*31st EPS Conference on Plasma Phys. London, 28 June - 2 July 2004 ECA Vol.**28G**, P-1.020 (2004)*

Modelling of plasma-solid interaction at low and medium pressures

R. Hrach[1,2], S. Novak[1], V. Hrachova[2]

[1]*Department of Physics, J. E. Purkyne University, Usti nad Labem, Czech Republic*
[2]*Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic*

1. Introduction

The understanding of processes in the boundary layer between low-temperature plasma and immersed substrates is very important both in modern plasma-chemical technologies and in Langmuir probe diagnostics of plasma. The detailed description of processes taking part during plasma-solid interaction is rather difficult and the interpretation of probe characteristics is complicated as the substrates/probes perturb their local surroundings.

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. However, in this regime the experiments and practical applications outstripped the theoretical and computational studies; therefore the application of Langmuir probe diagnostics of such plasmas is limited due to the lack of interpretation of obtained results.

At low pressures for collisionless or slightly collisional plasmas there exist theories, which can be used for this purpose. When the collisions start to be important, the computer experiments are now widely used as they proved to be very convenient tool for the study of processes taking part during plasma-solid interaction. There exist two basic approaches – either the fluid modelling or the particle simulation techniques. At higher pressures the fluid models are typically used (e.g. [1]–[3]), however the comparison of both approaches reveals that the particle simulation codes give much deeper insight into studied problems. Therefore, in the present contribution, the combination of molecular dynamics and Monte Carlo methods was used for the study of sheath evolution at low and medium pressure plasmas and for the determination of trajectories of charged particles both in the sheath and presheath.

2. Experimental

The input data for simulation were obtained by experiments performed in the positive column of dc glow discharge in argon as well as from the literature. The electron concentration (see Fig. 1, [4]) and information about scattering processes in argon plasma [5] was the information transferred into our model.

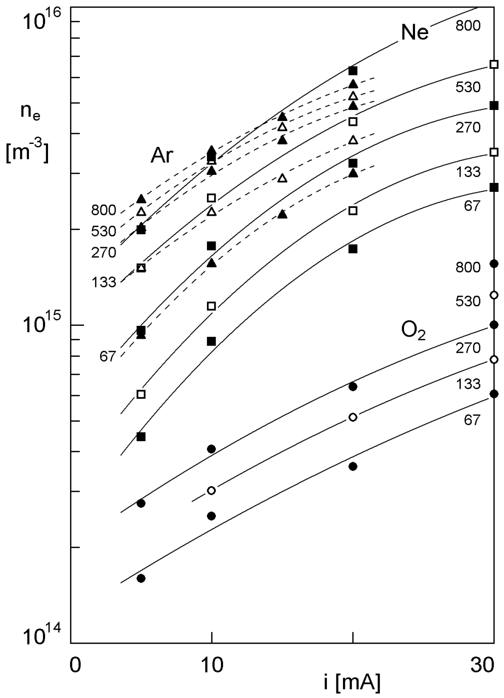

Fig. 1: Experimentally derived electron density n_e in the dependence on discharge current i for three gases – argon, neon and oxygen. Parameter: gas pressure in the range 67–8800 Pa.

3. Model

The particle model of plasma-solid interaction consisted of the following parts:

- Source of particles: Undisturbed plasma consisting of electrons, positive argon ions and argon atoms. Maxwell distribution of particles, different temperatures T_e and T_i are used.
- Interactions: The cross-sections for the interactions of charged particles with neutrals were used with characteristics taken from [5] – elastic collisions, excitation and ionisation for electrons, elastic collisions and charge transfer interactions for Ar^+ ions.
- Trajectories of particles: The trajectories of particles between scattering events were simulated by the molecular dynamics method, i.e. the Newton´s equations of motion were solved by means of a leap-frog scheme. The scattering of particles was simulated by the Monte Carlo method with the help of null-collision technique.
- Force calculations: The local forces acting on individual particles were calculated by the standard PIC-MC technique in CIC modification. The distribution of electric potential was derived by solving the Poisson equation.
- Advanced computational techniques: The leap-frog scheme handles the problem discretely in time with constant time step Δt. In order to speed-up calculations different time steps for electrons and heavier particles were used, 10^{-11} to 10^{-12} s and 10^{-8} to 10^{-9} s. In order to obtain more efficient code some further techniques were introduced – variable

numbers of particles increasing in the course of simulation and variable statistical weights of particles depending on their positions.

The model was written in FORTRAN 95 programming language and processed by the PC. The total number of particles in the model treated simultaneously was 2×10^5 (in special cases even more than 1×10^9) and the number of time steps was about 1×10^6.

One of the questions, which must be taken into account during interpretation of experimental data, is the geometry of studied problems. It was observed (e.g. [6]) that the derived plasma parameters depend not only on plasma properties but also on the probe used. In the paper [7] was proved that although the application of models with simplified geometries influences some plasma characteristics (as sheath thickness), the internal processes in the sheath (energy and angular distributions of charged particles, fluxes of particles to substrate, etc.) are influenced by in a negligible way. Therefore, in our simulation we used the one-dimensional model corresponding to planar geometry of metal substrate.

4. Results

The increase of gas pressure influences the model in two ways – the number of charged particles in plasma is increased (due to changes in ionisation degree this increase is not too high – see Fig. 1) and scattering processes are more intensive (proportionally to pressure variations). In Figs. 2 and 3 some results of our simulation are presented.

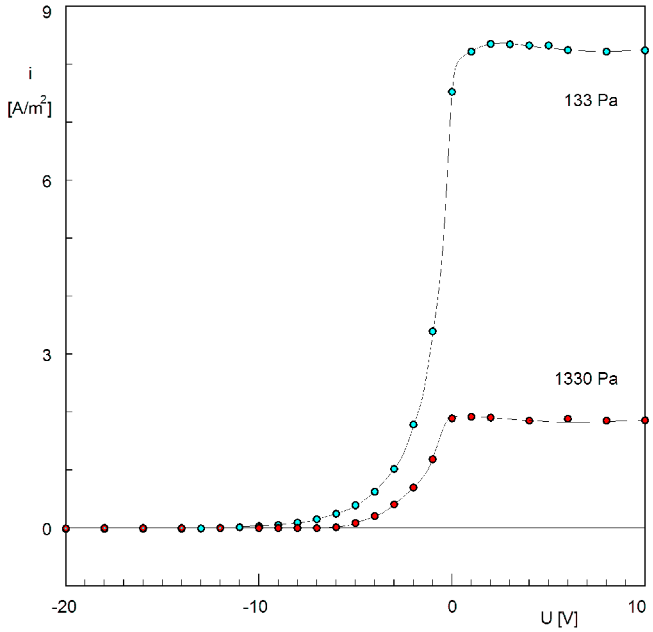

Fig. 2: Simulated current-voltage characteristics at two pressures of argon plasma. The decrease of current flowing to probe suggests that the mobility of charged particles is highly reduced at medium pressures.

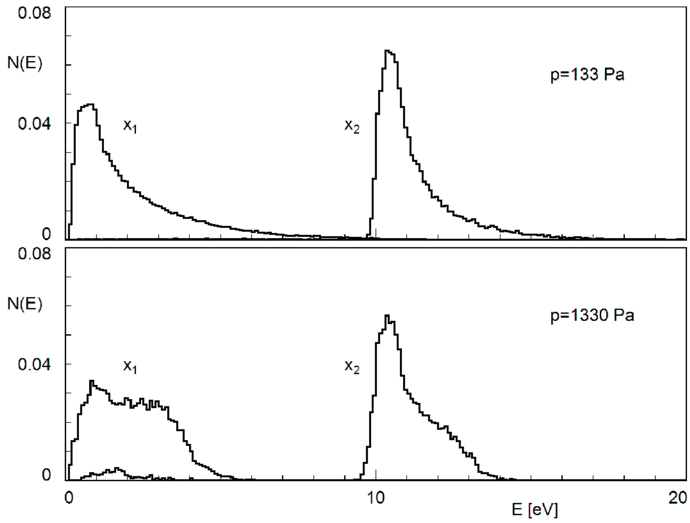

Fig. 3: Energy distributions of electrons in two positions – near the boundary between sheath and presheath, x_1, and on the substrate, x_2. Parameters: pressure p, bias +10 volts.

5. Conclusion

In our computer experiment it was found that the PIC-MC technique could be extended to plasmas with medium pressures. However, the modelling is extremely time-consuming as the movement of charged particles changes its character from the ballistic transport in electric field at low pressures to chaotic. To handle this problem effectively, it is necessary to introduce new and more sophisticated simulation techniques. The promising seems to be the hybrid modelling combining the best of both particle and fluid codes [8].

Acknowledgement:

The work is a part of the research program MSM 113200002 that is financed by the Ministry of Education of the Czech Republic. The research has been supported by the grant GAUK–296/2004 of the Grant Agency of Charles University Prague (authors R. H. and V. H.). The author S. N. acknowledges the support of the research intent No. MSM 1343000001.

References:

[1] R.T. Farouki, S. Hamaguchi, Dalvie M.: Phys. Rev. A **45** (1992) 5913.
[2] S. Mukherjee: Physics of Plasmas **8** (2001) 364.
[3] J.J. Gonzalez, P. Freton, A. Gleizes: J. Phys. D: Appl. Phys. **35** (2002) 3181.
[4] R. Hrach, V. Hrachova, M. Vicher: Vacuum (2004) (in print).
[5] S.C. Brown: *Basic Data of Plasma Physics.* AIP Press, New York 1994.
[6] R. Hrach, V. Hrachova: Proc. XVII ICPIG, Budapest, Hungary (1985) 834.
[7] R. Hrach, P. Jelinek, J. Simek, O. Barina, M. Vicher: Czech. J. Phys. **54** (2004) C671.
[8] A. Bogaerts, R. Gijbels: Phys. Rev. E **65** (2002) 056402.