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Finite size effects on charging in dusty plasmas

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Abstract. A three-dimentional particle–particle particle–mesh (P3M) model for dusty plasma has been developed. The model implies a fully kinetic description for all species in the plasma, being able to resolve the finite size effects for dust grains. The model was used for simulation of charging process for the dust grains in a capacitive radiofrequency discharge.

1. Introduction

In previous work [1, 2] we have studied the formation of dust structures in a capacitively coupled radiofrequency (RF) discharge with a self-consistent particle simulation. For this purpose, a three-dimensional particle-in-cell code with Monte Carlo collisions (PIC MCC), resolving also the sheath in front of the wall including all relevant species (neutrals, ions, electrons) and their reactions, was developed and applied [1]. In the simulation, dust particles trapped in the sheath over the lower electrode formed vertical strings, in which negative particles are attracted due to polarization of the ion flow (wake-field effect). A quasi-two-dimensional (simple hexagonal) structure was formed by the dust in which layers with hexagonal symmetry are vertically aligned due to the unidirectional ion background flow towards the electrode in the sheath.

2. Concept of the P3M code

Although PIC simulation has proved to be a powerful tool for studying dusty plasmas, the PIC method has a considerable drawback. The space resolution in the PIC scheme is limited by the size of the grid which is typically of the order of a Debye length (a fraction of a millimeter for RF plasmas). The size of the dust grains used in the laboratory experiments is much smaller than this within the micrometer–nanometer range. The particles in the conventional PIC algorithm are represented by charged clouds of the grid size, being able to penetrate each other [3]. This leads to high inaccuracy for interparticle interaction when the distance becomes smaller than the cell size. In Fig.1, we show the dependence of the interparticle interaction force on the distance, where the distance is normalized to the cell size, as calculated with the PIC model. The interaction force is strongly deviating from the Coulomb force for small distances and tends to go to zero as the inter-particle distance decreases.

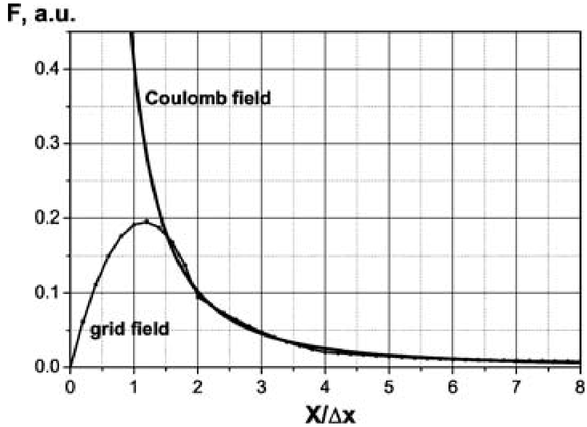

Figure 1. Interaction force between two charged particles in the PIC model. Here Δx is the cell size.

Therefore, the PIC model, being able to resolve long-range interaction between the particles (in the order of the Debye length), misses the close-range part for distances comparable with the radius of the dust grains.

In order to resolve close-range interaction between dust grains and plasma particles accurately, we extended our PIC model, combining it with the molecular dynamic (MD) algorithm. In the resulting particle–particle particle–mesh (P3M) model, the long-range interaction of the dust grains with charged particles of the background plasma is treated according to the PIC formalism. For particles which are closer to the dust grain than a Debye length, their interaction force is computed according to a direct particle–particle MD scheme using the exact Coulomb potential. This is implemented in the following way: in the computational domain, the cell in which the dust grain is located together with the neighboring cells form the 'MD' region. All particles outside the MD region are treated according to the conventional PIC scheme. For plasma particles (electrons and ions) inside the MD region the electric field is calculated as $\mathbf{E} = \mathbf{E}_{\text{grid}} + \mathbf{E}_{\text{dust}}$. Here for the calculation of the grid field $\mathbf{E}_{\text{grid}}$ we use the charge density as in the PIC part from which the dust grain contribution is subtracted. The dust contribution is accounted for through the exact Coulomb electric field $\mathbf{E}_{\text{dust}}$. In order to resolve particle motion on scales of the order of dust grain size, particles in the MD region are moved with time step smaller than in the PIC region. Particles which cross the dust grain boundary are assumed to be absorbed. The dust grain charge is updated each MD time step. This approach allowed us to follow the charged particles trajectories in the close vicinity of the dust grain and by this to include finite-size effects for dust grains, self-consistently resolving the dust grain charging due to the absorption of plasma electrons and ions. The P3M code is parallelized using the MPICH library.

3. Results

In this work we use a P3M model to investigate the dust grain charging process in a capacitive RF discharge in methane. The parameters of the simulation were chosen close to those used earlier for modeling of a three-dimensional dust crystal in a RF methane plasma [1]. As a background gas, methane with a density

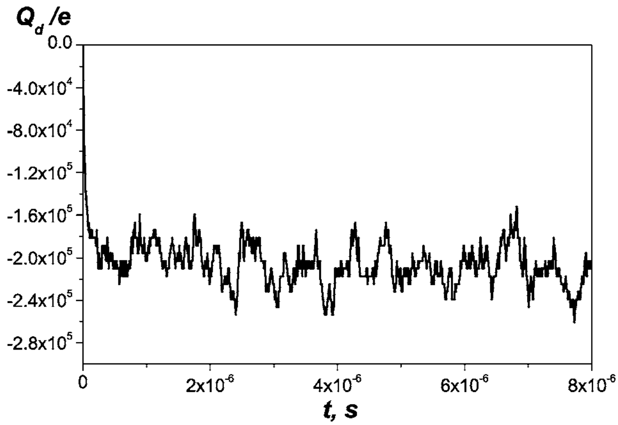

Figure 2. Charging of a dust grain with a radius of 30 μm in a capacitive RF discharge.

$n_{CH_4} = 7 \cdot 10^{14}$ cm^{-3} and temperature $T_{CH_4} = 500$ K was used. The initial electron density and temperature were chosen as $n_{e0} = 2.5 \times 10^9$ cm^{-3} and $T_{e0} = 20$ eV, respectively.

The computational domain represents a three-dimensional box with dimensions $Z_{max} = d = 32 \cdot \lambda_{D0} = 1.5$ cm, $X_{max} = Y_{max} = 8 \cdot \lambda_{D0} = 0.38$ cm, where Z corresponds to the vertical direction and d is the electrode spacing. The lower electrode at $Z = Z_{max}$ is grounded and the upper electrode at $Z = 0$ is powered with a sinusoidal voltage with frequency $f_{RF} = \omega_{RF}/2\pi = 13.56$ MHz. At the electrodes absorbing wall, boundary conditions for the particles were applied. In the X and Y directions periodic boundary conditions were applied, both for particles and the potential. The neutral gas was treated as a fixed background with constant density and temperature. Only the charged particle dynamics was followed. For simplicity, only Coulomb collisions between charged species and electron-impact ionization of methane were considered in the simulation.

A grid with spacing $\Delta x = \Delta y = \Delta z = \lambda_{D0}/2 = 0.0241$ cm and time step $\Delta t = 0.2/\omega_{pe} = 7 \times 10^{-11}$ s was used in the simulation.

In the simulation, the plasma was sustained self-consistently due to electron impact ionization of the neutral gas by the electrons accelerated in the applied RF voltage. In order to reach equilibrium discharge conditions, the amplitude of the RF voltage U_{RF} was automatically adjusted during the simulation using a feedback control loop [4]. The calculations were carried out on a Linux cluster with eight AMD Athlon 2700 + MHz processors. The duration of each run was about 40 h.

The dust particles with radii 3.75, 7.5, 15 and 30 μm were introduced into the system having zero charge. During the simulation dust grains, collecting plasma electrons and ions acquired negative charge. In Fig. 2 we present the evolution of the electric charge of a dust grain with a radius of 30 μm placed in a capacitive RF discharge. A fast initial charging takes place due to the collection of electrons, while equilibration takes place on the ion time scale. The equilibrium dust charge is subject to stochastic fluctuations due to the discrete nature of charge carriers (in the simulation, one computational particle represents the 3668 real electrons or ions).

The time averaged charge for particle with different radii is presented in Fig. 3 (circles).

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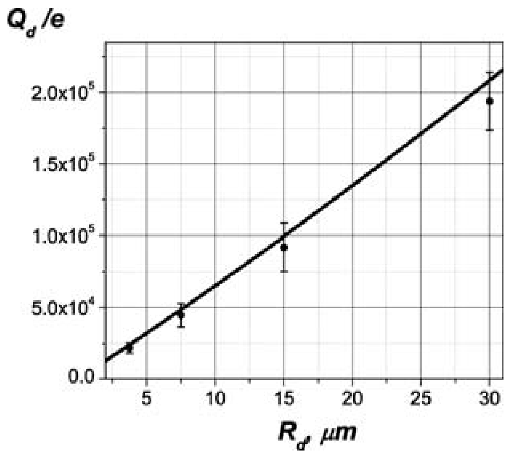

Figure 3. The dependence of the dust charge on the radius of the dust particle.

The charge of the dust grain in the plasma can be written as

$$Q_{\mathrm{d}} = 4\pi\epsilon_0 R_d\left(1 + \frac{1}{\lambda_{\mathrm{D}}}\right)U_{\mathrm{d}} \tag{3.1}$$

Here $C = 4\pi\epsilon_0 R_{\mathrm{d}}(1 + \frac{1}{\lambda_{\mathrm{D}}})$ is the capacitance of a spherical probe in the plasma [5], U_{d} is the dust floating potential, R_{d} is the dust radius, λ_{D} is the Debye length. According to the OML theory [6] the floating potential of a spherical grain in the methane plasma with electron temperature $T_{\mathrm{e}} = 4.35\,\mathrm{eV}$ and ion temperature $T_{\mathrm{i}} = 0.435\,\mathrm{eV}$ is $U_{\mathrm{d}} = 9.1\,\mathrm{V}$. Using this value in (3.1) we obtain the dependence of the dust grain charge on the radius (solid line in Fig. 3). As one can see, the data points obtained in the simulation are in very good agreement with the analytical prediction.

4. Summary

The three-dimensional P3M model for dusty plasmas was developed and tested. The model implies a fully kinetic description for all species in the plasma, being able to resolve the finite size effects for dust grains. The charging process for the dust grains in a capacitive RF discharge was simulated. The results obtained are in good agreement with analytical predictions.

References

[1] Matyash, K. and Schneider, R. 2004 *Contrib. Plasma Phys.* **44**, 157–161.

[2] Matyash, K., Fröhlich, M., Kersten, H., Thieme, G., Schneider, R., Hannemann, M. and Hippler, R. 2004 *J. Phys. D: Appl. Phys.* **37**, 2703–2708.

[3] Birdsall, C. K. and Langdon, A. B. 1985 In: *Plasma Physics via Computer Simulation.* New York: McGraw-Hill.

[4] Matyash, K. 2003 Kinetic modeling of multi-component edge plasmas. *PhD Thesis*, Ernst-Moritz-Arndt-University, Greifswald, Germany.

[5] Bouchoule, A. 1999 *Dusty Plasmas: Physics, Chemistry and Technological Impacts in Plasma Processing.* New York: Wiley.

[6] Allen, J. E. 1992 *Physica Scripta* **45**, 497.