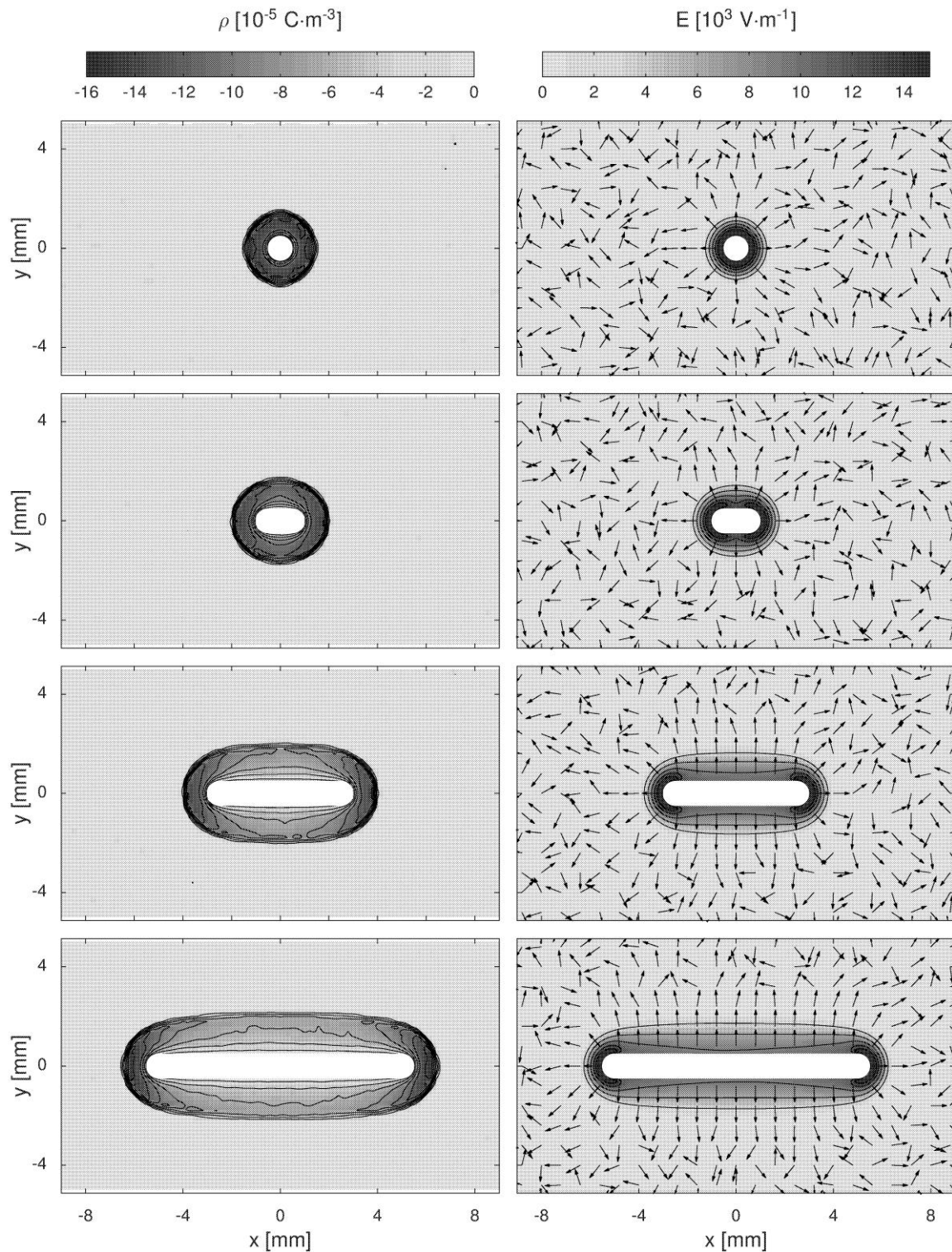


**Figure 1.** Electric field intensity (solid lines) and net charge density (dashed lines) in the vicinity of a single Langmuir probe with  $2 \times 10^{-4}$  m radius immersed in Ar/O<sub>2</sub> plasma. Two different biases of the probe  $U_p$  are presented. The results were compared to those for simplified electronegative plasma [6].

### 3. Computer simulations of Ar/O<sub>2</sub> plasma

First of all, the sheath around a single cylindrical Langmuir probe with  $2 \times 10^{-4}$  m radius was investigated. Two different biases of the probe with respect to the plasma potential were considered:  $\pm 10$  V. The results are depicted in the figure 1 and compared to those for simplified 50 % electronegative plasma [6]. (The term simplified electronegative plasma means in our context argon plasma in which O<sup>-</sup> ions are also present; therefore e<sup>-</sup>, Ar<sup>+</sup> and O<sup>-</sup> ions represent the only charged particles in this first approximation of Ar/O<sub>2</sub> plasma. The amount of O<sup>-</sup> ions is given by the electronegativity  $\alpha$  which is defined as:  $\alpha = n_{O^-} / (n_{e^-} + n_{O^-})$ , where  $n_{O^-}$  denotes number density of O<sup>-</sup> ions and  $n_{e^-}$  that of electrons.) Significant differences are observed for  $-10$  V bias of the probe. In this case O<sup>+</sup> ions play important role in shielding out of the negative probe potential since they are lighter than Ar<sup>+</sup> ions and more of them get into the sheath. As a result of their presence sheath becomes thinner and electric field increases. On the other hand, the situation in Ar/O<sub>2</sub> plasma is quite similar to that in electronegative plasma for  $+10$  V bias of the probe.

The next investigated problem is depicted in the figure 2. The sheath structures during the transition from a cylindrical Langmuir probe of  $5 \cdot 10^{-4}$  m radius to a semi-planar probe of  $5 \times 10^{-4}$  m thickness were examined for several widths of the semi-planar probe:  $(2; 6; 11) \times 10^{-3}$  m. It can be observed that the parameters of the sheath (thickness and magnitude of electric field) near the rounded edges of the semi-planar probe remains the same as in the case of sheath near the cylindrical probe. However, the sheath structure in the middle part of the semi-planar probe significantly changes with



**Figure 2.** Net charge density and electric field intensity in the sheath structure around a cylindrical probe and a semi-planar probe immersed in  $\text{Ar}/\text{O}_2$  plasma. Bias of the probes:  $+10$  V. Only  $(1.8 \times 1.0) \times 10^{-2}$  m middle part of the computational domain is depicted. The solid lines mark isolines of the charge density with  $1 \times 10^{-5} \text{ C}\cdot\text{m}^{-3}$  step and isolines of the electric field intensity with  $3 \times 10^3 \text{ V}\cdot\text{m}^{-1}$  step.

increasing width of the probe – electric field intensity decreases and sheath thickness increases. The cylindrical probe sheath solution passes into the solution of a planar probe in this area.

#### 4. Conclusions

Two dimensional PIC/MCC computer model of multicomponent Ar/O<sub>2</sub> plasma was used to investigate sheath structures in the vicinity of immersed solids. It was proven that O<sup>+</sup> ions significantly affect sheaths near the negatively biased solids and it was shown for negatively biased cylindrical Langmuir probe. The edge effects were evaluated for semi-planar probe of different width. It was demonstrated how the sheath structure corresponding to a cylindrical probe passes into the sheath of a planar probe in the middle part of the probe.

#### Acknowledgments

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