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Modeling dust in plasmas:
From 2d dust crystals to Coulomb balls

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A hierarchy of models is presented to study the basic physics of dust in RF laboratory plasmas in close connection to experiments. Here, the full spatial and temporal kinetics of all species is followed with different complexity in the inclusion of dust particles. The model results are compared to experimental findings.

We first present results of a simple model of Coulomb balls. For the recently discovered Coulomb (Yukawa) balls [1] classical molecular dynamics simulations as well as Monte Carlo simulations were performed to describe and analyze the structure and thermodynamics of these dusty plasmas. The dust particles are considered to interact with a screened Coulomb force while the surrounding plasma is included only in the screening parameter $\kappa = 1/\lambda_D$,

$$H = \sum_{i}^{N} \frac{p_i^2}{2m} + \sum_{i}^{N} \frac{\alpha}{2} r_i^2 + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{q^2}{r_{ij}} \exp\left(-\kappa r_{ij}\right) \qquad (1)$$

The Hamiltonian, with $r_{ij} = \left| r_i - r_j \right|$ as the interparticle distance and α as the confinement strength, will get dimensionless with the length scale $r_0 = \left(2q^2/\alpha\right)^{1/3}$ and the energy scale $E_0 = \left(\alpha q^4/2\right)^{1/3}$, the two particle equilibrium distance and energy for Coulomb interaction. Particles have equal masses *m* and charges *q*. The assumption of a spherical symmetric parabolic confinement is justified by experiments [2].

The molecular dynamics simulations with simulated annealing were used to compute the ground states of this Hamiltonian. These clusters show the same shell structure as in the experiment. Although the Coulomb ground state configurations [3] differ from the experimental observations, the same shell populations can be reproduced by increasing the screening parameter [4]. With increase of the screening the cluster not only is reduced in size but particles will also move from the outer shell to inner shells, shown in figure 1. The experiment was done at same plasma parameters with different number of dust particles. Monte Carlo simulations were used to analyze the effect of finite temperature on these configurations. It turned out that this effect is in the crystalline regime negligible compared against the effect of screening. Only at very high temperatures it shows the same effect of particles moveing from the outer shell to inner shells.

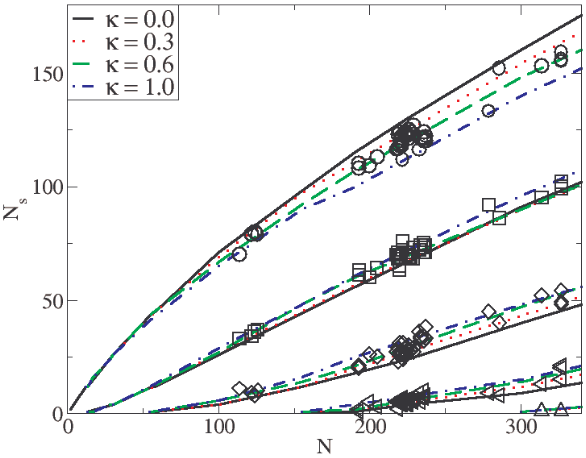

Figure 1. Number of particles on shells over the total number of particles. The lines are the MD simulation results for the ground states. The symbols are measured configurations in the experiment [1].

A further improvement requires the explicit treatment of electrons and ions. To this end we have developed a 2d3v Particle-in-Cell (PIC) code. The dust particles are introduced in the model as additional charged species, using the Cloud-in-Cell weighting formalism [5], so that no finite size effects for dust particles are considered. This code allows the study of the formation of “dust molecules” - vertical strings, in which negative particles are attracted due to polarization of the ion flow (wake-field effect) [6]. A 3d3v PIC code allows to investigate the formation of extended ordered structures in dusty plasmas. Layers with hexagonal symmetry are vertically aligned due to the unidirectional strong ion background flow towards the electrode in the sheath [6]. This closely resembles the experimental observations.

In order to include close-range interaction between dust grains and plasma particles, the PIC algorithm is combined with the molecular dynamic (MD) approach. In this Particle-Particle Particle-Mesh (P3M) model, the long-range interaction of the dust grains with the ions and electrons of the background plasma is treated according to the PIC formalism. For ions and electrons close to the dust grain the interaction force is computed according to a direct particle-particle MD scheme using the exact Coulomb potential. In order to resolve particle motion on scales of the order of dust grain size, particles in MD region are moved with time step smaller than in 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 absorption of plasma electrons and ions [7]. In figure 2 we present the evolution of the electric charge of a dust grain with a radius of 3.72 μm confined in capacitive discharge in Argon.

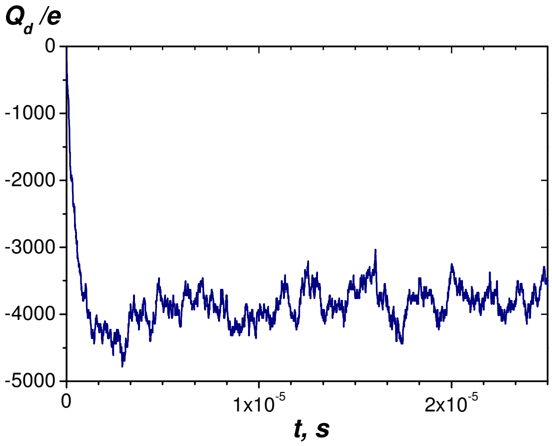

Figure 2. Charging of a dust grain with a radius of 3.72 μm in the bulk of a capacitive RF discharge.

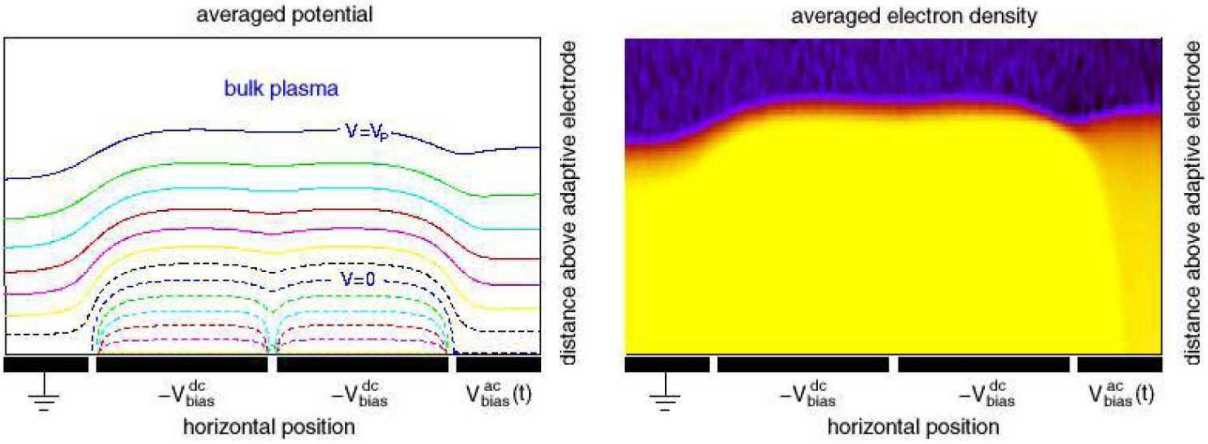

Figure 3. Zoom into the plasma sheath in front of the adaptive electrode. The time dependence of the ac bias is a sinusoidal variation around 0V. Shown is the averaged potential over one period of the rf-cycle (left panel) as well as the normalized averaged electron density (right panel).

The relevance of a detailed understanding of the dust charging becomes most obvious when we consider the particles as microscopic plasma probes and try to extract some information about the plasma out of the dust grains' behaviour. Due to their small size, the dust grains are ideal probes for regions in which a high spatial resolution is required, e.g. in the plasma sheath. Comparison of the simulation results with experiments on position and dynamics of the grains allows us to validate the charging models and to get better insight into the structure of the plasma sheath. This is of particular interest, if additional bias voltages are applied to some parts of the grounded electrode. By this means the local plasma parameters may be altered in a controlled way opening new possibilities for plasma processing in industrial applications as for instance etching. We applied a 2d3v-PIC code, which was developed starting from the xpdp2 code [8] to simulate the rf-discharge in the PULVA-INP device [9]. Incorporating the local bias voltages into the simulation via appropriate boundary conditions, we obtained results for the influence of the plasma parameters and the bias voltages on the structure of the sheath. Of particular interest are the differences in the local modifications if the applied biasing is of dc- or ac- type. While the ac-biasing only slightly influences the structure of the averaged potential, a clear effect is to be seen for the averaged electron density (see figure 3).

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