Effect of grain size on dust charging in an RF plasma

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The charge on the dust particles in a dusty plasma is a crucial parameter for the formation of Coulomb crystals, their structure and their dynamics. Here, a newly developed 3-dimensional Particle-Particle Particle-Mesh (P³M) code is applied to study the charging process of micrometer size dust grains confined in a capacitive RF discharge. In our plasma model, plasma particles (electrons and ions) are treated kinetically (Particle-in-Cell with Monte Carlo Collisions (PIC-MCC)), which allows to self-consistently resolve the electrostatic sheath in front of a wall. In order to accurately resolve the plasma particles’ motion close to the dust grain, the PIC technique is supplemented with Molecular Dynamics (MD), employing an analytic electrostatic potential for the interaction with the dust grain. This approach allows to follow the plasma particle trajectories in the close vicinity of the dust grain and by this to include finite-size effects for dust grains. Thus, the dust grain charging due to collection of plasma electrons and ions is resolved in a self-consistent manner. Here, the charging of dust grains in a capacitive RF discharge and its dependence on the size and position of the dust is investigated. The results are compared with laboratory measurements.

In previous work [1, 3] we have studied the formation of dust structures in low temperature laboratory plasmas with a self-consistent particle simulation. For this purpose a 3D 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]. Although PIC simulation proved to be a powerful tool for studying the 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 the Debye length (fraction of a millimeter for low temperature plasmas). The size of the dust grains is typically in the micrometer range and thus much smaller than the grid size. In conventional PIC algorithms, the particles are represented by charged clouds of the grid size and are able to penetrate each other [3]. This leads to high inaccuracies for interparticle interaction when the distance becomes smaller than
the cell size. In this case the interaction force is strongly deviating from the Coulomb force for small distances and tends to go to zero as the interparticle distance decreases. Therefore, conventional PIC models are able to resolve long range (larger than the Debye length) interaction between the particles, but fail to resolve the close-range interaction for distances comparable with the radius of the dust grains.

In order to accurately resolve close-range interactions between dust grains and plasma particles, 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: \( \mathbf{E} = \mathbf{E}_{\text{grid}} + \mathbf{E}_{\text{dust}} \). 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 by the exact Coulomb electric field \( \mathbf{E}_{\text{dust}} \).

In order to resolve particle motion on scales of the order of the dust grain size, particles in MD region are moved with time step smaller than in the PIC region. Plasma particles which cross the computational dust grain boundary are assumed to be absorbed. The dust grain charge is updated each MD time step.

We have applied the P3M model to investigate the dust grain charging process in a capacitive RF discharge in the argon. The parameters of the simulation were chosen to represent the conditions of the experiments with Coulomb balls (see Ref. [4]). As a background gas, argon with a pressure \( p = 50 \text{ Pa} \) and temperature \( T_{\text{Ar}} = 300 \text{ K} \) was used. The initial electron density and temperature were chosen as \( n_{e0} = 1 \times 10^9 \text{ cm}^{-3} \) and \( T_{e0} = 2.5 \text{ eV} \) respectively.

The computational domain represents a 3D box with dimensions: \( X_{\text{max}} = d = 64 \lambda_{D0} = 2.38 \text{ cm} \), \( Y_{\text{max}} = Z_{\text{max}} = 4 \lambda_{D0} = 0.15 \text{ cm} \), where \( X \) corresponds to the vertical direction and \( d \) is the electrode spacing. The lower electrode at \( X = 0 \) is grounded and the upper electrode at \( X = X_{\text{max}} \) is powered with a sinusoidal voltage with frequency \( f_{\text{RF}} = \omega_{\text{RF}} / 2\pi = 13.56 \text{ MHz} \) and the amplitude \( U_{\text{RF}} = 50 \text{ V} \). At the electrodes absorbing wall boundary conditions for the
particles are applied. At boundaries in the Y and Z directions periodic boundary conditions are applied, both for particles and the potential. The neutral argon was treated as a fixed background with constant density and temperature. Only the charged particle dynamics was followed. Coulomb collisions between charged species, electron-impact ionization, efficient excitation, electron-argon elastic collisions and momentum transfer charge-exchange collisions were taken into account in the simulation. A grid with spacing $\Delta x = \Delta y = \Delta z = \lambda_{d0}/2 = 0.019$ cm and time step $\Delta t = 0.2/\omega_{pe} = 1.21 \cdot 10^{-10}$ s was used. 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.

Dust particles with radii $R_d = 1.86, 3.72, 7.44, 11.16$ and $14.88$ $\mu$m were introduced into the discharge with zero starting charge. The position of the dust particles was fixed at four different positions: dust grain in the sheath $X_d = 8.5 \Delta x$, at the sheath border $X_d = 24.5 \Delta x$, and in the bulk $X_d = 40.5 \Delta x$ and $X_d = 56.5 \Delta x$. In all cases $Y_d = Z_d = 3.5 \Delta y$. During the simulation the dust grains acquired a negative charge by the collection of plasma electrons and ions.

![Figure 1](image.png)

**Figure 1.** Charging of a dust grain with a radius of $3.72$ $\mu$m in the bulk of a capacitive RF discharge.

In Fig. 1 we present the evolution of the electric charge of a dust grain with a radius of $3.72$ $\mu$m at $X_d = 56.5 \Delta x$. A fast initial charging takes place due to the collection of electrons, while equilibration takes place on the ion time scale (of the order of microseconds). The
equilibrium dust charge is subject to stochastic fluctuations due to the discrete nature of charge carriers (in the simulation one computational particle represents 171 real electrons or ions).

In Fig. 2 the dust charge as a function of position in the discharge is shown for dust grains of different radius. It is seen that the charge number is reduced in the sheath and at the sheath edge compared to the bulk value. This is due to the reduced electron flux to the dust particles near and in the sheath. The dust charge scales roughly linearly with the dust radius as expected from the capacitor model. The dust charge from the simulations is decisively smaller than calculated from the simple collisionless OML model, but is in general reasonable agreement with experiments [4, 5]. In experiments on Yukawa balls with particles of 1.7 µm radius a charge of about 2000 is found [4], whereas the simulations yield 1400 charges for a particle of 1.86 µm. From melting experiments, a charge of about 9000 is measured for a 4.7 µm radius particle. Here, the simulations suggest a value of about 6000.

![Figure 2](image-url)

**Figure 2.** Dependence of the dust grain charge on the radius and the axial position.

References