Simulation of Interaction of Low-Temperature Plasma with Immersed Solids

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Abstract: The computer simulation has become a widely used technique for the study of various problems in the field of plasma physics. Despite the increasing performance of computers, fully three-dimensional particle simulations still have got extremely high demands on hardware and computer time. Although many problems could be solved be fluid models, results obtained by these methods lack detailed information about individual particles. To overcome these difficulties, hybrid models combining several basic techniques have been introduced. The presented model allows us to solve complex problems demanding the three-dimensional geometry, such as interaction of low-temperature plasma with uneven substrates or plasma propagation to porous solids in the presence of magnetic field.

Keywords: Plasma-solid interaction, hybrid model, magnetised plasma, uneven substrates

1. Introduction

In our contribution, we present a hybrid model designed to solve interaction of low-temperature plasma with immersed solids. Generally, hybrid models combine more techniques in order to gain advantages from each part, however some disadvantages are inevitable [1].

The presented model is based on an iterative alternation of a fluid part and a particle part. Fluid models are relatively fast, but their results are expressed only in macroscopic quantities, such as number density and temperature. Self-consistent particle models have got high requirements on hardware and time; however, their results include detailed information about individual particles. A combination of these methods may significantly increase the efficiency of the simulation.

2. Numerical Model

The fluid part of the hybrid model is based on a set of partial differential equations including Poisson's equation (1) and continuity equations for all types of charged particles in plasma, e.g. electrons (2) and ions (3) in the case of electropositive plasma [2]

$$\Delta\varphi = -\frac{e}{\varepsilon_0}(n_\mathrm{i} - n_\mathrm{e}) \qquad (1)$$

$$\frac{\partial n_\mathrm{e}}{\partial t} + \nabla \cdot \vec{\Gamma}_\mathrm{e} = 0 \qquad (2)$$

$$\frac{\partial n_\mathrm{i}}{\partial t} + \nabla \cdot \vec{\Gamma}_\mathrm{i} = 0 \qquad (3)$$

where n_e and n_i are number densities of electrons and ions, Γ_e and Γ_i are their fluxes and φ is the electric potential. The expression for fluxes depends on the configuration of the problem. In the case of collisional low-temperature plasma at middle pressures, the drift-diffusion approximation is used

$$\vec{\Gamma}_k = \frac{q_k}{m_k \nu_k} n_k \vec{E} - \frac{1}{3\nu_k}\overline{c_k{}^2}\nabla n_k \qquad (4)$$

where k denotes the type of particles, q is the charge of particle, m is its mass, v is the mean frequency of collisions with background gas and c^2 is the mean chaotic velocity of particles. Spatially dependent parameters v and c^2 are determined in the particle part. Assuming a fixed external magnetic field is present, the flux is given by expression (5) [3]. When a stationary solution of equations (1) to (3) is computed, the spatial distribution of electric potential is passed to the particle part.

In the particle part, individual particles are traced under the influence of electric and optionally magnetic forces [4]. As the model is non self-consistent, the direct interaction between charged particles is neglected. This approximation is valid, only if the collective forces and collisions with background gas are dominant. During the motion of particles in the computational domain, various quantities are sampled, including v and c^2 and fluxes to boundaries. After a sufficient number of particles is traced, these quantities are used in next

$$\vec{\Gamma}_k = \left[\frac{q_k}{m_k \nu_k} n_k \vec{E} + \left(\frac{q_k}{m_k \nu_k} \right)^2 n_k \left(\vec{E} \times \vec{B} \right) + \left(\frac{q_k}{m_k \nu_k} \right)^3 n_k \left(\vec{E} \cdot \vec{B} \right) \vec{B} - \frac{1}{3\nu_k} \overline{c_k}^2 \nabla n_k \right.$$
$$\left. - \frac{q_k}{m_k \nu_k} \cdot \frac{1}{3\nu_k} \overline{c_k}^2 \left(\nabla n_k \times \vec{B} \right) - \left(\frac{q_k}{m_k \nu_k} \right)^2 \frac{1}{3\nu_k} \overline{c_k}^2 \left(\nabla n_k \cdot \vec{B} \right) \vec{B} \right] / \left[1 + \left(\frac{q_k B}{m_k \nu_k} \right)^2 \right] \quad (5)$$

iteration of the fluid part. Whole procedure converges usually in several iterations.

3. Use of COMSOL Multiphysics

COMSOL Multiphysics proved to be a useful tool for solution of the fluid part, especially when the three-dimensional approach is required. The Poisson's equation (1) is solved in the Electrostatics application mode and the continuity equations (2) and (3) in PDE General Form mode with appropriate expressions for the flux.

The particle part is based on a standalone application in C++ with OpenMP parallelization. The spatial distributions of quantities interchanged between the fluid and particle part are passed as text files containing data on a rectangular grid.

4. Results and Discussion

The presented hybrid model has been used to solve various problems of interaction of low-temperature plasma with solids, e.g. [5]. As an example of a configuration with magnetic field, we present selected results of a study of plasma propagation to a cylindrical hole in a conductive substrate. The geometry is shown in Figure 1. As the orientation of homogeneous magnetic field is arbitrary, the three-dimensional approach is necessary. The undisturbed plasma of DC glow discharge in argon at 133 Pa is attached to the top boundary of the domain. The substrate is biased to -0.5 V. In Figure 2, the distribution of ion density and the ion flux in the domain is shown. The magnetic field enhances the propagation of ions to inner parts of the hole. However, the propagation of charged particles is also influenced by E×B drifts, making the analysis more complicated.

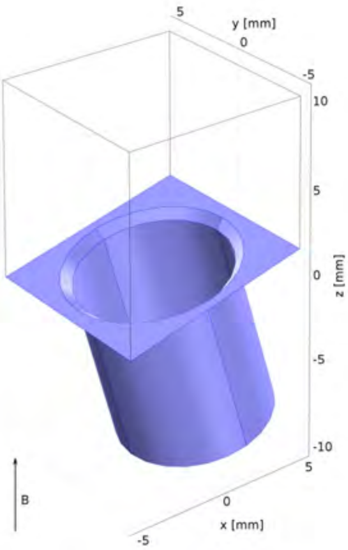

Figure 1. The geometry of the substrate and of the computational domain used in the study of plasma propagation to a cylindrical hole

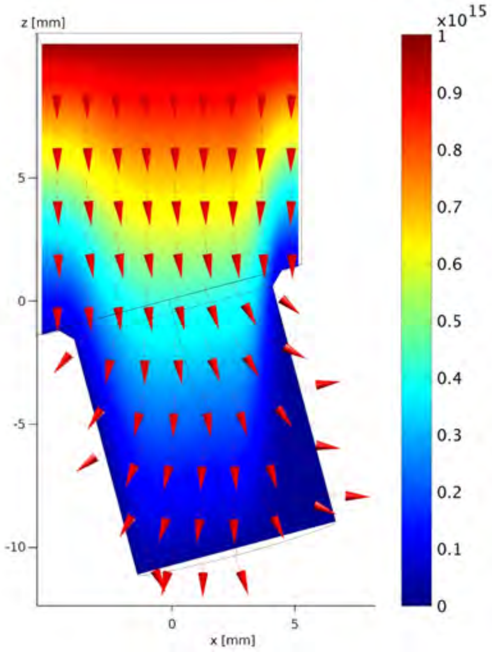

Figure 2. The propagation of ions to the cylindrical hole. The patch shows the number density of ions in m^{-3}. Red arrows are drawn in the direction of ion flux.

The hybrid model was also used to a study of plasma interaction with uneven substrates. Physical conditions in the vicinity of unevenness strongly influence plasma treatment of solids in various technologies. In Figure 3, the magnitude of electric field at the surface with a matrix of semi-cylindrical protrusions is shown. Parameters of plasma are the same as in the previous case. The conductive substrate is biased to +5.0 V. The electric field is enhanced at the top of protrusions; moreover, the field is minimal between them. The flux of charged particles follows the electric field and the plasma treatment of the surface is not uniform. The computational simulation helps to quantify these effects.

5. Conclusions

The presented iterative hybrid model of plasma-solid interaction is a competitive technique offering more detailed and accurate results with reasonable time and hardware requirements. One configuration can be solved in 6 to 12 hours on a PC (Intel Core i7 940 at 2.98 GHz), while a comparable particle model would require weeks.

The hybrid model can be used to solve various problems; however, its scope is limited to steady-state problems and collision-dominated plasmas.

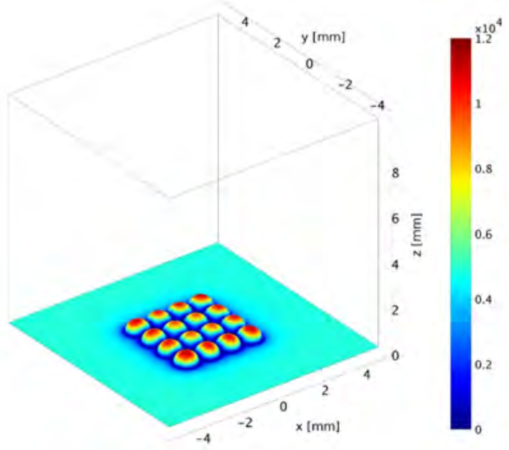

Figure 3. The magnitude of electric field E [V m^{-1}] at the surface of an uneven substrate

6. References

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7. Acknowledgements

The work is a part of the research plan MSM0021620834 financed by the Ministry of Education of the Czech Republic. The authors acknowledge the support of the Grant Agency of Charles University in Prague, project GAUK18908/2008, and the Czech Science Foundation GA ČR, projects 202/08/H057 and P205/10/0979.