Differential cross section in PIC-MCC simulation of plasma-solid interaction

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Abstract. This paper focuses on the particle modelling of the interaction of low-temperature plasma with immersed cylindrical Langmuir probe. Particle modelling gives comprehensive information about the system, which is being analyzed, but the simulations are highly time-consuming. Especially in the high-pressure plasma the interactions between charged and neutral particles play an important role and they are often simulated by the Monte Carlo method. For this paper we prepared a simulation, which contains these interactions in as accurate way as possible, including the angular dependence of the electron-neutral elastic collision. We showed the effect of neglecting this angular dependence as well as the energy dependences of the cross sections of all included interactions.

1. Introduction
To understand plasma-solid interaction is essential in modern plasma-assisted technologies as well as for the interpretation of plasma probe diagnostics. The theoretical analyses of processes taking place in low-temperature plasmas are complicated especially due to the collisions. Hence, computer simulations present a good possibility to describe the examined systems.

The particle simulations of plasma provide results in both macroscopic and microscopic scales. Their time requirements are, however, very high and many techniques are being developed to speed up the calculations. The simulations based on Particle in Cell technique with Monte Carlo collisions (PIC-MCC) are widely used. So far, the PIC-MCC simulations have included collisions with either constant or energy-dependent cross sections. Recently, the Monte Carlo collision model has been improved in accuracy and speed [1] and the effect of further improvement of this model in sense of adding the angular dependencies of the cross sections is presented in this contribution.

Three simulations of interactions between the charged particles and the neutral ones with different levels of accuracy are compared and presented as a part of the PIC-MCC simulation. The simulated system is electropositive argon plasma in DC glow discharge with immersed Langmuir probe.

2. Description of the simulation
The simulation is based on the combination of molecular dynamics (MD) and Monte Carlo (MC) techniques. The trajectories of the charged particles (electrons and argon ions) are determined by the numerical solution of the Newton’s second law of motion, which includes the electrostatic interactions between the charged particles and with the probe. The interactions with neutral particles are included as random events using the Monte Carlo technique.
2.1. The molecular dynamics simulation

The two-dimensional working area is square-shaped with the side of 2 cm. In the centre of the area there is a cylindrical probe with positive bias and in the undisturbed plasma outside the working area we assumed Maxwell-Boltzmann distributions of argon ions and electrons.

For the integration of Newton’s equations of motion we used the velocity Verlet algorithm [2]. In order to speed up the relaxation time we implemented different time steps for electrons $1 \times 10^{-12}$ s and for argon ions $1 \times 10^{-9}$ s. The force acting on the charged particles is obtained in each time step by solving Poisson’s equation on the grid of $200 \times 200$ nodes. The algorithm we used is usually called Particle in Cell - Nearest Grid Point (PIC-NGP) algorithm and it is described in details in [3]. For numerical solving of the Poisson’s equation the C library UMFPACK [4] was used.

The main input parameters of the undisturbed argon plasma and infinite cylindrical Langmuir probe are shown in table 1.

Table 1. The parameters of the MD part of the simulation.

| Parameter                  | Value       |
|----------------------------|-------------|
| probe radius               | 100 μm      |
| probe bias                 | +10 V       |
| plasma number density      | $3.22 \times 10^{22}$ m$^{-3}$ |
| electron number density    | $1 \times 10^{15}$ m$^{-3}$ |
| electron mean energy       | 3 eV        |
| argon ion mean energy      | 39 meV      |

2.2. The Monte Carlo simulation

The Monte Carlo part of the simulation is responsible for the interactions between the charged particles and the neutral argon atoms. For electrons we chose elastic collision, excitation to the first excited level (11.55 eV) and ionization (15.755 eV). For argon ions it is elastic collision and charge transfer. The cross sections of the electron interactions were obtained from [5] and for the argon ions from [6]. The angular dependency of the electron-argon elastic collision was taken from [7].

The most accurate version of simulation contains all dependencies that have been mentioned including the angular dependency and in the resulting graphs it is called “angle”. For the generation of electron random free path $\xi$ we could use the simplified formula

$$\xi = -\lambda \ln \gamma$$

where $\lambda$ is the mean free path of electrons and $\gamma$ is uniformly distributed random number from the interval (0;1). The equation (1) can be used only if the velocity of scattering centers can be neglected and the mean free path is independent of energy. The second requirement we fulfilled using the “null collision” method [8] by adding a virtual collision. During the simulation, if the elastic collision was chosen, we randomly chose the scattering angle with the probability distribution, which corresponds to the angular cross section dependency for particular electron energy.

For the ion interactions the velocity of the neutral argon atoms cannot be neglected. Therefore, we used the “advanced null collision method” [9]. The null collision cross section is chosen in such a way that the expression $v \sigma(v)$ is constant for all relative velocities $v$ that might occur in the system. The probability that during the time step $\Delta t$ an electron undergoes collision is then given by the formula

$$P = 1 - \exp(-nv\sigma\Delta t).$$
The simulation “energy” shows the effect of neglecting angular dependency of the electron-argon elastic cross section and in the simulation “constant” the cross sections of all interactions are constant. Using numerical integration we computed mean values of the cross sections of each interaction. In this case for electrons the equation (1) could be used without applying the null collision method.

3. Results and discussion
In order to show the effect of the described simplifications we chose several output parameters. Through these parameters we compared the simulations “angle”, “energy” and “constant”.

3.1. Electrostatic potential and electron number density

![Figure 1. Radial distribution of potential near the probe. The shaded area shows the location of the probe.](image1.png)

![Figure 2. Radial distribution of electron number density. The shaded area shows the location of the probe.](image2.png)

The figures 1 and 2 show the radial distributions of the electrostatic potential and electron number density near the probe. The results are similar for simulations “energy” and “angle”. The simulation “constant” leads to a broader sheath region. The distributions of the electron number density have a similar tendency in the simulations “angle” and “energy”. The simulation “constant” leads again to biased results – the maximum near the probe is lower and it is followed by a faster radial increase. The local maximum near the probe is the result of cylindrical geometry and it was already presented as a result of other particle and fluid simulations, e.g. [10].

3.2. Electron angular distribution function
The figures 3 and 4 compare the angular distributions of electrons. The angle 0° represents the direction towards the probe. We chose two different locations for comparison – the first one (figure 3) is located directly at the probe, thus in the sheath region and the second one (figure 4) is located 2 mm from the centre of the working area in the pre-sheath region. The results of simulation “angle” are in these comparisons significantly different from the results of the other simulations, especially in the direction near 0°. As we can see on the graphs, there are fewer electrons heading towards this probe and more ones heading in the perpendicular directions. In the direction from the probe, which is not as important for the applications, the simulation “energy” gives the most biased results.
4. Conclusion

The results of the three simulations with different inclusion of collision processes were compared. We compared radial distributions of electrostatic potential, electron number densities and distributions of the velocity direction. As expected, the angular distribution was quite strongly influenced by the use of the angular dependence of electron-argon elastic collision.

In the other comparisons, the angular dependency does not play such an important role and the most biased results are produced by the simulation, which assumed the constant cross sections. On the example of the argon plasma we have shown that using differential cross sections in the particle simulations of plasma-solid interaction is essential if the angle-dependent results are needed, otherwise the previously used Monte Carlo simulation, as used e.g. in [1], are sufficient. The simplification of constant cross sections is in all cases unsatisfactory.

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