One-dimensional hybrid model of plasma-solid interaction in argon plasma at higher pressures

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Abstract. One of problems important in the present plasma science is the surface treatment of materials at higher pressures, including the atmospheric pressure plasma. The theoretical analysis of processes in such plasmas is difficult, because the theories derived for collisionless or slightly collisional plasma lose their validity at medium and high pressures, therefore the methods of computational physics are being widely used. There are two basic ways, how to model the physical processes taking place during the interaction of plasma with immersed solids. The first technique is the particle approach, the second one is called the fluid modelling. Both these approaches have their limitations - small efficiency of particle modelling and limited accuracy of fluid models. In computer modelling is endeavoured to use advantages by combination of these two approaches, this combination is named hybrid modelling. In our work one-dimensional hybrid model of plasma-solid interaction has been developed for an electropositive plasma at higher pressures. We have used hybrid model for this problem only as the test for our next applications, e.g. pulsed discharge, RF discharge, etc. The hybrid model consists of a combined molecular dynamics - Monte Carlo model for fast electrons and fluid model for slow electrons and positive argon ions. The latter model also contains Poisson's equation, to obtain a self-consistent electric field distribution. The derived results include the spatial distributions of electric potential, concentrations and fluxes of individual charged species near the substrate for various pressures and for various probe voltage bias.

1. Introduction
In recent years low-temperature plasmas are being used in a large number of application fields, e.g. plasma etching of surfaces, plasma deposition of thin films, medical applications, etc. To obtain a better theoretical understanding of the discharge processes and mechanisms several modelling approaches were performed in former times.

Firstly two more often used approaches of computer modelling were applied. The first one is to deal with plasma as a fluid. Technique used for these calculations is called fluid modelling. This assumption is not really valid for so-called “fast” electrons, so the fluid modelling is only an approximation. In spite of this fact this method is often used by many authors mainly because this approach is very fast or in case when the collision processes are not so important. The second possible and often used technique is called self-consistent particle simulation. This method is more precise than the first above mentioned one, on the other hand this approach is more time consuming than the previous technique. This fact is caused by high number of particles in the computer model and basic idea of this approach – to calculate the new position and velocity for every particle separately. This unpleasant matter is manifested even more strongly
in modelling of problems of plasma physics at higher pressures due to stronger interaction of charged particles with neutral background. Recently some combination of fluid and particle models were developed. This approach is called hybrid modelling and it takes advantages of both referenced methods. By means of this model the “fast” electrons are simulated by the particle-in-cell Monte Carlo (PIC – MC) model whereas “slow” electrons and ions are calculated by means of fluid approach.

In this work we present one-dimensional hybrid model. The calculation was performed for planar geometry of the probe, immersed into plasma. We concentrate on an argon gas, because the collision processes and discharge mechanisms in this type of plasma are transparent and relatively simply. Our hybrid model as mentioned above consists of two parts. Self-consistent particle model where the positions and velocities of “fast” electrons are calculated by means of Verlet algorithm [1] and obtained collision rates are used as input to the fluid model. The second part of hybrid model, i.e. the fluid model, works with “slow” electrons and positive argon ions, and calculates new electric field based on Poisson equation.

Typical results of our calculations are distribution of electric field and distribution of electric potential as a function of distance from the probe, concentrations and fluxes of charged particles. We have obtained the fast electron energy distribution function in the frame of this model, too.

Below the description of hybrid model and physical assumptions, (boundary conditions, collision processes, etc.), in the model are mentioned. The results of our calculations and comparison of these results are also shown. Finally, some conclusions and discussions are presented.

2. Description of the model

2.1. Particle model

As mentioned above particle model calculates new positions and velocities for so-called “fast” electrons, it means electrons with ability to ionise neutral argon atoms. We assume all particles have Maxwell velocity distribution, so the number of “fast” electrons was calculated by means of incomplete gamma function:

\[ \Gamma(x, a) = \int_0^x t^{a-1}e^{-t}dt. \]  

(1)

Afterwards we can calculate the new positions and velocities for these electrons based on solution of Newton’s law of motion by means of Verlet algorithm. As the results of these calculations we obtained the collision rates of slow electrons and argon ions, \( r_e \) and \( r_i \), which serve as an input to the equations (2) and (3) in fluid part of hybrid model.

The collision processes for fast electrons were treated stochastically by means of null-collision technique. Detailed information about this method could be found in [2] or [3]. The collision processes assumed in our model can be seen in table 1, i.e. the electron elastic collisions with argon atoms, excitation and ionization of argon atoms [2]. The analytical expressions of the

| electrons + Ar neutral atoms |  
|-----------------------------| 
| \( e + Ar \rightarrow e + Ar \) | Elastic scattering  
| \( e + Ar \rightarrow e + Ar^* \) (\( E_{ex} = 11.55 \) eV) | Excitation  
| \( e + Ar \rightarrow e + Ar^+ + e \) (\( E_{ion} = 15.76 \) eV) | Ionization |
collision cross sections for electrons with neutral argon atoms can be found in [4].

2.2. Fluid model

The fluid model for the positive argon ions and for the slow electrons consists of following set of partial differential equations for both types of charged particles. Continuity equations (2), (3), the particle flux equations, [equations (4) and (5)] for ions and electrons, respectively and the Poisson equation (6):

\[ \frac{\partial n_i}{\partial t} + \nabla j_i = r_i, \quad (2) \]
\[ \frac{\partial n_e}{\partial t} + \nabla j_e = r_e, \quad (3) \]
\[ j_i = -\mu_i n_i E - D_i \nabla n_i, \quad (4) \]
\[ j_e = \mu_e n_e E - D_e \nabla n_e, \quad (5) \]
\[ \nabla^2 U = -\frac{e}{\varepsilon_0} (n_i - n_e - n_{e,\text{fast}}). \quad (6) \]

The values of diffusion coefficients \( D_i, D_e \) and mobility of electrons \( \mu_e \) were taken from [5]. The mobility of ions was calculated from the Frost formula [6]. The next quantities in above mentioned equations are concentrations of positive argon ions and “slow” electrons, \( n_i \) and \( n_e \), the concentration of “fast” electrons is \( n_{e,\text{fast}} \), \( j_i \) and \( j_e \) are the corresponding particle fluxes, \( r_i \) and \( r_e \) are collision rates as a result of particle simulations.

The solution of these coupled differential equations is a difficult numerical problem. These five equations can be reduced to three equations for \( n_e, n_i \) and \( U \) if we insert equations (4) and (5) into equations (2) and (3), respectively. For the solution of this problem we have used the method called Scharfetter – Gummel exponential scheme [7]. This method is widely used by many authors for the spatial discretization of the transport equations of gas discharges.

The boundary conditions for these equations were \( U = U_{\text{probe}} \) on the surface of the probe, \( U = 0 \) V at the end of work region, \( \frac{\partial n_e}{\partial x} = 0, \frac{\partial n_i}{\partial x} = 0 \) at the probe and \( n_e = n_{0e}, n_i = n_{0i} \) at the end of work region.

2.3. Hybrid model

Coupling of both above mentioned models is the base for so-called hybrid model. In this model we start with fluid model and we calculate distribution of electric field by means of equation (6) from uniform distribution of charged particles in undisturbed plasma at the beginning of calculation. Afterwards we use particle model and we calculate collision rates of electrons and positive argon ions. These creation rates are used as an input to the fluid model. Then the fluid model calculates new electric field and this procedure is repeated until convergence is reached.

2.4. Physical assumptions of the model

Our calculations were performed for DC discharge in an argon plasma. The “fast” electrons in the particle model have had Maxwell distribution of velocity and their temperature was \( 2 \text{ eV} \approx 23200 \text{ K} \). The work area was 1.0 cm long. Probe bias was firstly set to \(+10 \text{ V}\) and in the second run to \(-10 \text{ V}\), the gas pressure was 1 Torr and then 10 Torr for both of the probe biases. The time step for “fast” electrons in the particle model \( 10^{-11} \text{ s} \) was considered. In the fluid model the same time step for “slow” electrons and for positive argon ions was used. At
the beginning of the calculation the Maxwell distribution of velocities for “fast” electrons in the particle model was considered.

3. Results and discussion

In this chapter we present results of our simulations obtained by means of our hybrid model. As we mentioned above we have performed the calculations for two various probe voltages and for two various argon gas pressures. So, in the following figures can be seen the results obtained under described conditions, as well as the comparison among these results. Some discussions of results shown in these figures are also presented.

![Figure 1.](image1.png) **Figure 1.** Fluxes of “slow” electrons for two different pressures; probe bias +10 V.

![Figure 2.](image2.png) **Figure 2.** Fluxes of positive argon ions for two different pressures; probe bias +10 V.

In the figures 1, 2 and 3 the fluxes of all charged particles in our model are shown. These results were obtained for positive probe bias - +10 V and for various pressures of argon gas - 1 Torr and 10 Torr. From figure 1 can be seen that the flux of “slow” electrons is higher at higher pressure than at low one. On the other hand, in figure 3 you can see that the flux of “fast” electrons is higher at lower gas pressure. This effect is caused by the fact that at higher pressure there is more collisions between charged particles and neutral background and the “fast” particles are becoming slower, then the flux of “slow” particles is higher, whereas the flux of “fast” electrons is lower.

For the same reason the flux of positive argon ions in figure 2 is lower with increasing gas pressure, because of a lot of collisions at higher pressures.

In figures 4, 5 and 6 the concentrations of charged particles are shown. These results were obtained for two various probe biases - +10V and −10 V and for gas pressure of 10 Torr. From figures where the “slow” particles are depicted, you can see that theirs concentrations strongly depend on applied probe bias. The depicted curves in these figures correspond to the analytical solution of the diffusion equation in planar case. On the other hand in the figure 6 there are not great differences in dependence on applied probe voltage. Only small difference between concentrations can be seen in this range of gas pressure. For smaller gas pressures there are greater differences and the concentrations of “fast” electrons are lower than in higher pressures. It is probably caused by the fact that when the positive probe bias is applied, many fast electrons impinging the probe surface and total number of these electrons is lower than in the case when the negative probe bias is applied, and this effect is more manifested at lower pressures than at higher pressures.
In figures 7 and 8 you can see the distributions of electric field and electric potential as the function of distance from the planar probe. The distribution of electric field is calculated for two various probe biases +10 and −10 V and for gas pressure of 10 Torr. The distribution of electric potential is calculated for probe bias +10 V and for pressures 1 and 10 Torr. From the last figure can be seen that the thickness of sheath is smaller for higher pressure than for lower pressure. It is in good accordance with the theory and it is caused by higher ions density near planar probe in consequence of higher number of collisions of positive argon ions with neutral argon atoms.

4. Conclusion
The one-dimensional hybrid model, i.e. combined particle and fluid technique for planar geometry, is presented. The results obtained by means of this model as, e.g. potential distribution, distribution of intensity of electric field, concentrations of “fast” and “slow” electrons, positive argon ions and fluxes of these particles for various combination of probe
biases and gas pressures, are shown. This work is the continuation of our previous work [8].
Our present calculations with one-dimensional hybrid model will serve as the base for more
dimensional hybrid models. Mainly, we are going to create two-dimensional model in cylindrical
geometry because in many physical problems we can use their cylindrical symmetry. Thereafter,
we will be able to use our hybrid model for some calculations in surfatrons, magnetrons or
some other reactors where the cylindrical symmetry could be assumed. The next goal of our
calculations by means of hybrid modelling is the modelling of some dynamical problems in
plasma physics, e.g. RF discharges, etc., all problem will be solved for various ranges of gas
pressures.

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