*33rd EPS Conference on Plasma Phys. Rome, 19 - 23 June 2006 ECA Vol.**30I**, P-4.017 (2006)*

Computational study of plasma-solid interaction in low-temperature plasma: Surface processes at higher pressures

R. Hrach[1,2], V. Hrachová[1], S. Novák[2]

[1] *Department of Electronics and Vacuum Physics, Faculty of Mathematics and Physics Charles University, Prague, Czech Republic*

[2] *Department of Physics, Faculty of Science, J.E. Purkynje University Ústí nad Labem, Czech Republic*

1. Introduction

Understanding of processes in the boundary layer between plasma and immersed substrates is very important both in probe diagnostics and in plasma chemical technologies. In the last few years the challenging problem for plasma science and technology started to be the surface treatment at higher pressures including the atmospheric pressure plasma (e.g. [1], [2]). However, the applications in this field outstripped the theories, which were derived for collisionless or slightly collisional plasmas and lose their validity in this pressure range. Therefore the methods of computational physics are being widely used for such problems, like fluid modelling or particle simulation techniques.

2. Experimental

The structure and properties of the discharges in various gases are intensively studied for a very long period. In our laboratory, the measurements were performed in positive column of the dc glow discharge. The plasma consisted of rare gases – argon, neon and helium, either pure ones or in the mixture with oxygen. Main parameters of our experiments were the total pressure of the mixture, the composition of mixtures and the discharge current. For the study of plasma properties various diagnostics were used – optical, microwave and probe diagnostic. Some experimental results obtained in our laboratory can be found e.g. in [3].

In our experiments, the positive column of dc glow discharge was studied in the pressure range 67 to 800 Pa. All plasma parameters were measured in the dependence on the discharge current (for discharge tube with diameter 0.02 m). In Fig. 1 the dependencies of electron densities n_e determined by microwave toroidal resonator method on various experimental parameters are shown.

These results as well as some other experimental characteristics were used as both input data for modelling and data for testing of results of our computer experiment.

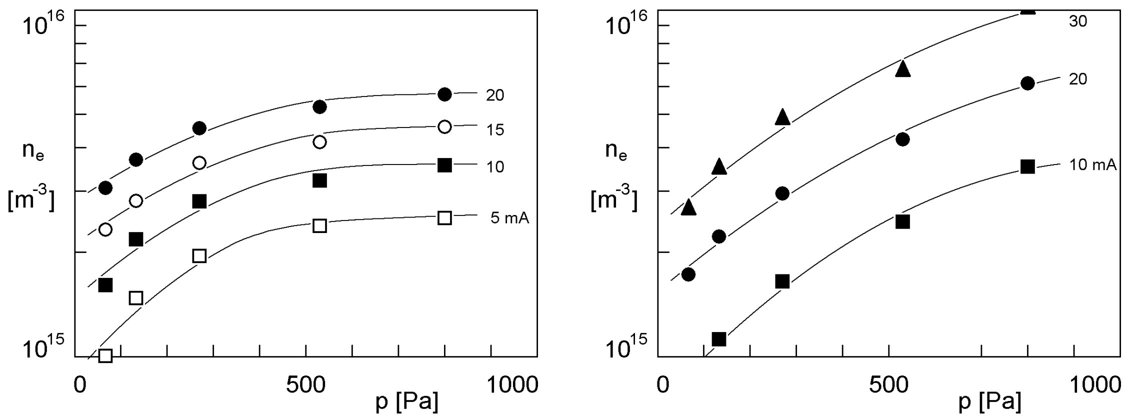

Figure 1: Measured electron density n_e in Ar plasma (left) and in Ne plasma (right) in the dependence on plasma pressure p. Parameter: discharge current.

3. Computer experiment

Computational approach was used for the study of trajectories of charged particles both in the sheath and presheath at various pressures in the contribution. The results of computer experiments were compared with experimental data obtained in the dc glow discharge in argon.

In our computer experiment the attention was given both to physical problems – formation of sheath at various pressures, energy and angular distributions of charged particles during their transition from the undisturbed plasma to the substrate, fluxes of particles impinging surfaces of immersed solids, etc.; and to problems of computational physics – efficiency of computer algorithms and its changes at higher pressures, influence of scattering processes, etc.

A main model based on the self-consistent particle simulation approach was prepared for this purpose. The combination of deterministic molecular dynamics simulation (determination of movement of charged particles in both external and local electric fields) and stochastic Monte Carlo simulation (description of interactions between charged and neutral particles) was used in the model. This model is based on standard PIC-MC technique and involves well-known algorithms as Thomas algorithm for solving Poisson equation, Verlet algorithm for molecular-dynamics part of model and null-collision method for treatment of energy dependent scattering. The model is limited to simplified geometries taking into account the symmetry of studied problems – [4] and [5]. There exist several modifications of this self-consistent particle model. All modifications are either one- or two-dimensional in space and differ in geometries – planar, cylindrical or spherical – corresponding to various forms of probes or substrates.

Next particle model was a non self-consistent one, when the electric forces acting on charged particles in the vicinity of probes are given externally. The results of self-consistent modelling, i.e. spatial distribution of electric potential, were used in most cases.

Both models were written in FORTRAN 95 programming language and processed by the PC computer. The number of particles treated simultaneously was 2×10^5 to 2×10^6 in the self-consistent model and the number of time steps was about 1×10^5. The number of particles is determined by the studied problem in the non self-consistent model and ranges from 1×10^4 for the determination of probe characteristics to 1×10^6 for precise determination of energy and angular distributions of charged particles in the sheath.

4. Results and discussion

The dependence of plasma-solid interaction on the pressure in an electropositive plasma was studied in the contribution. We supposed that the cross-sections of interactions of charged particles with neutrals change linearly with pressure, while the concentrations behave according to experimental data (Figs. 1).

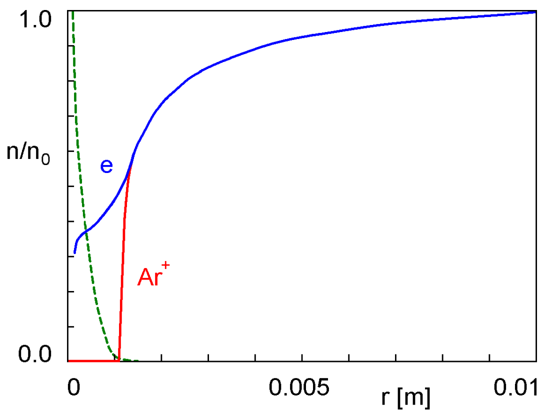

Figure 2: Spatial distributions of electrons (blue) and positive ions (red) near the cylindrical probe (radius 1×10^{-6} m). Dashed line denotes the potential distribution. Voltage bias +10 V.

Some examples of derived results are shown in following figures. The present simulations were performed for cylindrical and for planar probes. In Fig. 2 the spatial distributions of both electric potential and concentrations of charged species are shown at 133 Pa. It was found that these quantities are strongly influenced by the plasma pressure – see our other contribution [6]. On the other hand, the change of plasma pressure in studied limits has less pronounced impact both on the velocity distributions of electrons and ions as well as on fluxes of particles impinging surfaces – see Fig. 3 for energy distributions.

The particle simulation at higher pressures is much more difficult from the computational point of view as the intensive scattering of charged particles by neutrals influences their trajectories, so the deterministic modelling starts to be very inefficient.

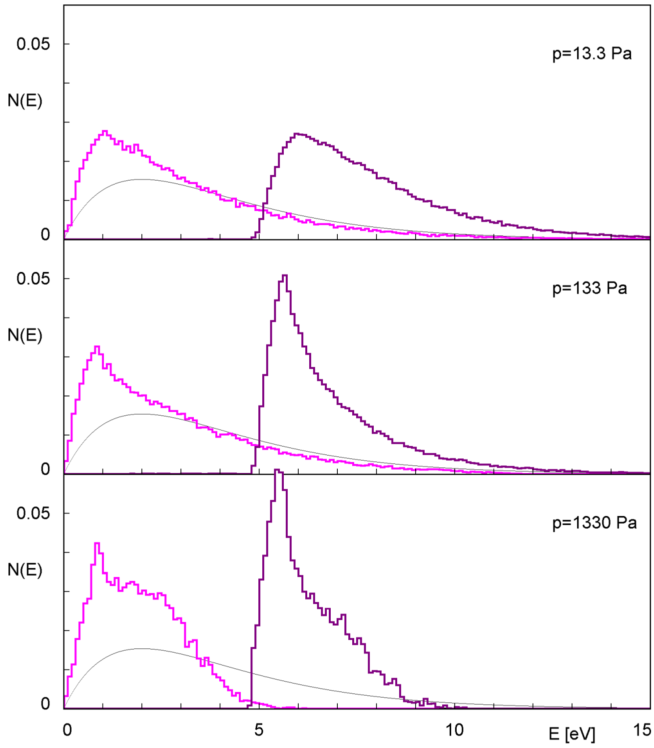

Figure 3: Pressure dependence of energy distributions of electrons. Positions: left – boundary presheath-sheath, right – surface of probe. Voltage bias +5 volts. Planar geometry.

Acknowledgement

The work is a part of the research plan MSM0021620834 financed by the Ministry of Education of Czech Republic. Authors R.H. and V.H. acknowledge the support of the Grant Agency of Charles University Prague, Grants No. GAUK-296/2004 and GAUK-220/2006, and authors R.H. and S.N. acknowledge the support of the Ministry od Education of Czech Republic – Projects COST 0C 143 and LC 06041.

References

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

[2] G.E. Georghiou, A.P. Papadakis, R. Morrow and A.C. Metaxas, J. Phys. D: Appl. Phys. **38**, R303 (2005)

[3] R. Hrach, V. Hrachová, M. Vicher and J. Šimek, Proc. 16th Intern. Symp. on Plasma Chemistry ISPC-16, Taormina, Italy, 145 (2003)

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

[5] P. Jelínek, R. Hrach, J. Šimek and D. Sedlák, Proc. 32nd EPS Conf. on Plasma Physics, Tarragona, Spain, ECA **29C**, P-4.126 (2005)

[6] R. Hrach, J. Šimek and V. Hrachová: *Study of plasma-solid interaction in electronegative gases at medium pressures*, Proc. 33th EPS Conf. on Plasma Physics, Roma, Italy (2006).