3D particle simulations of plasma-solid interaction: magnetized plasma and a cylindrical cavity

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Abstract.
In this contribution we report the results obtained using a newly developed self-consistent fully 3D Particle-In-Cell code for modelling of plasma-solid interaction.
The model presented here involves a hollow cylindrical chamber opened to the plasma, with an external magnetic field limiting access of charged particles to the cylindrical wall. This model layout might provide more insight into processes taking place during magnetron deposition of thin films onto porous media. It is also a basis for probe diagnostics in fusion plasma research.
The magnetic field is inclined with an angle of either 15° or 30° with respect to the cylindrical axis. Several different pressures of the ambient neutral Ar gas are considered to model the diffusion of ions across the magnetic field in the presence of a solid surface.

1. Introduction
Self-consistent Particle-In-Cell (PIC) simulations provide more realistic and detailed information about modelled plasma processes than fluid simulations do. This benefit is, however, balanced by far greater demands in terms of computational resources. In the past PIC computations were usually accelerated using the intrinsic symmetry of the particular modelled phenomenon. This approach led to 1D and 2D PIC models with many successful applications.

Nevertheless, a large class of plasma-solid interactions cannot be precisely described by this simplified approach. Often the reason is the magnetic field which in certain configurations decreases symmetry of otherwise regular structures of the solid surface such as a hollow cylindrical bore. In these cases a seemingly reasonable approximation would be e.g. to disregard small deviations of the magnetic field from the axis of symmetry of the cavity and thus transform the simulation into a feasible 2D PIC model. Our previous work [1] demonstrated that this assumption is in certain configurations incorrect and that even minor deviations of the magnetic field can have significant impact on measured quantities, such as density distributions of ions impinging on the inner walls of the cylinder.

1.1. Motivation and novel approaches
The primary purpose of this contribution is not to model a particular plasma device, setup or experiment. Our goal is slightly different: we would like to investigate an effect which is rather difficult to measure in actual experiments, i.e. the relative change of ion distribution on the concave cylindrical wall depending on the ambient gas pressure (and thus ionization degree).
Our secondary goal is to evaluate usefulness of 3D PIC codes in configurations similar to that of our model. Diffusion of ions across the magnetic field due to collisions might have a significant impact in certain cases of plasma-solid interaction. An example is given in Fig. 1, where we consider a relatively highly magnetized plasma entering a cylindrical cavity. The inclined magnetic field channels the charged particles along its direction and forces them to impinge preferentially onto a certain part of the inner cylindrical wall.

Collisions of ions with neutral particles present in the plasma cause an opposite effect which randomly scatters guiding centers of ions and allows them to cross the magnetic field and enter otherwise shielded areas of the cylindrical wall.

The results [1] were obtained using our newly developed self-consistent 3D PIC code for a model configuration of fully ionized isothermal hydrogen plasma. Since our group has a substantial experience in modelling low-temperature slightly ionized Ar plasma and its collisions [4], we have decided to extend this research to account for collisions and to model Ar plasma, where the parameters such as scattering cross-sections are relatively well understood. The 3D model was also extended with a multigrid solver enhancing the LU decomposition solver used previously. Both the solver and the collision model will be now briefly described.

2. Poisson equation solver

There is a large number of methods for solving PDEs such as the Poisson equation. Direct methods are usually faster but more difficult to implement and extend, while also requiring more computational resources such as computer memory. Iterative solvers are easier to implement and use, but their performance is usually lower (the most notable exception being the multigrid solver).

Our first contribution to the field of 3D models utilized a direct, LU decomposition-based solver. Since then we extended this solver with a technique utilizing the multigrid method, which is essentially an union of a direct and an iterative approach leading to the PDE solution.

The multigrids [2],[3] are based on a set of grids with different sizes, each grid size is usually twice as coarse in each dimension as the previous one. The particle density and potential is computed on the finest grid, the residual error is smoothed and extinguished on each grid, thus utilizing the optimal smoothing properties for frequencies corresponding to the characteristic cell size of each grid size.

3. Collision model

The effect of collisions is incorporated into the model using the Monte Carlo method. The usual approach to computation of probability of collisions is based on random generation of the free path (FP) between collisions. This method requires the knowledge of the mean FP, which is well defined only if the velocity of scattering centers is negligible in comparison to the velocity of the scattered particle. Otherwise the expected FP depends on actual velocity of particles, which would require computing the collision probability at every timestep. Moreover, as the particle velocity decreases the expected FP approaches zero, which further complicates use of this method.
In case of electron-neutral collisions, the computation of random FP is simple because the electron velocity is by orders of magnitude higher than the neutral particle velocity. In case of ions the situation is different. The thermal velocities of ions and neutral particles are of the same order, therefore the description of collisions using the random FP is not suitable and can result in a strong deformation of velocity distribution [4].

In order to describe the ion-neutral collisions, the collisional frequency of ion in the neutral gas was calculated. With the knowledge of collisional frequency, we were able to generate random time between collisions (instead of random free path). For description of processes with velocity dependent collisional frequencies we used modified null collision method [5] to make the collisional frequency constant.

At the moment of collision, an interacting particle is picked randomly. Based on the collisional frequency corresponding to relative velocity of particles, we decide the occurring interaction. It can be shown that this method exactly (in terms of probability distribution) describes frequency of collisional processes and velocities of interacting particles.

4. Plasma model and its parameters
The goal of this paper is to investigate the effects of collisions on diffusion of ions across the magnetic field. In order to model this phenomenon we developed a configuration as described in Fig. 1. The parameters of the geometry: \( r_C = 4 \text{ mm}, \ l_C + l_A = 9.5 + 0.5 \text{ mm}, \) the whole model area spans \( 10 \times 10 \times 20 \text{ mm} \).

The modelled plasma consisted of Argon ions with the temperature \( T_i = 300 \text{ K} \) and electrons with \( T_e = 21600 \text{ K} \). Charge density was constant for all computations, \( n_0 = 1 \times 10^{15} \text{ m}^{-3} \), ambient gas pressures were \( 1.33 \times 10^{-4}, 1.33, 13.3 \) and \( 133 \text{ Pa} \), which corresponds to ionisation degrees between \( 3.1 \times 10^{-8} \) and \( 3.1 \times 10^{-2} \). Magnetic field \( B = 0.1 \text{ T} \) was inclined with an angle \( \alpha = 15^\circ \) or \( 30^\circ \).

The dimensions of the grid were \( 60 \times 60 \times 120 \text{ cells} \), the Poisson equation solver was a two-level multigrid with full weighting for both restriction and prolongation, with the Gauss-Seidel method smoothing and with the LU decomposition-based solver [1] providing the solution on the coarsest level. The multigrid subroutines were parallelized using the OpenMP technique.

The ratio of particles to macroparticles was \( 1 \times 10^3 \), the timestep for electrons was \( 1 \times 10^{-11} \text{ s} \), for ions \( 1 \times 10^{-9} \text{ s} \).

5. Results and their discussion
The results presented in fig. 2 show both complex and understandable behaviour. For both inclinations of the magnetic field the angular distribution of ions is slightly shifted from its symmetrical position, this phenomenon is caused by the helical motion of charged particles which leads to a preferred direction from which the ions impact the inner cylindrical wall.

As the diffusion through collisions for the pressure of \( 133 \text{ Pa} \) becomes dominant, the angular distribution becomes even. At the same time, the axial distribution shows that for the highest pressure the magnetic field loses its channeling abilities and ions spread randomly with the net result of less ions reaching the bottom of the cavity.

Thus, for these model settings we have identified a transient region of pressure where the influence of the magnetic field is lessened by collisions with the neutral particles. At the same time we can derive from results that for lower pressures (and thus higher ionisation degrees) the influence of collisions is fairly negligible. This observation might be significant in considering relevance of collisions e.g. in plasma diagnostic probes used in fusion devices.

The model of plasma presented here is by no means complete. It lacks several potentially significant phenomena, such as a non-zero probability of ion reflection from the surface, the effects of secondary emission etc. Also, the relatively modest size of the modelled region prohibits use of more aggressive biasing.
Figure 2. The angular (left) and axial (right) distributions of ions on the inner cylindrical wall, with the magnetic field inclination $\alpha$ and ambient gas pressure as parameters.

However, many of these phenomena are material dependent and their proper incorporation is a problem in any plasma model and as such should be addressed mainly in models of particular experiments. Future improvements might also further enhance the 3D model performance and thus enable modelling of more complex setups.

6. Conclusion
We have demonstrated the behaviour of plasma in presence of two competing phenomena, the magnetic field and the ambient neutral gas, which influence the particle trajectories in vicinity of a complex solid surface. We have also demonstrated feasibility of self-consistent 3D PIC models and their deployment in investigations of plasma device setups which lack exploitable symmetry.

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