Numerical investigations of sheath structure in presence of magnetic field

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Abstract. The contribution is focused on a computational study of the plasma-solid interaction in DC glow discharge in argon plasma with a special interest in the inclusion of external magnetic field and its effects on the sheath structure. In addition, the properties of the sheath and the presheath region have been analyzed in order to estimate the influence of pressure and size of a solid substrate immersed in plasma. The problem is assumed to be two-dimensional and the attention is also given to the efficiency of computer codes in two dimensions.

1. Introduction
The sheath structure and the sheath formation during the interaction of plasma with a solid surface is a fundamental phenomenon of plasma science. During the past decades, the behaviour of the sheath and the presheath region has been a topic of many investigations [1].

Regarding the complexity of studied problems, the computational approach is now being widely used to supplement experimental and theoretical investigations. Moreover, the theoretical description lose its validity in some conditions (e.g. collisional plasma at high pressures) and in this case the computational approach proved to be the best solution.

The contribution presents a computational analysis of the plasma-solid interaction in DC glow discharge in argon plasma in the presence of external magnetic field. The magnetic field significantly influences the sheath and the presheath region, its size and shape. Some of modern plasma technologies employ magnetic fields and the movement of charged particles in these fields is of scientific interest. In addition to the effects of the magnetic field, the influence of pressure and size of a solid surface immersed in plasma on the sheath structure is analyzed.

Besides these physical questions the attention was given to problems of computational physics, concerning the performance of individual algorithms in more dimensions and realistic assumptions about physical processes taking place during the plasma-solid interaction. The problem is considered to be two-dimensional and it is studied using a fluid description of plasma species dynamics. The fluid model of plasma describes an evolution of macroscopic plasma parameters such as plasma density and average plasma velocity and since it is based on solving a set of macroscopic partial differential equations (PDEs), it is not as time-consuming as a particle simulation where the trajectories of all the individual particles are being traced. Therefore, it is particularly suitable for any kind of extended analysis where the particle approach would be too time demanding.
2. Fluid model of plasma-solid interaction

2.1. Basic features of the model

The model uses a square computational domain \((x, y)\) with a regular grid in Cartesian coordinates together with the assumption of translational symmetry along the axis perpendicular to the plane of the model. The model solves the dynamics of plasma species in the vicinity of a cylindrical probe placed in the \(z\) direction, perpendicular to the computational plane. Magnetic field \(\mathbf{B} = (B_x, 0, 0)\) is set to be parallel with the \(x\) axis. These assumptions allow us to work in two dimensions.

The model is solved for each plasma species – electrons and argon ions. Collisions with neutral background are approximated in a simple way as elastic scattering with a given collision frequency. This frequency is constant for each particle species.

Boundary conditions correspond to an assumption of undisturbed plasma at the outer boundaries of the computational domain, while the internal boundary with electrode has to represent an interface with a metal immersed in plasma.

2.2. Mathematical background

Mathematical description is based on a fluid model governed by partial differential equations (PDEs), which can be derived taking velocity moments of the Boltzmann equation. This computational study uses the continuity equation (1) for plasma density \(n\) and momentum transfer equation (2) for average velocity of plasma species \(u\). The conservation equations describing a transport of mass and momentum are solved for electrons (\(k=e\)) and ions (\(k=i\)).

\[
\frac{\partial n_k}{\partial t} + \nabla \cdot (n_k u_k) = 0 \tag{1}
\]

\[
m_k n_k \frac{\partial u_k}{\partial t} + m_k n_k (u_k \cdot \nabla) u_k = q_k n_k (\mathbf{E} + u_k \times \mathbf{B}) - \nabla p_k - m_k n_k \nu_k u_k. \tag{2}
\]

Quantities in equations (1) and (2) have their usual meaning – density \(n\), average velocity \(u\), pressure \(p\), mean collision frequency \(\nu\), mass \(m\), charge \(q\) and electric and magnetic field \(\mathbf{E}\) and \(\mathbf{B}\). The system of equations is completed by Poisson’s equation for electric potential \(\varphi\)

\[
\triangle \varphi = \frac{e}{\epsilon_0} (n_e - n_i) \tag{3}
\]

\[
\mathbf{E} = -\nabla \varphi. \tag{4}
\]

The model is simplified by an assumption of constant temperature and the energy balance is not solved. Viscosity effect are neglected and only scalar pressure is taken into account \(p = nkT\). Collision processes are simplified assuming only elastic scattering with constant collision frequency \(\nu\). Considered approximation follows an intent to carry out a qualitative analysis, while more precise model with improved treatment of collisions and the energy equation taken into account is described and solved e.g. in [2]. Compared to other papers, where the momentum equation is strongly simplified, this model works with full momentum equation. It is usual, under certain assumptions being fulfilled, to cancel the inertial and convective terms and to work with a drift-diffusion approximation [3]-[5], which has an algebraic form and describes a flux composed of the drift and the diffusion. In such a case, Scharfetter-Gummel scheme [6] is commonly proposed to solve PDE of the drift-diffusion type.

2.3. Boundary conditions

Boundary conditions of the equations (1)-(3) imposed on density, velocity and electric potential are summarized in Table 1. The problem is fixed by Dirichlet boundary conditions imposed...
Table 1. Boundary conditions.

|                | $n_e$ | $n_i$ | $u_e$ | $u_i$ | $\varphi$ |
|----------------|-------|-------|-------|-------|-----------|
| exterior (undisturbed plasma) | $n_e = n_0$ | $n_i = n_0$ | open | open | $\varphi = 0$ |
| interior (solid surface)       | open  | open  | open  | open  | $\varphi = U_p$ |

on electric potential, assuming biased electrode with a positive voltage $U_p$ and assuming undisturbed quasineutral plasma on the exterior of the computational domain. Dirichlet boundary condition is used also for plasma density at the outer boundary, setting the density to an experimental value of undisturbed plasma density. All the other conditions are kept open, i.e. we extrapolate values from nearest grid points inside of the computational region to the boundary (see [7]).

2.4. Computational technique
The system of equations (1)-(3) is solved using the finite difference approach. The equations are discretized on a regular rectangular grid of size $L \times L$ with uniform grid spacing in both dimensions $h = \Delta x = \Delta y$.

The fluid equations (1) and (2) can be written in general form as

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(fv_x) + \frac{\partial}{\partial y}(fv_y) = F$$

with $f = (n, u_x, u_y)$. The same form of the continuity and momentum equations allows us to apply the same method of solution. The equations are discretized in a similar way using the flux-corrected transport (FCT) algorithm [8]-[9] and the solution is being updated to converge to a steady state. The numerical implementation involves three steps: advection, diffusion and anti-diffusion. To update the solution, any traditional high-order numerical scheme can be used, e.g. the two-step Lax-Wendroff discretization is implemented here. Then the diffusive flux is computed using a diffusivity coefficient and the solution is advanced. Final step to update the solution to next time level is to anti-diffuse the solution using a flux limiter. The whole procedure enable to smooth oscillations arising in the numerical solution and steep gradients can be resolved. Detailed description of the implementation is beyond the scope of the paper and it is presented e.g. in [8].

The Poisson’s equation (3) is discretized using the traditional five-point stencil

$$\varphi_{i+1,j} + \varphi_{i-1,j} - 4\varphi_{i,j} + \varphi_{i,j+1} + \varphi_{i,j-1} = \frac{h^2}{\epsilon_0} (n_e - n_i).$$

The resulting system of linear equations is solved using the UMFPACK library [10]-[11], where the solution of systems of linear equations is based on direct LU decomposition solver.

3. Application of the model and input parameters
The fluid model described above was applied to simulate the interaction between plasma and an immersed solid substrate – a cylindrical probe. The model works with plasma composed of electrons and argon ions on a neutral background of argon atoms. Collisions of charged particles with neutrals are simplified assuming elastic scattering with constant collision frequency $\nu_e$ and $\nu_i$. The simulation was performed for various values of external magnetic field $B_x$, probe radius $R_p$ and pressure $p$. Pressure corresponds to certain values of undisturbed plasma density.
The input parameters of the model are summarized as follows: size of the computational domain \( L = 0.01 \) m, probe voltage \( U_p = 10 \) V, electron temperature \( T_e = 23210 \) K and ion temperature \( T_i = 300 \) K. The main subject of interest is to analyze the effect of magnetic field and the influence of pressure and the probe size on the sheath structure. Simulations were performed for various values of \( B_x, R_p \) and \( p \) and only few simulations were selected to illustrate the effects considered here. Values of analyzed parameters used for results in the paper are listed as follows: magnetic field strength \( B_x = 0 \) T and \( B_x = 0.001 T \), probe radius \( R_p = 1 \times 10^{-4} \) m and \( R_p = 5 \times 10^{-4} \) m and pressure \( p = 500 \) Pa \( (n_0 = 1.9 \times 10^{15} \text{ m}^{-3}, \nu_e = 3.9 \times 10^9 \text{ s}^{-1}, \nu_i = 2.0 \times 10^7 \text{ s}^{-1}), p = 1000 \) Pa \( (n_0 = 2.7 \times 10^{15} \text{ m}^{-3}, \nu_e = 7.8 \times 10^9 \text{ s}^{-1}, \nu_i = 3.9 \times 10^7 \text{ s}^{-1}) \) and \( p = 2000 \) Pa \( (n_0 = 3.9 \times 10^{15} \text{ m}^{-3}, \nu_e = 1.6 \times 10^{10} \text{ s}^{-1}, \nu_i = 7.8 \times 10^7 \text{ s}^{-1}) \).

4. Results

![Figure 1](image1.png)

**Figure 1.** From left to right – electron density \( n_e/n_0 \) (1), ion density \( n_i/n_0 \) (2), \( x \) component of electron velocity \( u_e^x [10^6 \text{ m/s}] \) (3) and \( x \) component of ion velocity \( u_i^x [10^5 \text{ m/s}] \) (4). \( B_x = 0 \) T, \( p = 1000 \) Pa, \( R_p = 5 \times 10^{-4} \) m.

The results of a basic fluid model without magnetic field are shown in Figure 1. The distribution of plasma density and electric potential is symmetric around the probe axis. The radial dependence of plasma density in the presheath region is logarithmic (Figure 2), which is predicted also by a simple theoretical model – analytic solution of the diffusion equation and it corresponds also to experimental investigations.

![Figure 2](image2.png)

**Figure 2.** From left to right – radial dependence of plasma density for \( R_p = 1 \times 10^{-4} \) m (1) and \( R_p = 5 \times 10^{-4} \) m (2) for \( B_x = 0 \) T and \( p = 1000 \) Pa. Ion density \( n_i/n_0 \) for \( R_p = 1 \times 10^{-4} \) m (3) and \( R_p = 5 \times 10^{-4} \) m (4) for \( B_x = 0.001 \) T and \( p = 1000 \) Pa. The radial coordinate \( r \) ranges from \( r = R_p \) to \( r = 5 \) mm.

The structure and the size of the sheath region depends on the probe size, as it is illustrated in Figure 2 together with the effect of the magnetic field. Concerning the simulation without magnetic field, the sheath size becomes larger with increasing probe radius. The radial dependence of plasma density in the presheath region becomes more linear than logarithmic.
and it is not so steep. The effect of the magnetic field on the sheath structure is clearly seen. The shape of the sheath region is elongated in the $x$ direction, parallel with the magnetic field $B_x$. Obviously, the extension is larger with increasing magnetic field strength.

![Figure 3](image_url)

**Figure 3.** From left to right – radial dependence of plasma density for $p = 500$ Pa (1) and $p = 2000$ Pa (2) for $B_x = 0$ T and $R_p = 1 \times 10^{-4}$ m. Ion density $n_i/n_0$ for $p = 500$ Pa (3) and $p = 2000$ Pa (4) for $B_x = 0.001$ T and $R_p = 1 \times 10^{-4}$ m.

The effect of pressure on the sheath structure can be seen in Figure 3. Simulation without magnetic field shows that pressure influences the width of the sheath region and for lower pressure density of electrons on the probe surface is higher as well as their velocity. The collision processes significantly influence the sheath shape in presence of magnetic field. For lower pressure, when plasma is less collisional, the magnetic field affects the sheath elongation much more strongly in comparison with more collisional plasma.

The spatial resolution of the grid was $400 \times 400$ grid points or $200 \times 200$ in some simulations. The time resolution was given by Courant-Friedrichs-Lewy (CFL) stability condition and proper value is automatically computed in the code run. Minimum time steps in calculations satisfying the CFL criterion were $\Delta t_e \sim 1 \times 10^{-11}$ s and $\Delta t_i \sim 1 \times 10^{-8}$ s. The efficiency of the fluid code depends on considered physical conditions. One iteration of the simulation in Figure 1 with $400 \times 400$ grid points takes 0.35 s (Intel compiler, Intel Core2 Duo 2.4 GHz CPU) and sufficient number of time steps to reach a steady state solution was $3 \times 10^4$.

5. Discussion and conclusions

The size and the shape of the sheath region surrounding a solid substrate embedded into plasma depends on plasma properties and processes taking place during plasma-solid interaction. In particular, the magnetic field strength and pressure (rate of collision processes) strongly influence the sheath structure. Even in the case of relatively weak magnetic field the effect can be clearly seen.

The presented model was simplified by neglecting non-elastic collisions and assuming constant temperature. These aspects could influence the results quantitatively, but the qualitative effect and the tendency would remain the same. More exact model from this point of view has been also developed and it was described elsewhere [2]. However, the model presented in [2] doesn’t take into account the magnetic field, the equations are simplified in different manner and the numerical technique is different. It would be rather straightforward to upgrade the model described here and include the energy balance and better treatment of collision processes. On the other hand, the model solves full momentum equation compared to common approach, when the momentum equation is simplified and an algebraic expression for flux is used [4].

It should be stated, that for collisionless plasma in presence of the magnetic field it is characteristic to observe the perturbation of the sheath and the presheath region relatively far from the solid surface. In such a case of strong extension of the sheath shape by the magnetic field, the ratio of the width of the perturbed region in the direction of magnetic field lines and in the direction perpendicular to magnetic field lines can be one order of magnitude. In these
conditions, the validity of the model is limited by an assumption of undisturbed plasma outside of the computational region and then a proper boundary conditions should be used or the size of the grid should be modified to correspond to physical conditions. In this study we keep the magnetic field and pressure in such a range to satisfy the boundary conditions.

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