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MD SIMULATIONS OF DUSTY PLASMA CRYSTAL FORMATION: PRELIMINARY RESULTS

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INTRODUCTION

In the last few years, a number of laboratory experiments involving dusty plasmas have shown that a crystalline structure can be produced under certain conditions¹⁻⁴. The experiments involve a weakly ionized rf discharge plasma and take advantage of the fact that the dust grains collect in “electrostatic traps”, i.e., regions of the discharge where the electric, ion drag, and gravitational forces balance. Typically, the dusty plasma crystal is only a few layers thick, but can extend for many (~ 100) lattice spacings in the transverse directions. Because the grains charge negatively to relatively large values, $Q_d > 1000e$, where e is the electron charge, the coupling parameter can be very large, $\Gamma > 1000$.

In this paper we present some preliminary calculations of plasma crystal formation using molecular dynamics (MD) methods. A Yukawa potential is used to model the interaction of the charged grains shielded by the plasma, while an external potential is added to model effects imposed by the discharge. The external potential is based on the forces (electric, ion drag, gravity) experienced by charged grains in the trap region⁵ and is modeled as a (asymmetric) Morse potential in the direction (x) normal to the electrode. This is in contrast to the model of Totsuji *et al.*⁶, who assume a parabolic potential. At present, our calculations do not include the effect of shielding due to ions streaming toward the electrodes. This process has been shown via particle orbit studies² and crystal formation simulations that include ion dynamics³ to be a potentially important effect to explain the observed crystalline structure. Some preliminary studies of this effect are described below.

MD SIMULATIONS

We assume the parameters of a typical rf discharge (plasma density $\sim 10^9 \text{cm}^{-3}$, electron and ion temperatures, $T_e \sim 2 \text{eV}$ and $T_i \sim 0.03 \text{eV}$, and rf voltage $\sim 100 \text{V}$) to calculate profiles for the density, temperature, and electric field across the steady-state discharge. Given these profiles, we then calculate⁵ the profiles of the electric, ion drag, and gravitational forces and the resulting potential $U(x)$ acting on an individual dust grain, assumed to have a radius of $2 \mu\text{m}$ and a (constant) charge of $-2000|e|$. The gravitational and ion drag forces push the dust grain toward the electrode ($x = 0$), while the electric force pushes the the negatively charge grain away from the electrode, leading to a minimum in the potential near $x \sim 4 \mu\text{m}$ from the electrode.

Some idea of the steady state configuration in the trap potential can be gotten from MD simulations neglecting the angular dependence due to ion streaming effects and using pure Yukawa potentials of the form,

$$u(r) = \epsilon \left(\frac{r_0}{r} \right) \exp(-\alpha(r/r_0)), \quad (1)$$

for the pair-wise interaction between charged dust particles. We have taken $\alpha = 1$ corresponding to using the electron Debye screening length. The initial nearest neighbor separation is denoted by r_0 and $\epsilon = Z^2 e^2 / r_0$. Both of these quantities are determined from the temperature and $\Gamma = Z^2 e^2 / k_B T r_{WS}$, where r_{WS} is the Wigner-Seitz radius for the dust particles. In these calculations we have taken $\Gamma = 1000$. The external potential is modeled with a Morse potential of the form:

$$U(x) = 2\epsilon_M \left(1 - e^{-\alpha_M(x/r_0)} \right) - \epsilon_M \left(1 - e^{-2\alpha_M(x/r_0)} \right), \quad (2)$$

with $\epsilon_M = 7\epsilon$ and $\alpha_M = 0.25$. ϵ_M has been adjusted so that the interplanar spacing is ≈ 1 . We have taken a computational volume which is periodic in the transverse directions and started from a (thermodynamically unstable) cubic lattice of 1024 particles at temperature $k_B T / \epsilon = 0.0015$. A Nosé-Hoover thermostat was used to keep the global temperature equal to this value on average. Yukawa systems have a marked tendency toward planar ordering⁷ and we find that after a time of order $100 - 200 t_0$, a planar order appears perpendicular to the x-axis. Here, $t_0 = r_0 \sqrt{m/\epsilon}$ where m is the dust particle mass. The order within the planes is hexagonal but defective with dislocations. The structure of the planes becomes very diffusive as distance increases outward from the minimum of the Morse potential. These effects are shown in Fig. 1 and Fig 2. Consistent with this change from two-dimensional planes to a disordered three-dimensional outer cloud are changes in the local distribution of kinetic energy. We have divided our system into four Lagrangian volumes containing 256 particles each, extending outward from the electrode. The average position $\langle x \rangle$, the out-of-plane temperature $\langle T_{xx} \rangle$, and the in-plane temperature $\langle T_{yy} + T_{zz} \rangle / 2$, as defined by $3Nk_B \langle T_{\alpha\beta} \rangle = \sum m \langle \nu_\alpha \nu_\beta \rangle$, are plotted in Fig 3. The out-of-plane temperature is lower than the in-plane temperature, consistent with the defective planar order, and these approach each other linearly with distance from the electrode as the diffuse region is approached.

ION SHIELDING

We have also studied the uniformity of the dust particle charge including ion flow. The charging of a dust particle immersed in an ambient plasma is studied with the CELESTE-2D particle in cell code. The electrons and ions are governed by the Vlasov-Poisson model and interact with the dust surface. To model accurately a dielectric dust particle, the electrons and ions that hit the surface are captured locally on the exact point where they hit; this effect can lead to nonuniform charge distributions over the dust surface⁸. Figure 4 shows the equilibrium ($\omega_{pi}t = 30$) potential around a dust particle. The electrons (ions) are distributed initially according to a nondrifting (drifting) Maxwellian. The plasma parameters are: $T_i/T_e = 5$, $m_i/m_e = 100$, $a/\lambda_D = 0.25$, where λ_D is the linearized Debye length $\lambda_D = \left(\frac{1}{\lambda_{De}^2} + \frac{1}{\lambda_{Di}^2}\right)^{-1/2}$ and a is the dust radius. Note that the nonuniformity of the surface charge and of the surface potential is important.

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Figure 1. The configuration at $t = 122t_0$: (a) view parallel to the electrode (with the electrode at the bottom), (b) in plane view of one of the hexagonal planes.

Figure 2. The configuration at $t = 322t_0$: (a) view parallel to the electrode (with the electrode at the bottom), (b) in plane view of one of the hexagonal planes.

Figure 3. Normal and transverse temperature distribution at $t = 420t_0$.

Figure 4. Electrostatic potential around a dust particle at $\omega_{di}t = 30$. The ion drift velocity, toward positive x , is $v_{di} = 3v_b$, where $v_b = (k_B T_e / m_i)^{1/2}$ is the Bohm velocity. The electron drift speed is zero.

Fig. 1a

bottom

Fig 1b.

bottom.

Fig 2a

bottom

26.

bottom

Fig. 3.

Fig 4

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