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Techniques for computational study of plasma–solid interaction at higher pressures

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Abstract

Several techniques of computational physics used in low-temperature plasma simulations at higher pressures are presented in our contribution. The first approach is called fluid modelling, the second one hybrid modelling and the third technique—particle modelling presented here is realized as a part of hybrid model. There are several techniques applicable in computational plasma physics but some of these methods have explicit limitation. For example, time consumption of standard particle-in-cell Monte Carlo (PIC-MC) particle simulation is increased profoundly with increasing pressure of plasma. Hence, we have used the fluid and hybrid modelling. Hybrid model consists of two parts—particle model, simulating fast electrons while fluid model simulates slow electrons and positive argon ions. In particle model, the positions and velocities of fast electrons are calculated by means of deterministic Verlet algorithm while the collision processes are treated by the stochastic way. For solution of fluid equations, the Scharfetter–Gummel exponential scheme was used. Typical results of our calculations are electric field distribution, fluxes and collision rates of charged particles near the planar probe.

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Keywords: Plasma–solid interaction; Hybrid modelling; Plasma simulations; Low-temperature plasma; Plasma at higher pressures

1. Introduction

The interaction of low-temperature plasma with immersed substrates takes part both in plasma diagnostics and in many technological applications of plasma, therefore the detailed knowledge of corresponding physical and chemical processes is very important. One of challenging problems of contemporary plasma physics is plasma processing of materials at higher pressures including the atmospheric pressure plasma [1–3].

Therefore, in our contribution the transport of electrons and ions to metal substrates immersed into plasma is studied by computer experiment using fluid [4,5] and combination of the fluid and particle modelling. The particle (particle-in-cell Monte Carlo (PIC-MC)) models provide a deeper insight into studied problems while their efficiency is low compared to fluid models, the efficiency being the crucial question at both higher pressures and more dimensions.

The assumption of fluid modelling 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.

The next possible and often used technique is called self-consistent particle modelling, e.g. see our results in [6]. This method is more precise than the fluid modelling, on the other hand this approach is more time consuming than the previous one. This fact is caused by high number of particles in the computer model.

Recently some combination of fluid and particle models were developed. This approach is called hybrid modelling [7] and it takes advantages both of fluid and particle methods. By means of this model the ‘‘fast’’ electrons are simulated by the PIC-MC method whereas ‘‘slow’’ electrons and ions are calculated by means of fluid approach.

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In this work we present one-dimensional models. The calculation was performed for planar geometry of the probe, immersed into argon plasma.

Typical results of our calculations are distribution of electric field as a function of distance from the probe, collision rates and fluxes of charged particles for various pressures.

The description of our models and physical assumptions (boundary conditions, collision processes, etc.), in the model are mentioned. In the next part of our contribution, results and discussions of our calculations are shown. Finally, we present some conclusions.

2. Computer model

2.1. Fluid model

The fluid model consists of following equations, i.e. continuity Eqs. (1), (2), the flux equations, [Eqs. (3) and (4)] for ions and electrons, respectively, and the Poisson Eq. (5)

$$\frac{\partial n_i}{\partial t} + \nabla \boldsymbol{j}_i = r_i, \quad (1)$$

$$\frac{\partial n_e}{\partial t} + \nabla \boldsymbol{j}_e = r_e, \quad (2)$$

$$\boldsymbol{j}_i = -\mu_i n_i \boldsymbol{E} - D_i \nabla n_i, \quad (3)$$

$$\boldsymbol{j}_e = \mu_e n_e \boldsymbol{E} - D_e \nabla n_e, \quad (4)$$

$$\nabla^2 U = -\frac{e}{\varepsilon_0}(n_i - n_e - n_{e,fast}). \quad (5)$$

In the "classical" simple fluid model we assume the collision rates $r_i = 0$, $r_e = 0$ and concentration of "fast" electrons $n_{e,fast} = 0$, the physical quantities n_i and n_e are concentrations of charged particles—electrons and ions, $\boldsymbol{j}_i$ and $\boldsymbol{j}_e$ are the corresponding fluxes.

On the other hand in the hybrid model, we assume r_i, r_e and $n_{e,fast}$ are nonzero. As we mentioned above, $n_{e,fast}$ is concentration of "fast" electrons, such electrons have energy higher or equal to ionization energy in argon, i.e. $E_i \geqslant 15.76\,\text{eV}$. The Eqs. (1)–(4) are now used for "slow" particles, i.e. electrons with $E < E_i$ and positive argon ions.

Finally, D_i, D_e, μ_i, μ_e are diffusion coefficients and mobilities for ions and electrons, respectively. The values of D_i, D_e and μ_e were taken from [8]. The coefficient μ_i was calculated by means of Frost formula [9].

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

The solution of these coupled 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 Eqs. (3) and (4) into Eqs. (1) and (2), respectively. For the solution we use method called Scharfetter–Gummel exponential scheme [5]. This method is widely used for the spatial discretization of the transport equations of gas discharges.

2.2. Particle model

As mentioned above particle model calculates new positions and velocities for so-called "fast" electrons, it means electrons with ability of ionising 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

$$\Gamma(x, a) = \int_0^x t^{a-1} e^{-t}\, dt. \quad (6)$$

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 r_e and argon ions r_i calculated from the collisions between "fast" electrons and neutral argon atoms, which serve as an input to the Eqs. (1) and (2) in fluid part of hybrid model. Some of "fast" electrons become "slow" one because of the collisions and some of them can create ions; then the total number of newly created "slow" electrons in one time step is r_e and the number of newly created ions is r_i. In our model we assume the source of "fast" electrons with Maxwell distribution of velocities, incoming in each time step from undisturbed plasma.

The collision processes for "fast" electrons were treated stochastically by means of null-collision technique. Detailed information about this method could be found in [10] or [11]. The collision processes assumed in our model are the electron elastic collision with argon atoms, excitation and ionization with argon atoms. These processes are schematically shown in Table 1.

2.3. Hybrid model

Coupling of fluid and particle models is the base for so-called hybrid model. In this model we start with fluid model and we calculate distribution of electric field. Afterwards we use particle model and we calculate collision rates of electrons and positive argon ions. These creation rates r_i and r_e 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.

The total time of calculation on computer AMD Athlon 64 3500+ 1 GB RAM was in average 2 min for fluid model

Table 1
Scattering processes—"fast" electrons

(1) $e + Ar \rightarrow e + Ar$
(2) $e + Ar \rightarrow e + Ar^*$, ($E_{ex} = 11.55\,\text{eV}$)
(3) $e + Ar \rightarrow e + Ar^+ + e$, ($E_i = 15.76\,\text{eV}$)