CHARGING OF A GRAIN IMMERSED INTO PLASMA: STUDY BY COMPUTER SIMULATIONS

Petr Bartoš, Josef Blažek, Petr Špatenka

University of South Bohemia, Department of Physics, Jeronýmova 10, 371 15 České Budějovice

Abstract

In our contribution we describe the computer model written in the MATLAB programming language that is based on the particle modelling technique. Although this approach is not in the computational point of view the most powerful one, physically it could be very interesting. It minimizes some drawbacks of recently used methods, like the assumptions of Maxwellian electron energy distribution function, constant diffusion coefficients and coefficients of mobility in particle and energy fluxes and others. Moreover, important physical phenomena, like photo-emission, secondary electron emission or thermo-emission can be precisely described and considered in the model. Both the surface charge and dependent quantities can be determined by this way with relatively high accuracy.

1 Introduction

In recent years computer simulations are playing an important role in theoretical investigations in various branches of human activities. Similar is the situation in the research of complex (dusty) plasma [1] that is interesting not only for astronomers (interstellar clouds, comet tails etc.) but it found the place also in complicated technological processes like powder modification, plasma etching of semiconductor devices or plasma diagnostic. The understanding of processes like charging and dynamics of dusty particles is necessary for the effective developing of technological devices.

If a micron-sized grain is immersed into a positive column of electropositive low-temperature DC glow discharge, it became negatively charged. This effect is caused due to the different velocities of electrons and positively charged ions. The light and more moveable electrons reach the solid surface in shorter time than heavy and less moveable positive ions. The electric field generated in the vicinity of the grain by the negative grain surface charge causes that in the steady state the particle fluxes are equal.

The grain surface charge is the essential quantity that should be determined as precisely as possible, because it significantly influents the results of computer experiments in other areas – micro-particles interaction, grain dynamics in plasma sheaths, the formation of plasma crystals etc. Therefore, the charging of particles immersed into plasma attracts a lot of attention in recent theoretical and experimental studies.

Computer modelling techniques, which are usually used in simulations in plasma physics, can be divided into three groups – particle, fluid and hybrid simulations. The particle approach describes the processes on the level of particles, movement of every particle is studied individually and – because of large number of studied particles – the calculation took several hours or days. In contrast to this technique, the description of collision processes on the level of atoms and charged particles make the simulation precise.

Fluid modelling techniques describe the plasma like a system of several fluids. During the calculation a system of several partial integro-differential equations is solved numerically and the computation can be performed relatively quickly (in several seconds or minutes), but the description of collision processes can be done under many non-physical assumptions decreasing the precision of results.

In order to minimize the drawbacks of particle and fluid simulations and to keep the precision of the calculation relatively high, hybrid modelling techniques are sometimes used in recent years. Such computer models can be further divided into several groups, but the main idea is to describe the plasma fluidly and to perform the collision processes by the particle simulation.

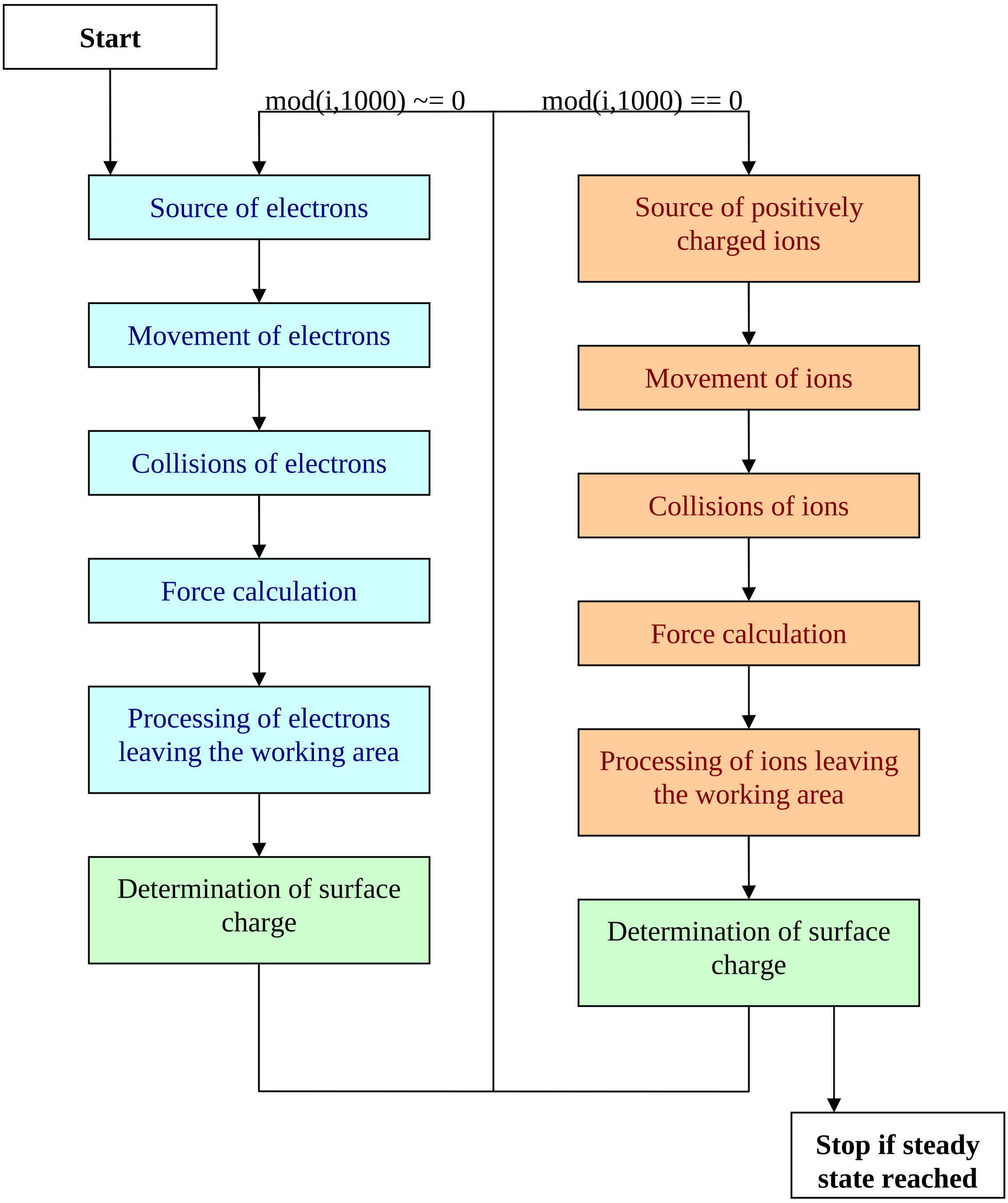

Figure 1: Model scheme

Most of recent theories describing grain charging use the fluid modelling technique and they are usually based on the comparison of particle fluxes to the grain surface. The most simply one compares both the electron and the positive ion fluxes that can be analytically deduced under the assumption of Maxwellian electron energy distribution function.

In such a case we can write the particle fluxes in the form [2]

$$j_{\mathrm{e}} = n_{\mathrm{e}} \sqrt{\frac{k_{\mathrm{B}} T_{\mathrm{e}}}{2\pi m_{\mathrm{e}}}} \exp\left(-\frac{e_0 V_{\mathrm{floating}}}{k_{\mathrm{B}} T_{\mathrm{e}}} \right) \qquad (1)$$

$$j_{\mathrm{i}} = n_{\mathrm{i}} \sqrt{\frac{k_{\mathrm{B}} T_{\mathrm{i}}}{2\pi m_{\mathrm{i}}}} \left(1 - \frac{e_0 V_{\mathrm{floating}}}{k_{\mathrm{B}} T_{\mathrm{i}}} \right) \tag{2}$$

and the floating potential V_{floating} can be found easy as the numerical solution of the equation

$$j_{\mathrm{e}} = j_{\mathrm{i}} \,. \tag{3}$$

Photoemission, thermo-emission and ion impact secondary emission on the particle surface are usually neglected. Afterwards, the surface charge is determined as a function of the floating potential

$$Q = 4\pi\varepsilon_0 r V_{\mathrm{floating}} \,.$$

In this approximation the surface charge decreases linearly with the probe radius (see Figure 2, the temperature of electrons $T_{\mathrm{e}} = 23.200\ \mathrm{K}$, temperature of positively charged ions $T_{\mathrm{i}} = 300\ \mathrm{K}$). This is in contrast to the experimental results that were obtained in many measurements (Fortov [3], Walch [4], etc).

Therefore the more precise theories are used in recent studies. They are usually based on the drift-diffusion approximation of particle fluxes. The influence of various physical phenomena on the grain surface (photoemission, thermo-emission, etc.) and the comparison of theoretical and experimental results can be found in the Ref. [5].

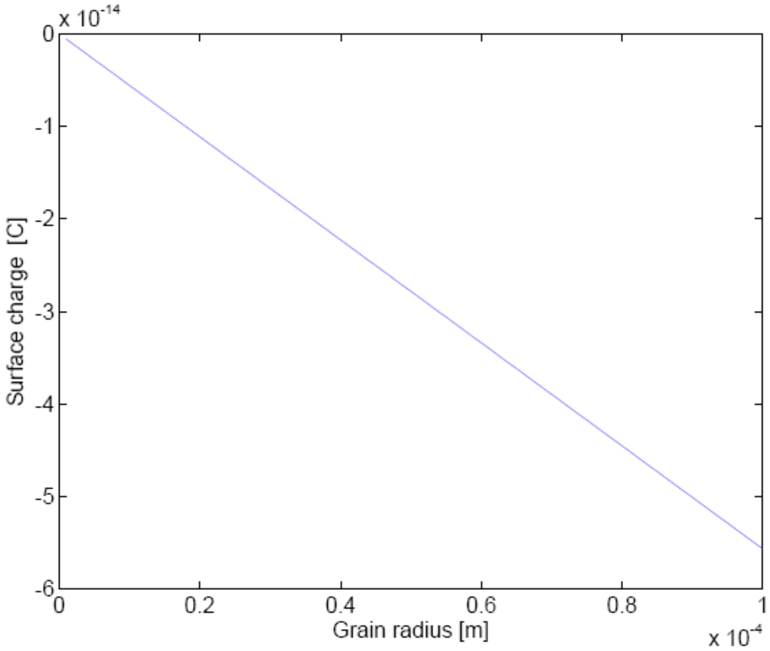

Figure 2: Surface charge as a function of the grain radius - output of the basic model.

2 Description of our model.

On our department we have developed a computer model based on the particle modelling approach. Model scheme is presented in the Figure 1. A positive column of DC glow discharge in argon containing micro-sized dusty particles is considered. The plasma consists of electrons, singly charged positive argon ions and neutrals. Other types of particles do not significantly affect other studied quantities.

The working area is a sphere with the radius given by the Debye length

$$\lambda_{\mathrm{D}} = \sqrt{\frac{\varepsilon_0 k_{\mathrm{B}} T_{\mathrm{e}} T_{\mathrm{i}}}{n e^2 (T_{\mathrm{e}} + T_{\mathrm{i}})}} \,. \tag{4}$$

Concentrically to this sphere there is placed the second one representing the dust particle. The source of both electrons and positively charged ions is around the working area. The energy distribution functions of charged species in this region are supposed to be Maxwellian.

The movement of charged particles is described by the Verlet's algorithm [6]:

$$\vec{r}_\mathrm{i}^{\,\mathrm{k+1}} = \vec{r}_\mathrm{i}^{\,\mathrm{k}} + \vec{v}_\mathrm{i}^{\,\mathrm{k}}\,\Delta t + \frac{1}{2m_\mathrm{i}}\vec{F}_\mathrm{i}^{\,\mathrm{k}} \tag{5}$$

$$\vec{F}_\mathrm{i}^{\,\mathrm{k+1}} = \ldots \tag{6}$$

$$\vec{v}_\mathrm{i}^{\,\mathrm{k+1}} = \vec{v}_\mathrm{i}^{\,\mathrm{k}} + \frac{1}{2m_\mathrm{i}}\left(\vec{F}_\mathrm{i}^{\,\mathrm{k}} + \vec{F}_\mathrm{i}^{\,\mathrm{k+1}}\right)\Delta t \tag{7}$$

In above equations $\vec{r}$ denotes the vector of space coordinates, $\vec{v}$ is the velocity of particle, Δt denotes the time step, m is the mass of particle and $\vec{F}$ is the force vector. The movement of negative species is neglected. Because of significantly different velocity of electrons and negatively charged ions various time steps are used. For electrons the time step length is $\Delta t_\mathrm{e} = 1\times10^{-11}\ s$, for positive ions $\Delta t_\mathrm{i} = 1\times10^{-8}\ s$.

If the charged particle travels the random free path λ_random that is generated according to the equation

$$\lambda_\mathrm{random} = -\lambda_\mathrm{total}\ln\gamma, \tag{8}$$

a collision occurs. Because the mean free path in Eq. (8) has to be constant, Null Collision method is used [6]. In our model following collision processes are considered:

a) Elastic scattering of electrons with neutrals

$$Ar + e^- \rightarrow Ar + e^- \tag{9}$$

b) Excitation of neutrals into all important energetic states:

$$Ar + e^- \rightarrow Ar^* + e^- \tag{10}$$

c) Ionisation of neutrals

$$Ar + e^- \rightarrow Ar^+ + e^- + e^- \tag{11}$$

d) Elastic scattering of positive ions

$$Ar + Ar^* \rightarrow Ar + Ar^* \tag{12}$$

e) Charge transfer

$$Ar + Ar^* \rightarrow Ar^* + Ar\,. \tag{13}$$

The collision type depends on the particle energy. The probability of a collision of the given type can be expressed as a function of the collision cross-section. In literature there can be found following dependencies for argon (all collision cross-sections are expressed in cm^2 by the relations (14)-(20), electron energy E is given in eV [7]):

- elastic collision:

$$\sigma_\mathrm{ela} = \left\{\left|\frac{6}{\mathrm{Y}_1} - \frac{1.1E^{1.4}}{\mathrm{Y}_2}\right| + \frac{0.05}{\left(1+\frac{E}{10}\right)^2} + \frac{0.01E^3}{1+\left(\frac{E}{12}\right)^6}\right\}\times10^{-16} \tag{14}$$

where

$$Y_1 = \left(1 + \frac{E}{0.1} + \left(\frac{E}{0.6}\right)^2\right)^{3.3} \tag{15}$$

$$Y_2 = \left[1 + \left(\frac{E}{15}\right)^{1.2}\right]\left[1 + \left(\frac{E}{5.5}\right)^{2.5} + \left(\frac{E}{60}\right)^{4.1}\right]^{0.5} \tag{16}$$

- excitation of neutral into all important energetic states (energy range from 11.5 eV) :

$$\sigma_{\text{exc}} = \frac{(E-11.5)^{1.1} \cdot \left[1 + \left(\frac{E}{15}\right)^{2.8}\right]}{2.94 \times 10^{17} \cdot \left[1 + \left(\frac{E}{23}\right)^{5.5}\right]} + \frac{2.3 \times 10^{-18}(E-11.5)}{\left(1 + \frac{E}{80}\right)^{1.9}} \tag{17}$$

- ionization of neutral argon atom by the fast electron in the energy range from 15.8 eV:

$$\sigma_{\text{ion}} = \frac{9.7 \cdot (E-15.8)}{10^{14} \cdot (70+E)^2} + 6 \times 10^{-18}(E-15.8)^2 \exp\left(-\frac{E}{9}\right). \tag{18}$$

- elastic scattering of ions

$$\sigma_{\text{ela}} = 42.887 E^{-0.1434} \times 10^{-16} \tag{19}$$

- charge transfer

$$\sigma_{\text{cht}} = 56.012 E^{-01403} \times 10^{16} \tag{20}$$

If the charged particle leaves the working area, the data are proceed and, afterwards, removed from computer memory.

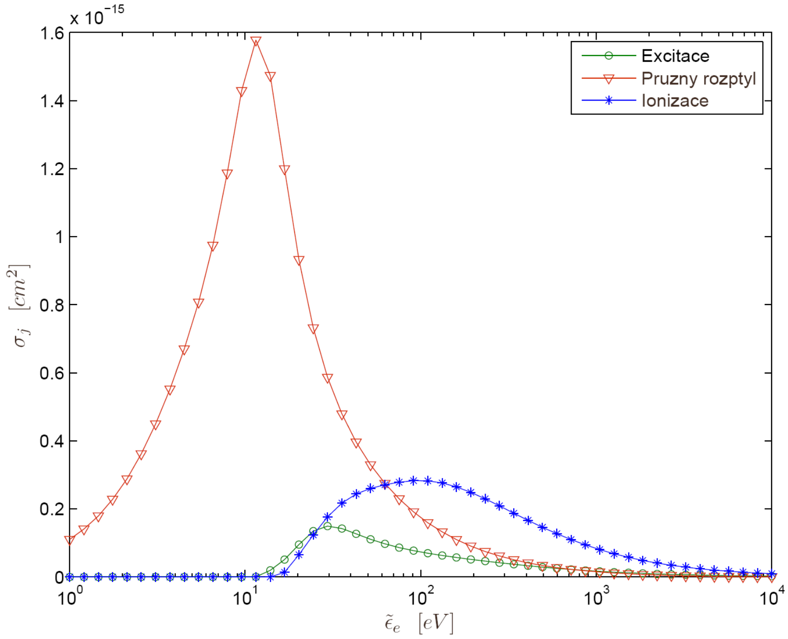

Figure 3: Collision cross sections for electrons – dependence on particle energy.

Results and discussion

The surface charge has been determined by the computer simulation for spherical grains of various radii in the range $5-10\,\mu\text{m}$ (see Figure 3). The comparison of theoretical and experimental results shows that the total charge on the grain surface predicted by our simulations is higher than the one obtained by measurements. The dissimilarity between our and experimental data is probably caused by the non-physical assumption that electrons and positively charged ions are absolutely absorbed when hitting the grain surface. Furthermore, secondary emission of electrons from the dust surface can play an important role, too. The tendency of the curve corresponds both to the predictions presented in [5] and the results presented by many authors.

We expect that in further versions of the computer model these processes will be included into model and the results will be well comparable to the experimental ones. This is indicated by recently performed simulations.

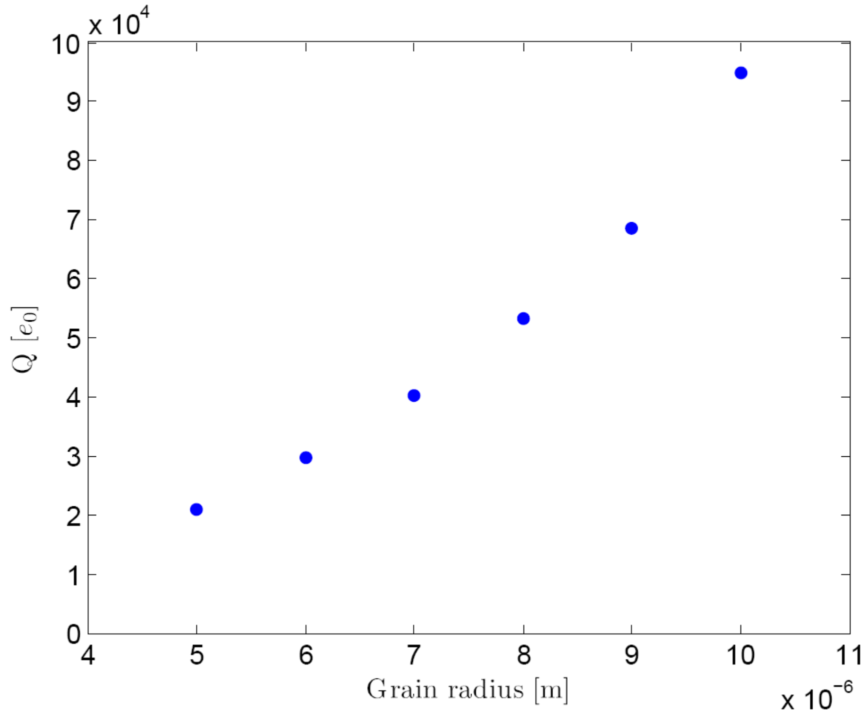

Figure 4: Dependence of the surface charge on the particle radii.

Conclusion

The presented computer model seems to be a good alternative to the fluid approaches that are frequently used in recent studies. However, the processes taking part on the grain surface have to be described more precisely in order to improve the precision of the calculation.

Acknowledgements

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Petr Bartoš
Pedagogická fakulta Jihočeské univerzity, Katedra fyziky
Jeronýmova 10
371 15, České Budějovice
Česká republika
e-mail: bartos-petr@seznam.cz

Josef Blažek
Pedagogická fakulta Jihočeské univerzity, Katedra fyziky
Jeronýmova 10
371 15, České Budějovice
Česká republika
e-mail: bla@pf.jcu.cz

Petr Špatenka
Pedagogická fakulta Jihočeské univerzity, Katedra fyziky
Jeronýmova 10
371 15, České Budějovice
Česká republika
e-mail: spata@pf.jcu.cz