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Two computational approaches for two-dimensional modelling of plasma-solid interaction

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Abstract

A numerical investigation of the plasma-solid interaction is presented. A formation of the sheath region in the vicinity of a cylindrical probe is simulated for conditions in a DC glow discharge with argon plasma. A fluid model and a particle model were developed to study the sheath structure. Results are compared and both techniques are discussed.

1. Introduction

The sheath formation during the interaction of a plasma with a solid surface is one of fundamental phenomena in plasma science. The understanding of processes in the boundary layer between the plasma and immersed substrates is very important in probe diagnostics and technological applications of plasma physics.

Besides experimental measurements and theoretical investigations, useful information can be obtained from the computer modelling. Plasma processes can be simulated using various computational techniques. Common computational methods differ in the time requirements, the accuracy or the applicability to a studied problem. The fluid models are applied to various kinds of problems in plasma physics. They describe the macroscopic evolution of plasma phenomena and therefore no direct evidence about the behaviour of individual particles can be obtained. The particle techniques solve trajectories of all constituent particles considered in a simulation and they provide microscopic information about processes in the plasma and give more detailed insight into the plasma behaviour. Such techniques are, however, computationally intensive, especially in more dimensions.

This contribution compares two techniques – the particle-in-cell method and the fluid modelling. Two models were developed to study the interaction of an argon plasma with a solid surface in the DC glow discharge. A two-component argon plasma is simulated (electrons and ions) and collisions with neutrals are simplified as the elastic scattering with a constant mean collision frequency. The models describe the interaction of the plasma with a cylindrical probe of the infinite length, which allows to reduce the dimensionality of the problem to two dimensions. Besides physical aspects and realistic assumptions about physical processes, the effort was focused on problems of computational physics and the attention was given to the performance of the individual algorithms in two dimensions.

2. Particle-in-cell simulation

The algorithm of the particle code combines a Molecular dynamics simulation of trajectories of charged plasma species and a stochastic Monte Carlo treatment of collisions of the electrons

and ions with neutrals. An undisturbed plasma with the Maxwell velocity distribution is considered at the outer boundary of the simulated region. The dynamics of the particles is driven by the electromagnetic force. An external electric field is not taken into account and the potential is calculated from the Coulomb interaction.

The plasma behaviour is described by the equations of motion which are numerically integrated to update the velocities $\mathbf{v}_i^{k+1/2} = \mathbf{v}_i^{k-1/2} + \mathbf{F}_i^k/m_i\,\Delta t$ and positions $\mathbf{r}_i^{k+1} = \mathbf{r}_i^k + \mathbf{v}_i^{k+1/2}\Delta t$ of the constituent particles (index i). The numerical integration and the calculation of a solution in the new time level $(k+1)$ is based on the Leap-frog algorithm.

The electrostatic interaction between the charged particles is calculated within the particle-in-cell (PIC) method. The computational domain is discretized to form a grid. The Cartesian coordinate system is used with a uniform grid spacing. The electric potential is described by Poisson's equation $\triangle\varphi = -\rho/\varepsilon_0$ and the boundary values are fixed to the probe voltage U_p on the probe and to zero on the exterior. Poisson's equation is discretized on the grid with the traditional five-point stencil and the resulting system of linear equations is solved using the UMFPACK library [1]. The electric field $\mathbf{E} = -\nabla\varphi$ is interpolated from the mesh points to particle locations and the electric force $\mathbf{F}_i$ is obtained.

3. Fluid model

Physical aspects of a fluid flow are governed by fundamental principles – the mass, momentum and energy conservation. The fluid model presented here is governed by partial differential equations (PDEs) describing macroscopic plasma parameters – the density n and average velocity $\mathbf{u}$. A transport of the mass and momentum for each plasma species (electrons k=e and ions k=i) is described by the continuity and momentum equations

$$\frac{\partial n_\mathrm{k}}{\partial t} + \nabla\cdot(n_\mathrm{k}\mathbf{u}_\mathrm{k}) = 0, \tag{1}$$

$$m_\mathrm{k} n_\mathrm{k}\frac{\partial \mathbf{u}_\mathrm{k}}{\partial t} + m_\mathrm{k} n_\mathrm{k}(\mathbf{u}_\mathrm{k}\cdot\nabla)\mathbf{u}_\mathrm{k} = q_\mathrm{k} n_\mathrm{k}\mathbf{E} - \nabla p_\mathrm{k} - m_\mathrm{k} n_\mathrm{k}\overline{\nu}_\mathrm{k}\mathbf{u}_\mathrm{k}. \tag{2}$$

The electric potential is solved from Poisson's equation. The quantities in the equations (1) and (2) have their usual meaning. We assume a constant temperature of the electrons and ions, the scalar pressure $p_\mathrm{k} = n_\mathrm{k} k T_\mathrm{k}$ and a constant collision frequency $\overline{\nu}_\mathrm{k}$. Non-elastic collisions are neglected. A fluid model with more precise treatment of collisions and solving the energy equation is presented in [2] and [3].

The system of the PDEs is solved using the finite difference approach. The equations are discretized on a regular rectangular grid with a uniform grid spacing. The electric potential is solved in the same manner as in the particle code and the UMFPACK library is used. The numerical algorithm to solve the fluid equations (1) and (2) is based on the flux-corrected transport scheme [4] involving three steps – an advection, a diffusion and an anti-diffusion and using the two-step Lax-Wendroff discretization for updating the solution.

Boundary conditions fix the density at the outer boundary to an undisturbed value n_0, while at the probe surface, the density is calculated as an extrapolated value from the nearest grid points. A similar boundary condition is imposed on the velocity at both boundaries.

4. Results

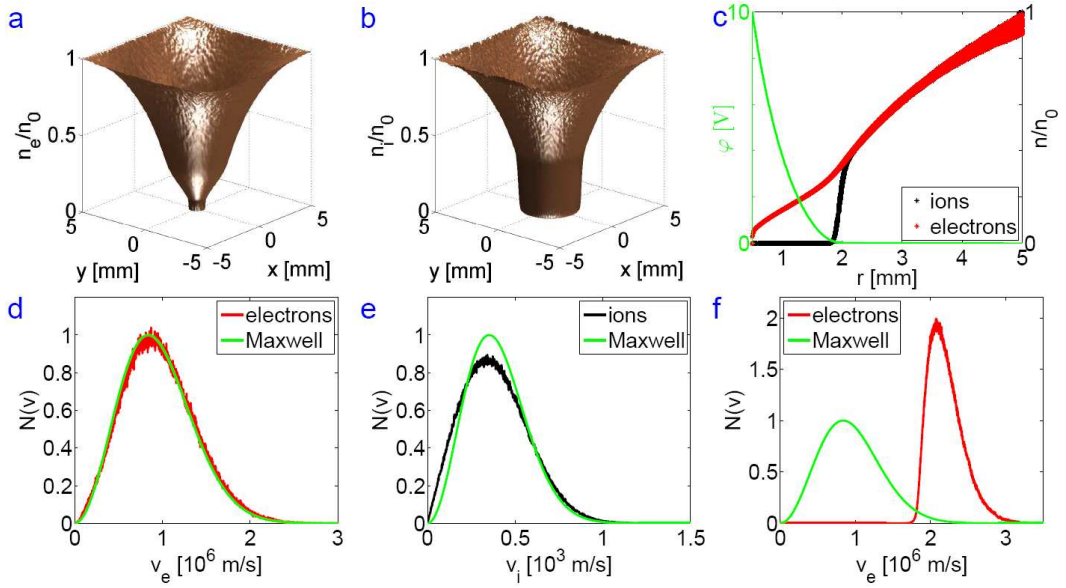

Figure 1: The normalized plasma density n_e/n_0 and n_i/n_0 (a, b, c), the electric potential φ [V] (c), the velocity distribution of the electrons and ions $N(v_e)$ and $N(v_i)$ in the whole region (d, e) and the electron velocity distribution $N(v_e)$ at the probe surface (f). The result of the PIC simulation.

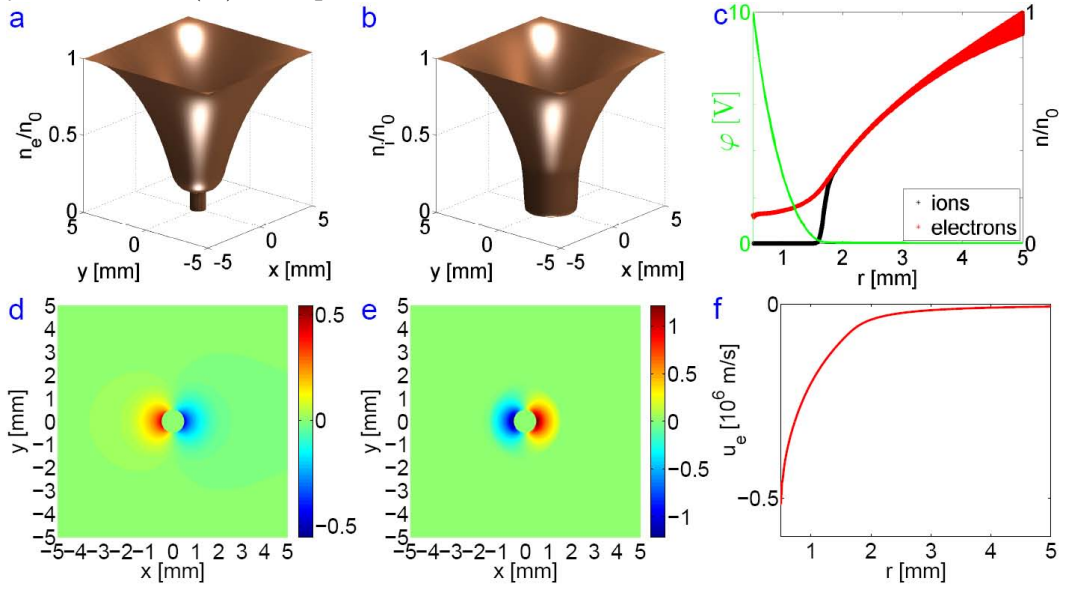

Figure 2: The normalized plasma density n_e/n_0 and n_i/n_0 (a, b, c), the electric potential φ [V] (c), the x component of the average electron velocity u_e^x [10^6 m/s] (d), the x component of the average ion velocity u_i^x [10^3 m/s] (e) and the average electron velocity u_e [10^6 m/s] (f). The result of the fluid model.

Let us summarize the parameters of the models. We consider a cylindrical probe of the infinite length with the radius $R_p = 5 \times 10^{-4}$ m and its axis perpendicular to the computational domain $L \times L$ of the size $L = 0.01$ m. The probe is biased at the voltage $U_p = 10$ V. We assume constant temperatures $T_e = 2$ eV and $T_i = 300$ K and the pressure $p = 1000$ Pa. The values of the undisturbed plasma density and the mean collision frequencies were derived from experimental data as $n_0 = 2.7 \times 10^{15}$ m^{-3}, $\overline{\nu}_e = 7.8 \times 10^9$ s^{-1} and $\overline{\nu}_i = 3.9 \times 10^7$ s^{-1}. The time steps in the PIC code were $\Delta t_e = 1 \times 10^{-11}$ s and $\Delta t_i = 1 \times 10^{-8}$ s. The time stepping in the fluid code is automatic and governed by Courant-Friedrichs-Lewy stability criterion, but the values of the time steps for the specified conditions were comparable with the PIC simulation.

Results of the models are shown in Fig. 1 and 2. The distribution of the plasma density and electric potential is symmetric around the probe axis. A sheath region develops, with a significant potential drop, where the quasi-neutrality condition is not fulfilled. The radial dependence of the density in the presheath region is logarithmic (Fig. 1 and 2 c), which is in an agreement with experimental investigations.

5. Discussion and conclusions

The sheath structure and formation in the vicinity of a solid surface are influenced by various physical processes, a plasma composition or a geometry of the immersed substrate. Two techniques are compared here for identical conditions.

The fluid model has been successfully implemented to give results in a good agreement with the particle simulation. In comparison to other authors, who use the drift-diffusion approximation, the model presented here involves the full momentum equation. The results of both techniques have the same character. The sheath is slightly larger in Fig. 1, the electron velocity at the probe is higher resulting in lower electron density. The fluid solution is characterized by boundary conditions and the particle flux at the probe is determined by a condition imposed on the density and velocity. Here boundary conditions similar to [5] were used, while some authors report a different approach [6]. In addition, the energy distribution of particles in the sheath is not Maxwellian due to the presence of a potential drop and the assumption of a constant temperature and collision frequency is not valid. As a summary, the particle method is preferable if a solution of the high accuracy is required. The fluid approach, due to the principle, can not describe microscopic phenomena which might be useful in some plasma technologies, but it is an optimal way to solve problems when obtaining effective and fast results is a priority.

The efficiency of both codes depends on physical aspects. For the conditions and parameters specified here, one time step of the PIC code for 6×10^6 particles on a grid with the resolution 200×200 takes 3.6 s and it requires about 1×10^5 iterations to converge to a steady state. One iteration of the fluid code for the same grid resolution and running on the same machine (Intel Core 2 Quad 2.83 GHz CPU) takes 0.07 s and the number of time steps to reach a steady-state solution is roughly 5×10^4. Even if the PIC simulation can be eventually further optimized or parallelized, it is much more computationally intensive than the fluid code.

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