Effective modelling of plasma sheath based on improved non self-consistent particle simulation technique

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Abstract

Two types of simulation techniques – non self-consistent and self-consistent particle models of plasma sheath in low-temperature plasma are described and obtained results are presented. For this purpose we processed data obtained by self-consistent simulations for various combinations of discharge parameters by the program based on evolutionary modelling. The following non self-consistent simulation of plasma-solid interaction for problems of similar types is not so time-consuming while the preciseness of results is increased radically compared to older non self-consistent calculations.

1. Introduction

Low-temperature plasma is used in plasma chemistry; therefore the good knowledge of processes, which take place during plasma treatment of materials, is important. The second motivation for the study of plasma-solid interaction is the probe diagnostics in both low-temperature and high-temperature plasmas. The computer modelling appears to be very powerful tool for these studies; however, both present computer hardware and methods of computational physics are not sufficient enough for the preparation of truly realistic models of plasma sheath. Especially during application of substrates and probes of complicated forms or in complex plasma mixtures – electronegative gases, chemically active plasmas, etc. – the choice of proper computational approach is very important [1]-[3].

Among various kinds of modelling the particle simulations are the most robust and accurate. The self-consistent particle models can bring sufficiently precise results but the computational requirements of standard algorithms, especially in higher dimensions, are very high. When the traditional non self-consistent particle simulation technique with distribution of electric potential near the substrate given analytically is used, the performance of resulting codes is increased [4]. However, in this case the accuracy of
derived results is rather low as it depends on simplified assumptions about the distribution of local electric field near the substrate used.

2. Computer model

There exist two possible ways how plasma-solid interactions can be modelled using particle techniques. The first approach is called self-consistent approach and the second one is non self-consistent modelling. Detailed description of these simulation techniques can be found e.g. in [5].

2.1. Self-consistent model

In this computational approach the electric potential in the vicinity of probe is derived from the space charge distribution in the working region by solving the Poisson equation. The standard technique of modelling is the PIC-MC method, where the movement of charged particles is calculated deterministically, while their interactions with neutral background are treated stochastically. This modelling is extremely time-consuming, because number of charged particles, which must be treated simultaneously, is very large.

2.2. Non self-consistent model

Non-self consistent modelling is based on the knowledge of electric field near the probe immersed into plasma. The forces acting on charged particles can be obtained by analytic expressions and the trajectories of particles can be computed separately. In this approach the movement of small number of charged particles is modelled. This technique is very fast, but the accuracy of derived results is given by the correctness of used assumption about the distribution of electric potential near the substrate.

Therefore, in our simulation first we derived a set of formulae for the electric field distribution in the sheath and presheath using the genetic algorithms. After that we were able to apply the fast non self-consistent approach, now with much higher accuracy.

3. Results of computer simulations

Some results of our simulations of plasma-solid interaction can be seen in Figs. 1 and 2. The results were obtained by both the self-consistent and non self-consistent calculations. The parameters of modelling correspond to positive column of the dc glow discharge in argon at 133 Pa. The probe bias was +10 volts.
Fig. 1.: Total velocity, x-component of velocity and angular distributions of electrons in the distance 0 mm from the probe – blue lines, red lines are theoretical Maxwell distributions. Voltage bias + 10 volts.

Fig. 2.: Total velocity, x-component of velocity and angular distributions of electrons in the distance 1 mm from the probe – blue lines, red lines are theoretical Maxwell distributions. Voltage bias + 10 volts.
During the modelling of plasma-solid interaction we derived the angular distribution of electrons, the \(x\)-component of electron velocity and the total electron velocity distributions. Results of our simulations are depicted for two various distances from planar probe immersed into plasma. The distances from substrate 0.0 mm and 1.0 mm were chosen. The first case corresponds to the position on the surface of planar probe; the second one corresponds to the half of thickness of the sheath region.

Discussion and conclusion

In the contribution the interaction of plasma with surfaces of immersed planar substrates was simulated by two different particles simulation techniques. During the simulation various information about the sheath region and about the behaviour of charged particles in the vicinity of biased substrates was obtained – spatial distribution of electric potential, fluxes of charged particles impinging substrate and the angular and velocity distributions, the last results being shown in the figures above.

The obtained results from non self-consistent modelling were compared with results obtained by means of self-consistent model. We can conclude that our non self-consistent model has provided expected results only the efficiency of computer codes differed profoundly. In 1D and 2D simulations the saving of computer time was about 3 orders of magnitude, while in 3D simulations the efficiency increased about \(10^6\) times.

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