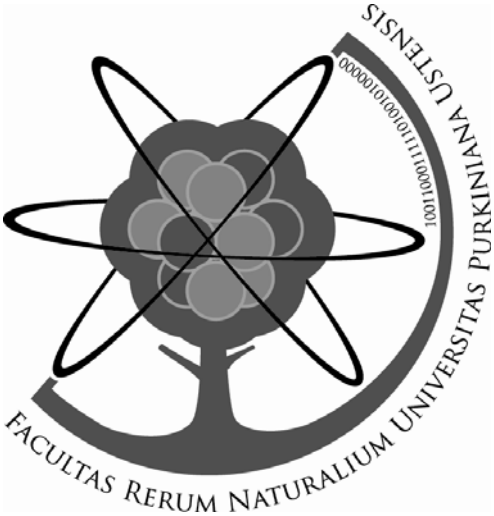
J. E. PURKINJE UNIVERSITY IN ÚSTÍ NAD LABEM

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

Abstract of Doctoral Thesis



COMPUTATIONAL STUDY OF PLASMA-SURFACE INTERACTIONS IN CHEMICALLY ACTIVE PLASMA

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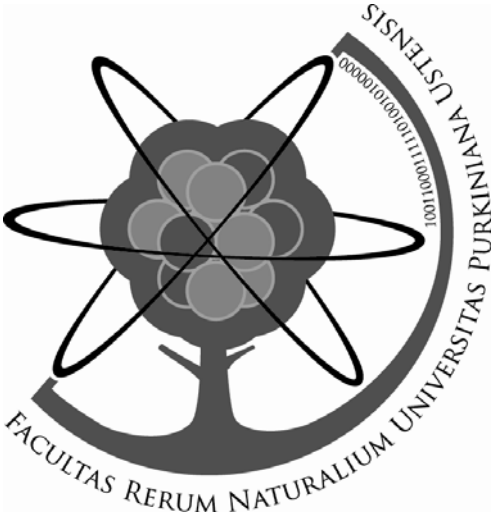

MODELOVÁNÍ INTERAKCE CHEMICKY AKTIVNÍHO PLAZMATU S VNOŘENÝMI PEVNÝMI LÁTKAMI

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CONTENTS

Abstract EN

This Ph.D. thesis is focused on investigation of a plasma-solid interaction with help of computer modelling methods. Two sets of models were created for this purpose. First of them is a fluid model based on a macroscopic kinetic approach. It simulates volume processes in a DC glow discharge in Ar/O_2 mixture. The kinetic scheme of the model contains 161 reactions between 16 neutral, charged, and excited species. As results, the time dependencies of concentrations of neutral, excited, and charged species were obtained for various discharge parameters. The second type of models are both one-dimensional and two-dimensional multicomponent particle models based on the PIC-MC technique; they are performed for the electronegative plasma of Ar/O_2 mixture with a cylindrical configuration. The results from the first model of volume processes are used as input concentrations of the species in the second model. The main attention is paid to a sheath development in dependences on various plasma parameters (gas ratio, pressure, probe radius, etc.), in both the steady and dynamic states.

Abstract CZ

Předkládaná práce je zaměřena na studium interakce nízkoteplotního plazmatu s vnořenou pevnou látkou za pomoci počítačového modelování. Za tímto účelem byly vytvořeny dva okruhy modelů. První z nich je spojitý model založený na makroskopickém kinetickém přístupu. Model simuluje fyzikální procesy, které se odehrávají v objemu plazmatu směsi Ar/O_2 v kladném sloupci stejnosměrného doutnavého výboje. Pro popis těchto procesů bylo použito 161 chemických reakcí mezi 16 neutrálními, nabitými a excitovanými částicemi. Výsledkem modelu bylo získání časových průběhu koncentrací neutrálních, nabitých a excitovaných částic pro různé výbojové parametry. Druhou částí modelů jsou jednorozměrné a dvourozměrné multikomponentní částicové modely založené na PIC-MC technice. Modely byly vypracovány pro elektronegativní plazma směsi Ar/O_2. Jako vstupní koncentrace pro tyto modely byly použity výsledky z předešlého modelu objemových procesů. V práci je hlavní pozornost věnována vývoji sheathu v závislosti na mnoha parametrech plazmatu (poměr plynů, tlak, poloměr sondy, atd.), a to jak pro statický režim, tak i dynamický.

1 Introduction

Understanding of physical and chemical processes taking place during a plasma-solid interaction is important for plasma chemical technologies as well as for probe diagnostics in a low-temperature plasma. While the analysis of experimental data is rather simple for collisionless or slightly collisional plasmas at low pressures as there exist both well-established theories (e.g. [1, 2]) and computational techniques [3, 4], the situation is quite different at higher pressures and for chemically active plasmas used in modern plasma science. The electronegative gases are used, especially, in various plasma-chemical technologies, however the presence of three-component plasma containing electrons, positive, and negative ions (e.g. [5]) influences the formation of a sheath and modifies the fluxes of the charged species to a substrate or a probe in this way.

In real conditions, there often exist more than one type of both negative and positive ions in the plasma, e.g. during a plasma oxidation process [6] in the Ar/O_2 gas mixture. For the analysis of such complex processes in so-called multicomponent plasmas, it was found that the computational approach is the best suited especially in a combination with experimental studies. Such types of problems was analysed by the fluid simulation in [7, 8], however, the particle simulation codes can give deeper insight into the processes in the sheath region according to our experience.

Therefore, transport of both electrons and ions to metal substrates/probes immersed into the multicomponent plasma was studied by a computer modelling based on a particle simulation technique, i.e., a combination of the molecular dynamics and Monte Carlo methods in this thesis. The macroscopic kinetic approach was chosen to study chemical processes in the electronegative plasma. The simulations were performed for both static and dynamic regime.

2 Aims of the thesis

Goal of the Ph.D. thesis is study of the interaction between a low-temperature plasma and a surface of immersed substrates during plasma oxidation processes by methods of computer modelling.

The goals can be summarized into the following parts:

- to create a computer model for simulations of chemical processes in an electronegative plasma and to obtain concentrations of all species involved into the simulations for various plasma parameters,
- to create one- and two-dimensional particle models of interaction between a multicomponent plasma and the immersed substrate; it is based on the previous results,
- to study properties of the plasma-solid interaction for both a static and dynamic regime
- to use the models created to study of a low-temperature plasma in Ar/O_2 mixture

3 Description of created computer models

Two sets of computer models – a model of volume processes and a model of plasma-solid interaction were created for achieving of the aims of the thesis. The main goal of the first model is to obtain concentrations of all species involved into the simulations for specific plasma parameters. Part of these results is consequently used as an input into the second set of models which simulate interactions between a multicomponent plasma and an immersed substrate.

3.1 Model of volume processes

The model simulates the processes in a positive column of a DC glow discharge in a mixture of Ar and O_2 gases. The model is based on a macroscopic kinetic approach, i.e. on a solution of continuity equations for all species introduced into the model. The set of equations is solved by the numerical Bader-Deuflhard method [9]. A kinetic scheme of the model contains 129 reactions between 12 neutral, charged, and excited species for pure oxygen (electrons, O, O_2, O_3, O^-, O_2^-, O_3^-, O^+, O_2^+, $O(^1D)$, $O_2(^1\Delta_g)$, $O_2(^1\Sigma_+)$), 12 reaction between 5 neutral, charged, and excited species for pure argon (electrons, Ar, Ar^+, Ar*, Ar_2^+) and 20 reactions between argon and oxygen gases. The chemical reactions and corresponding rate constants were obtained from both the literature [10-33] and our own calculations. The same rate constants depending on electron energy distribution function (EEDF) were calculated using the computer program ELENDIF [34] which simulates the EEDF in the dependence on discharge parameters. Phelps' cross sections [35] and some others [14, 28] were used as input data for the program ELENDIF. The whole list of the chemical reactions used with the rate constants and the used cross sections are available at the end of the thesis.

3.2 Model of plasma-solid interaction

Several one- and two-dimensional computer models, called 1d3v and 2d3v models respectively, were created for the study of plasma-solid interactions in multicomponent plasma. The models are based on a self-consistent particle simulation technique and combine the molecular dynamics and Monte Carlo methods. The simulations of the plasma-solid interactions were performed for a cylindrical probe.

The models consist of the following parts:

- *Source of particles:* Undisturbed plasma consisting of the subsequent charged species: Ar^+, O^+, O_2^+, electrons, O^-, and O_2^-. The concentrations of the charged particles were taken from the model of volume processes. It was supposed that both electrons and all kinds of ions have the Maxwell velocity distribution with corresponding temperatures in the undisturbed plasma.
- *Equations of motion:* Newton's equations of motion are solved by the second order Verlet algorithm [9].
- *Force calculations:* Movement of the particles is influenced by the self-consistent electric field created by all other particles and by the substrate bias. The input data for the Poisson equation were prepared by the standard Particle-In-Cell technique in a Cloud-In-Cell modification [36]. In the two-dimensional model is the Poisson equation solved with help of the Conjugate Gradients method (CG) [37].
- *Interactions:* Scattering of the charged particles by neutrals is handled stochastically by the Monte Carlo technique - Null collision method [38]. The set of possible interactions consists of elastic collisions for all kinds of particles, excitations, and ionizations of Ar, O, and O_2 by electrons, and of the charge transfer between Ar atoms and Ar^+ ions.
- *Boundary conditions:* The middle of the probe is located at $r = 0$ m (unless otherwise indicated); electron secondary emissions and escapes of the charged particles from the probe were not included. The undisturbed plasma is considered to be at a distance $r = 0.5\times10^{-2}$ m from the probe.

Different time steps for electrons and heavier particles are used for speeding-up the calculations in the static regime. The time steps were $\Delta t_e = 10^{-12}$ s for electrons and $\Delta t_i = 10^{-9}$ s for ions in our simulations of the plasma-solid interaction. However, this technique cannot be used for the simulations of dynamic properties of plasma. In this case, the time steps for all kinds of the particles were held between 10^{-11} and 10^{-12} s and the simulations were computed mainly on multiprocessor workstation to speed-up. Other parameters used were: the temperature of electrons $T_e = 2$ eV, temperature of ions and neutrals $T_i = 300$ K, the radius of cylindrical probe was mostly $R = 1\times10^{-4}$ m.

4 Main results

As mentioned above, the volume process model was developed for better understanding of the representation of particular species of the charged particles in Ar/O_2 mixture. Time dependences of the neutral, excited and charged particles concentrations for various discharge parameters are resulted from this model. The concentrations as a function of time for all included particles with specified experimental conditions are displayed in Fig 4.1.

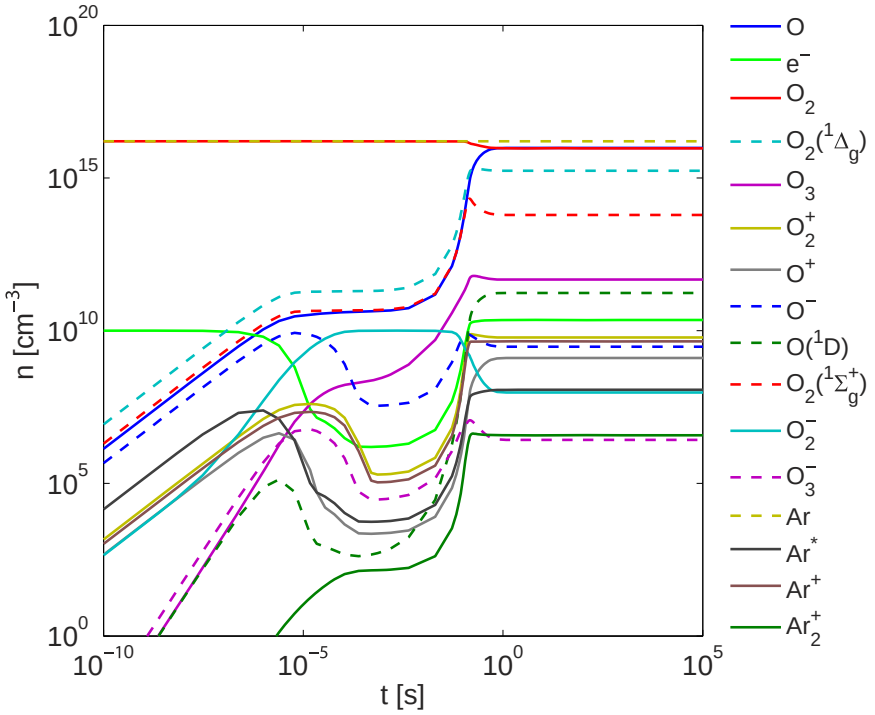

Fig. 4.1: Time dependences of concentrations of the species (discharge parameters E/N = 60 Td; pressure p = 133 Pa and gas ratio Ar:O_2 is 50:50).

We presume only oxygen and argon in the beginning (t = 0) of our simulation. After the discharge is applied, chemical reactions between the injected electrons and neutral oxygen or argon atoms cause a creation of the other particles. These particles chemically interact among them and create the other species. The time scale for these processes is to 1 s. The chemical equilibrium is then established and the concentration remains constant.

In simplified particle models of the plasma-solid interactions in electronegative plasma, only the most important charged species are typically used. As we can see from Fig. 4.1, the most important charged particles dominating in the sheath formation should be e^-, Ar^+, O_2^+, O^+, O^-, and O_2^- in this kind of plasma. Based on these results it was decided that above mention charged particles will be used for the following model of interactions between the multicomponent plasma and the immersed substrates.

In Figs. 4.2 and 4.3 the change of particle concentrations is seen in plasma when changing the ratio of oxygen and argon gas. The rapid decrease of the concentration of argon ions is caused by the increasing concentration of oxygen. This phenomena is also experimentally observed by adding a small amount of oxygen gas to argon plasma when changing the colour of the discharge.

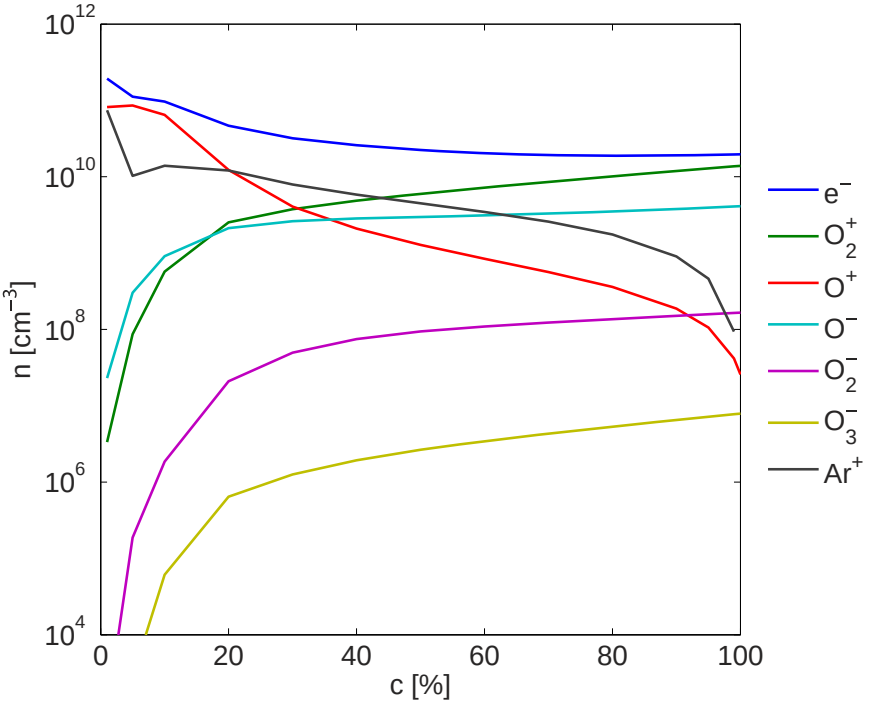

Fig. 4.2: Concentrations of charged particles for various O_2:Ar ratios. c = 0 % means pure argon plasma, c = 40 % means ratio 40:60 of Ar/O_2 mixture, c = 100 % means pure oxygen plasma. Discharge parameter E/N = 60 Td; pressure 133 Pa.

Next part of the results is about investigating both the static and dynamic properties of multicomponent plasma near the surface of immersed substrates for various pressures and discharge parameters. The potential distributions in the sheath and presheath were obtained and the spatial distributions and time evolutions of the concentrations of the most important charged particles were determined.

The concentrations of charged particles and the potential distribution in close vicinity of the probe as a function of the probe radius are displayed in Fig. 4.4. As can be seen, greater the radius is wider is the sheath. It is caused by a stronger electric field generated by the probe with smaller radius. Behavior of the charged particles is adhered to the gradient of electric potential near the probe.

Higher concentrations of negatively charged particles are observed on the left side of Fig. 4.4 where the probe radius is 50 μm. When increasing the probe radius the concentrations are

decreasing because of the above mentioned electric potential gradient. The high concentration at small radii is not caused only by the gradient of electric potential but also by accumulating of the negatively charged particles to a small volume in close vicinity of the probe. It is worth to mention that by unlimited increasing of the probe radius we change the configuration to planar.

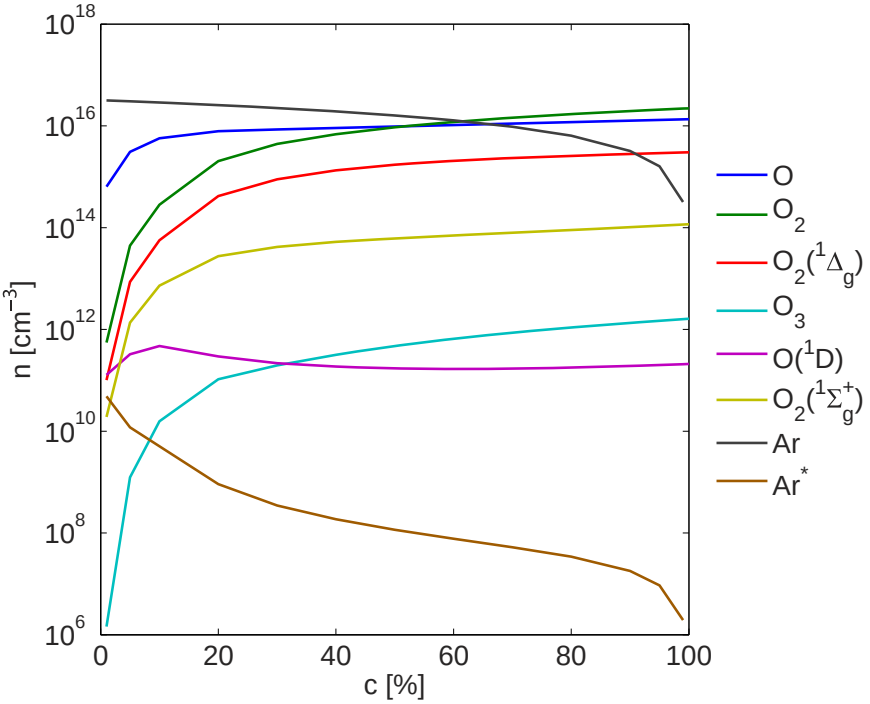

Fig. 4.3: Concentrations of particles for various O_2:Ar ratios. c = 0 % means pure argon plasma, c = 40 % means ratio 40:60 of Ar/O_2 mixture, c = 100 % means pure oxygen plasma. Discharge parameter E/N = 60 Td; pressure 133 Pa.

Energy and velocity distributions for electrons and negatively charged oxygen ions were measured in various distances from the probe. These distances are marked by ticks in Fig. 4.4 and results are described in detail in the thesis.

The following results are related to the study of the sheath structure forming of multicomponent plasma in the vicinity of the immersed probe. It is clear that the sheath dynamics depend on the mobility of individual species and therefore profoundly influence the fluxes both their magnitudes and composition of charged particles bombarding the surface of the substrates.

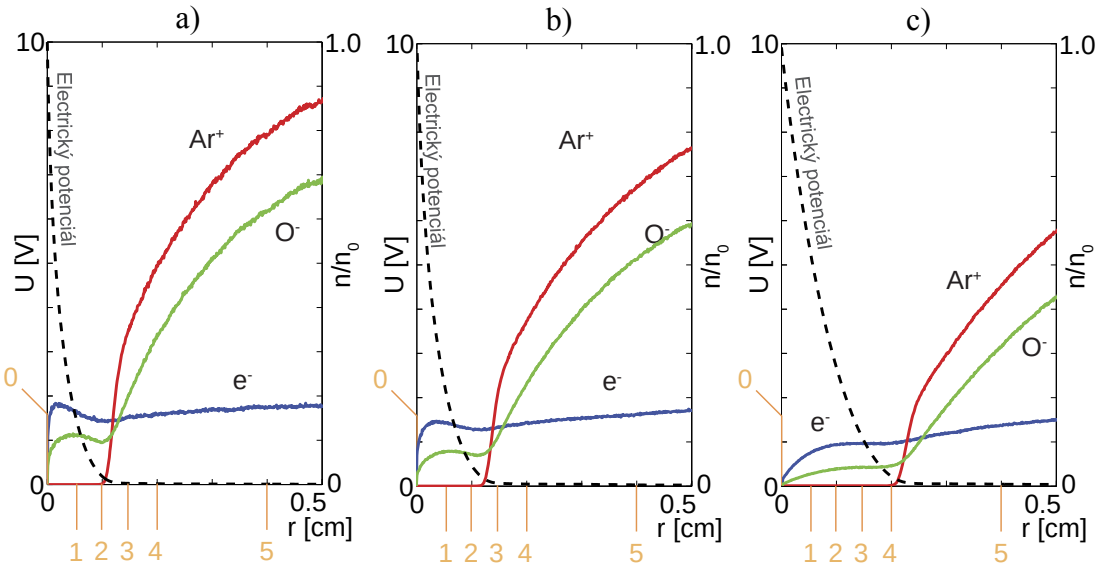

Fig. 4.4: Spatial distribution of charged species (solid lines) in the vicinity of cylindrical probe in electronegative plasma for various radii of the probe - a) 50 μm, b) 100 μm, c) 1 mm. Voltage bias +10 volts; pressure 133 Pa; fraction of oxygen ions 80%. The distribution of electric potential in the sheath is marked by the dashed line. In figures are marked places (0-5) where we obtained the energy and velocity distributions of electrons and negative oxygen ions. Distances from the probe are : 0 – probe surface, 1 - 0.5 mm, 2 - 1 mm, 3 - 1.4 mm, 4 – 2 mm, 5 - 4 mm.

In Fig. 4.5 the response of a multicomponent plasma to the application of a step voltage 0 V → +10 V is shown. The starting point of the simulation, $t = 0$, corresponds to the steady-state situation without any applied voltage when the spatial distributions of charged particles are given by the simple diffusion solution. From this figure it can be seen the formation of the sheath - the response of electrons is much quicker than the response of heavy particles, see both the concentrations of all species and the distribution of electric potential. Electrons are much more important for the compensation of a positive charge of positively biased electrode. Similarly, Fig. 4.6 shows the sheath structure forming but in the steady state of dynamic processes whereat a rectangular course of the voltage on the probe was used, with the frequency of 1 MHz. The behaviour of particles is similar to the previous case; however, the influence of different masses of particles is more important for the forming of the sheath structure. Behaviour of the charged particles is described in detail in the thesis.

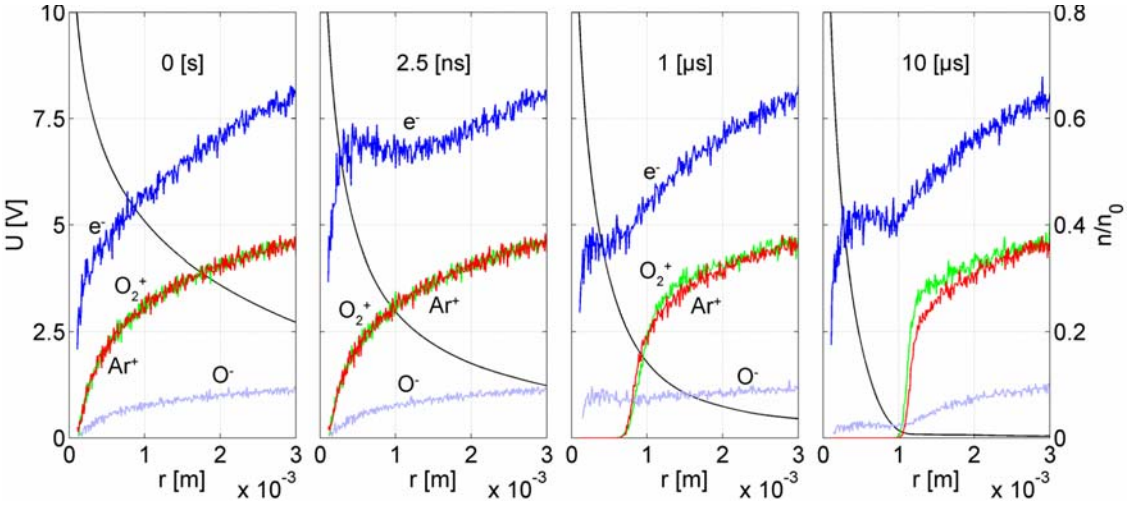

Fig. 4.5: The spatial distribution of charged species after applying the step voltage 0 → +10 volts at the time t = 0 s, together with the distribution of the electric potential near the electrode (full black line). Pressure 133 Pa.

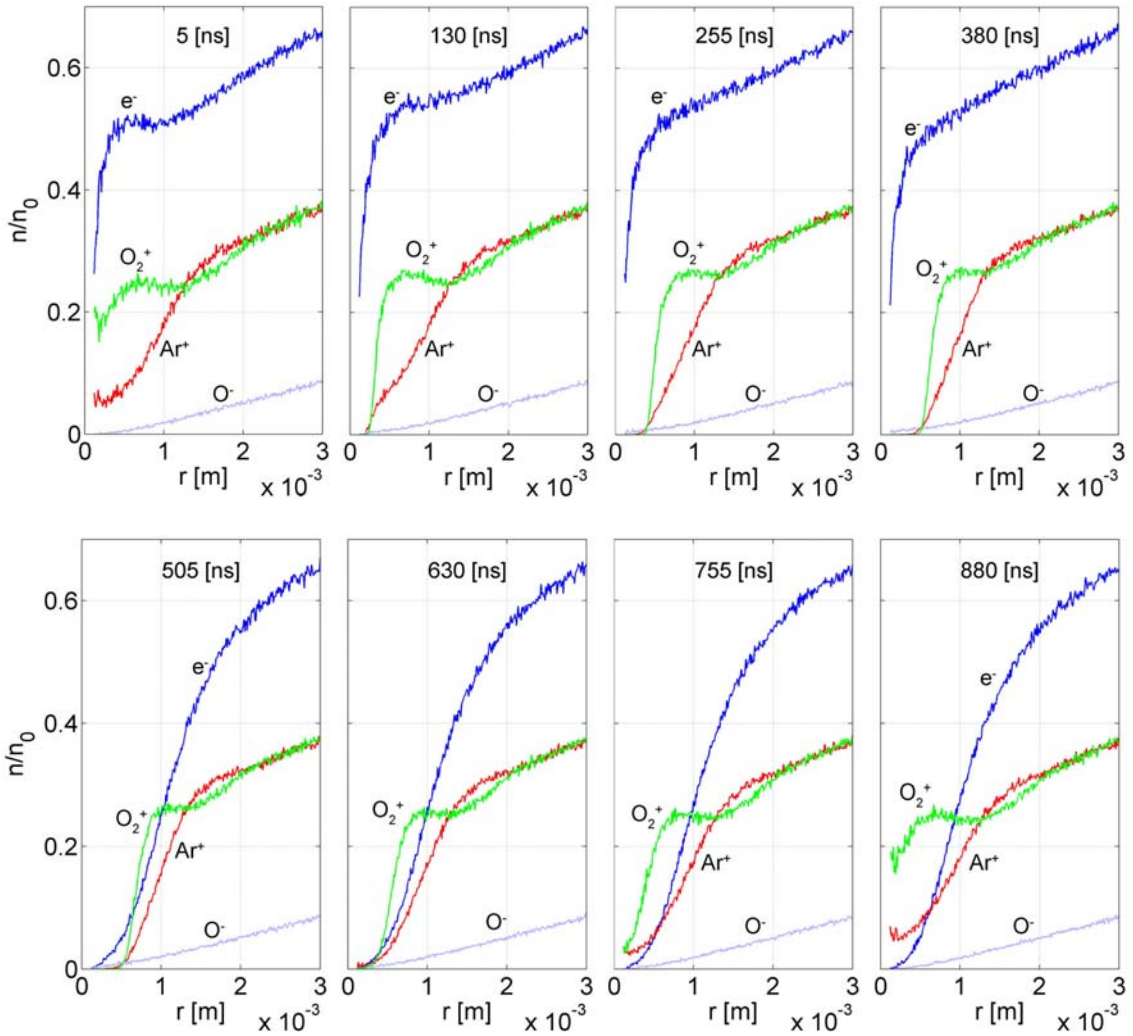

Fig. 4.6: The spatial distribution of charged species at the steady state of dynamic processes – top is first half of time period (jump -10 V to + 10 V at t = 0 ns) and bottom is second half of time period (jump +10 V to - 10 V at t = 500 ns). Rectangular course of voltage on electrode, frequency 1 MHz. Pressure 133 Pa.

We also tried other periodic courses. In Fig. 4.7 the time developments of electron concentrations near the substrate for the rectangular course (left) and sinusoidal course (right) of electrode voltage bias, both with frequency 1 MHz, are compared.

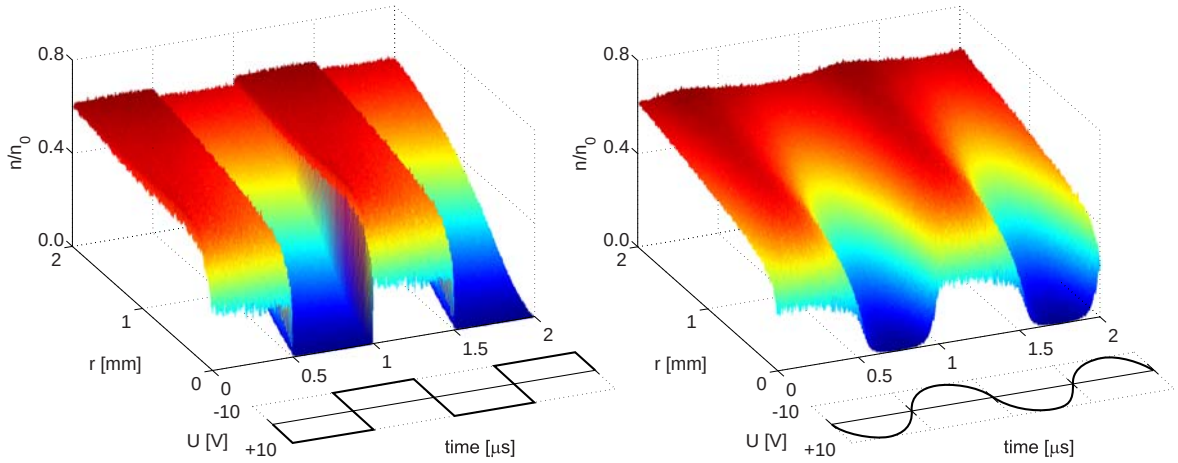

Fig. 4.7: Comparison of time developments of electron concentrations near the substrate. The rectangular and the sinusoidal waveform of the electrode voltage bias (frequency 1 MHz) are shown below. Pressure 133 Pa.

The two voltage courses were also compared from another point of view in Fig. 4.8. It illustrates the time developments of current densities of the charged species when rectangular (Fig. 4.8 left) and sinusoidal voltage bias (Fig. 4.8 right) is applied on the substrate. The behavior of charged particles is fundamentally determined by the particle signs and the differences between electron and ion masses. However, some positive ions can be found impinging the substrate even after changing the negative voltage bias to a positive one, which is caused by their inertial mass. Similar behavior is observed for the negative oxygen ions.

The results presented above were only for the pressure 133 Pa. In the rest of the paper, the results for different pressures are presented and compared together with their influence to the sheath structure.

The comparison is done for both the static regime when a constant value of the voltage bias +10 V on the electrode was kept, and the dynamic regime when the sinusoidal voltage bias was applied. Fig. 4.9 shows the spatial distributions of the charged species in the vicinity of the cylindrical probe biased +10 V in the electronegative plasma (Ar/O_2 mixture) for two pressures, 150 Pa and 600 Pa. Comparing these results we can see that the sheath region is smaller for the higher pressure. This difference is due to a higher volume density of the particles in the vicinity of electrode in the case of the higher pressure and hence, it follows a better shielding of the electrode voltage bias.

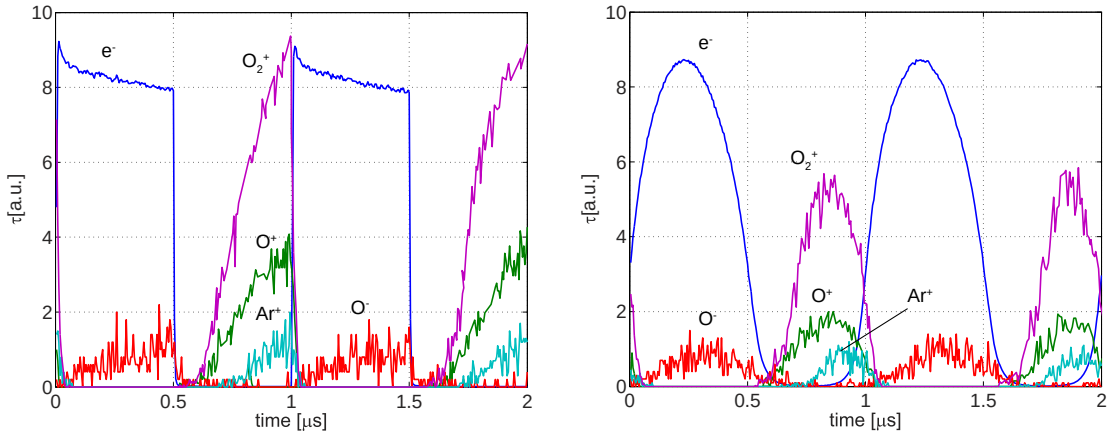

Fig. 4.8: Time developments of current densities of electrons, of negative and positive atomic oxygen ions (1000x magnified) and of positive molecular oxygen and argon ions (500x magnified) in Ar/O_2 plasma. Rectangular voltage bias (left) and sinusoidal voltage bias (right) is applied on the substrate. Ratio $Ar:O_2$ is 20:80, pressure 133 Pa.

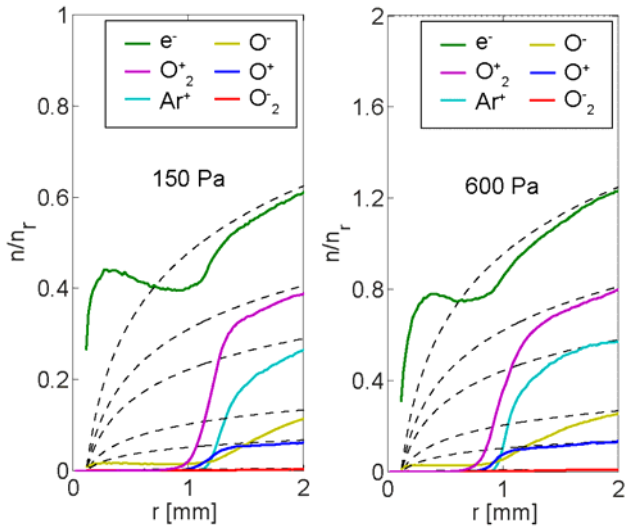

Fig. 4.9: Concentrations of charged species in the vicinity of cylindrical probe in electronegative plasma for $Ar:O_2$ ratio 50:50. Pressure 150 Pa (left) and 600 Pa (right). Voltage bias +10 V. All concentrations are divided by $n_r = 1\times10^{15}$ m^{-3}. Dashed lines show an analytical solution of diffusion equations. Probe is located at $r = 0$ mm.

Due to the higher volume density of the charged particles these differences can be better seen on the following figures. Fig. 4.10 demonstrates the time developments of concentrations of electrons and argon ions for two pressures (150 Pa and 600 Pa) in steady state of dynamic processes, whereat a sinusoidal course of voltage bias on the electrode was used; it changed at the frequency of 1 MHz. It can be seen different behaviour between electrons and argon ions due to their different masses, but there are mainly seen changes in behaviour of the charged particles for the higher pressure due to the higher volume density of the particles causing a smaller mobility of the particles. For example, if we compare the concentrations of electrons

in the immediate vicinity of the probe, we can observe, that concentration of electrons is much smaller in the case of higher pressure than in the case of lower pressure. As was mentioned before, it is due to the smaller mobility of electrons in the higher density plasma, where collisions between particles are occurring more frequently than in the case of lower pressure. If we look at the concentrations of argon ions for lower and higher pressures, we can see a bigger difference of concentration in the vicinity of the probe. In this case, there are two factors which are restricting mobility of argon ions: higher density (the same behaviour as in case of electrons) and much higher mass. In consequence of these restrictions, the argon ions are moving only up to 1 mm from probe.

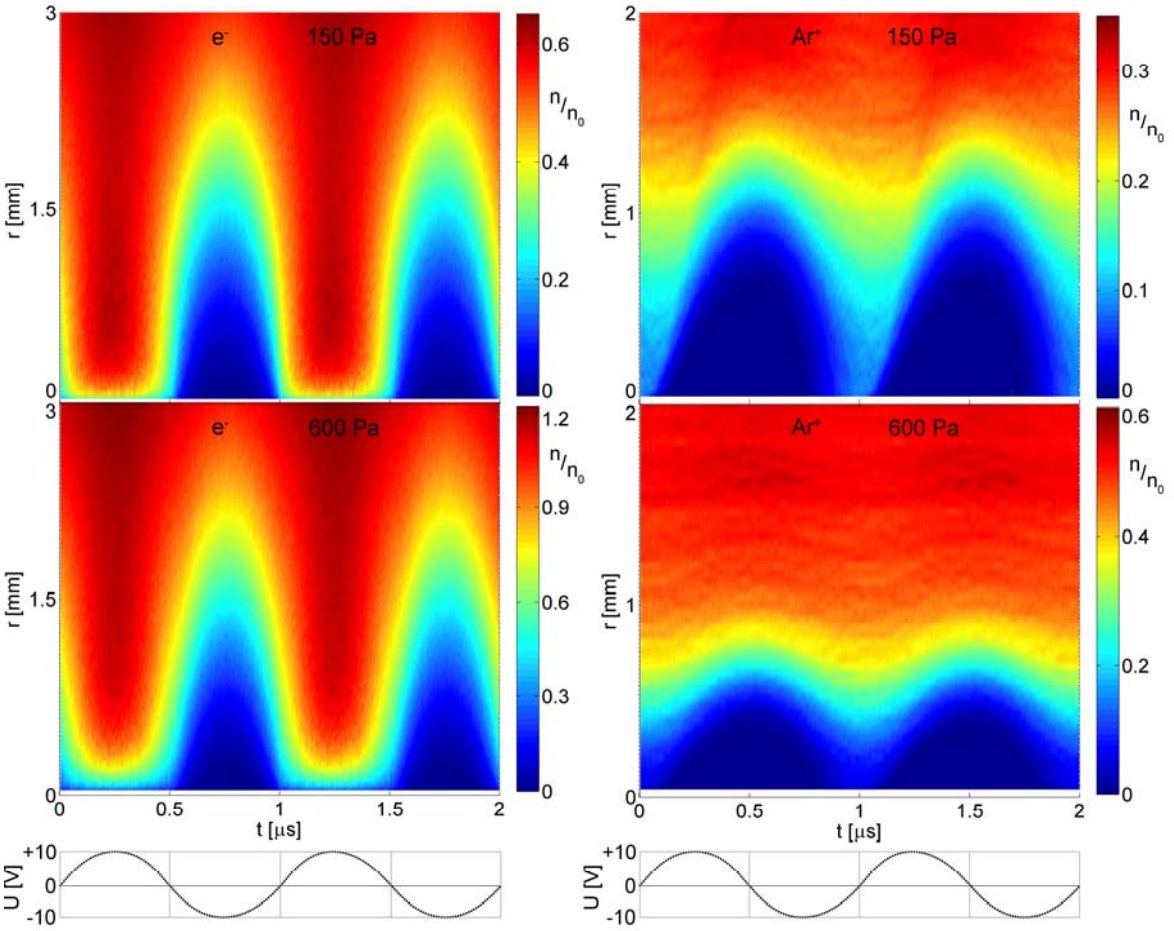

Fig. 4.10: Time developments of concentrations of electrons (left) and Ar ions (right) in the vicinity of substrate at the steady state of dynamic processes. Parameters: pressure 150 Pa (top) and 600 Pa (bottom), sinusoidal course of voltage bias on the electrode (shown below), frequency 1 MHz, Ar:O_2 ratio 50:50. Cylindrical probe with radius 1×10^{-4} m at $r = 0$ mm. All concentrations are divided by $n_0 = 1\times10^{15}$ m^{-3}.

Fig 4.11 shows the time developments of concentrations of other charged particles – negative oxygen ions and positive molecular oxygen ions. It can be seen, that these figures have not sharp borders as in case of argon ions. It is due to the using only elastic collisions for oxygen ions with other particles. In case of the negative oxygen ions it is also due to the smaller concentration of negative oxygen ions in the model. However, behavior of the particles is similar to behavior of the argon ions.

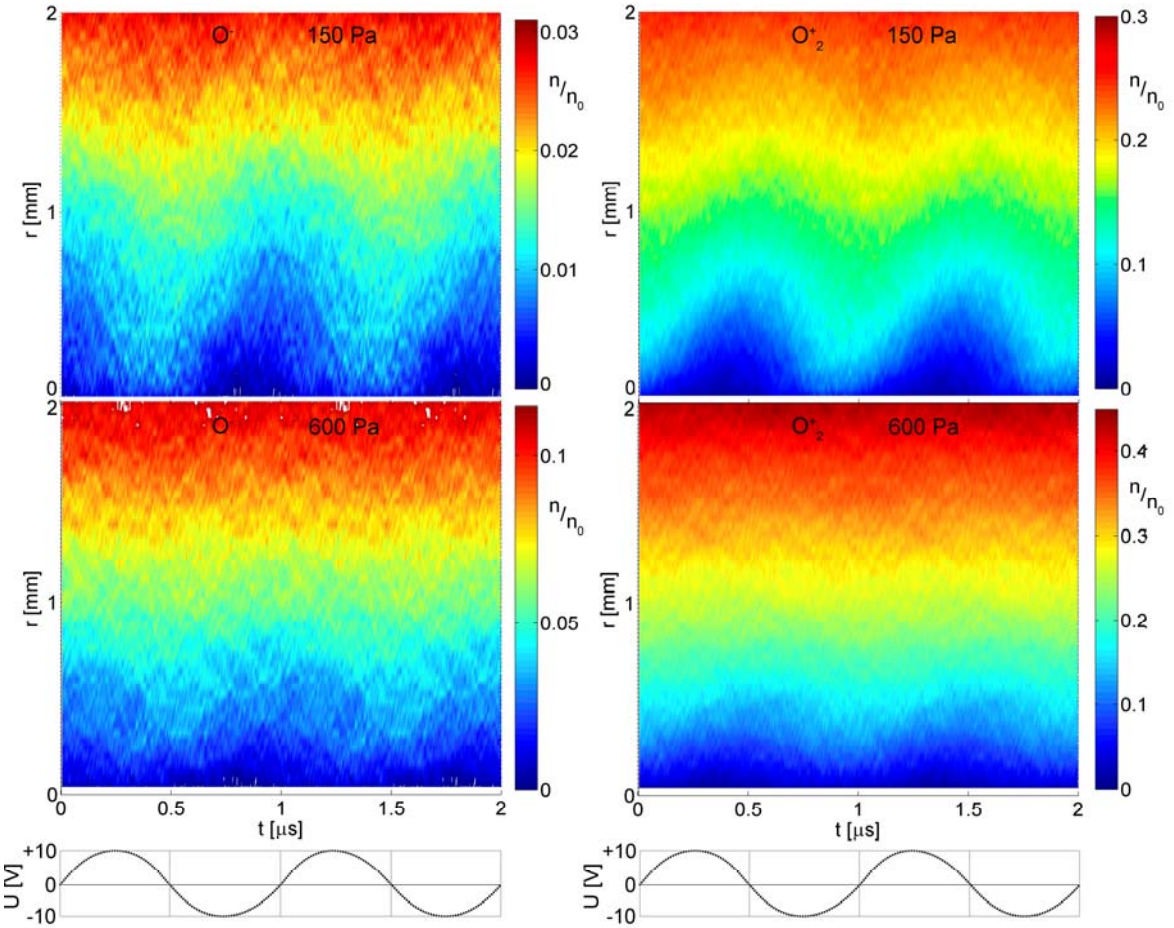

Fig. 4.11: Time developments of concentrations of negative oxygen ions (left) and positive molecular oxygen ions (right) in the vicinity of substrate at the steady state of dynamic processes. Parameters: pressure 150 Pa (top) and 600 Pa (bottom), sinusoidal course of voltage bias on the electrode (shown below), frequency 1 MHz, Ar:O_2 ratio 50:50. Cylindrical probe with radius 1×10^{-4} m at r = 0 mm. All concentrations are divided by n_0 = 1×10^{15} m^{-3}.

The same behavior of the charged particles described above can be seen on the last figure (Fig. 4.12), where the time developments of the current density of charged species for three pressures are shown. As we can see, the current density is decreasing with increasing pressure, which is due to the reducing mobility of the charged particles.

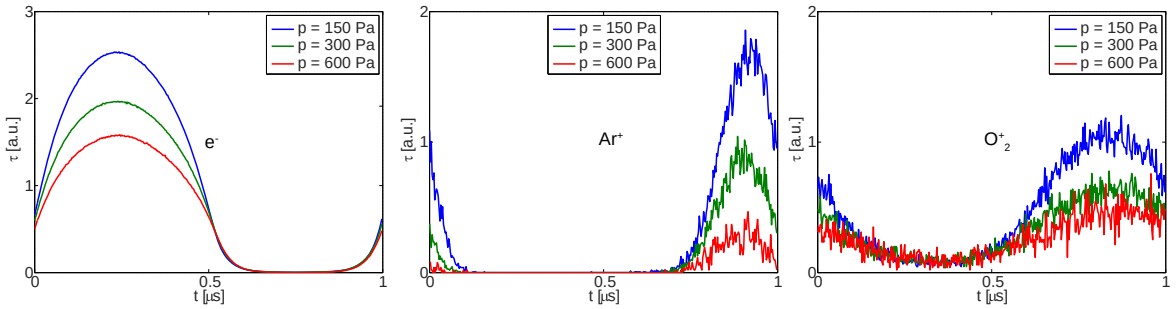

Fig. 4.12: Time developments of the current density of electrons (left), positive argon ions (middle) and positive molecular oxygen ions (right) – both the last 1000x magnified. Parameters: pressure 150 Pa, 300 Pa, and 600 Pa; sinusoidal course of voltage bias on the electrode; frequency 1 MHz; ratio Ar:O_2 50:50. Cylindrical probe radius 10^{-4} m.

5 Conclusions

This Ph.D. thesis is dealing with a computer modelling of the low-temperature plasma-solid interaction. Several computer models of electronegative multicomponent plasma were created together with several numerical approaches and with help of multiprocessor computers.

The model of volume processes was created to obtain the particle concentrations in a positive column of DC glow discharge in the mixture of Ar and O_2 gases. We observed a high sensitivity of our model to input data like rate constants of chemical reactions. This is mainly caused by discrepancies of experimental data found in the literature. Therefore, more experimental measurements will be needed.

Several models for description of the interaction between the electronegative low-temperature plasma and the immersed substrate were created. Simulations were run for a static regime where constant voltage bias on the substrate is hold, as well as for dynamic regime where the rectangular and subsequently the sinusoidal waveforms of the electrode voltage bias with frequency 1 MHz were applied. In case of the dynamic regime, parallel programming was used for speeding-up the programs.

Many results describing behavior of the charged particles in the vicinity of the substrate as well as the forming sheath and the response of the particles on alternating voltages were obtained. These results were generated for various parameters like the pressure, probe radius, ratio of Ar/O_2, etc.

The computer models presented in the thesis give valuable and deeper information about the physical processes whether in the bulk plasma or during the plasma-solid interactions. It is necessary to keep in mind that they are only models of actual physical processes. Their disadvantage is the lack of the necessary experimental data to complement or more precise the input parameters, e. g. the above mentioned rate constants or the cross-sections of scattering processes. However, we can use these models very efficiently to illustrate many physical processes. Therefore, the results of the models contribute to a better understanding of plasma behavior which is important in many technological processes.

The results were presented on several international conferences and in several impact journals. Its summary is in the end. Some of the results were used while solving of the projects GAČR P205/10/0979 “Study of the interaction of chemically active plasmas with

solid surfaces at medium and higher pressures", KAN101120701 "Nanocomposite films and nanoparticles prepared in low pressure plasma for surface modification" in "Nanotechnology for society" program, KAN40020701 "Hierarchical nanosystems for microelectronics" in "Nanotechnology for society" program and LC06041 "Preparation, modification, and characterization of materials by energetic radiation".

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Publications related to the thesis

Publications in impact journals:

[I1] Černý P., Novák S., Hrach R., Bruna P.: Study of sheath dynamics in multicomponent plasma. Contribution to plasma physics, 2008, **48**, pp. 424-429

[I2] Černý P., Novák S., Hrach R.: Dynamics of plasma-surface interactions in chemically active plasma. Vacuum, 2010, **84**, pp. 97-100

[I3] Černý P., Novák S., Hrach R., Hrachová V.: Study of material processing in chemically active plasmas. Surface and coatings technology (submitted).

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