A molecular dynamics study of dust cluster explosion in a complex plasma discharge afterglow

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The Coulomb explosion of clusters, as a source of multiply charged energetic ions, electrons, and photons, has been extensively studied in the past decade. Experiments by Barkan and Merlino in a Q-machine [1] have shown that micron sized negatively charged dust grains can be confined, in the electric field of anode double layer formed in the plasma discharge, in the form of a spherical cluster with roughly 1000 particles and inter-grain spacing $\sim$ 0.5 to 1.0 mm. It was noticed that when these confining fields were removed by switching off the anode voltage, the cluster exploded due to inter particle repulsion. Micron sized dust grains were seen to be accelerated up to $\sim$ 3g (where g is the acceleration due to gravity). Dust cluster explosion thus provides an efficient method of accelerating micron sized particles at the expense of plasma thermal energy. Dust cluster explosion has been suggested as a means for achieving micro propulsion in space using a plasma engine [2]. It is thus desirable to investigate and model dust cluster explosions in plasma discharges. Our present work is devoted to a molecular dynamics (MD) simulation study of the dust cluster explosion.

Our simulations study the dynamics of spherical clusters of negatively charged dust particles that are confined in a square well potential of variable volume. Prior to investigating explosions, we have verified the recently predicted Electrostatic-isothermal scaling $P_E \propto V_d^{-2}$[3] in the large volume limit, where the particle density is low and coupling effects are weak (here P_E is the electrostatic pressure acting on charged particles and V_d is the dust ball volume in which dust particles are confined). This study benchmarks our code.

To study the explosion dynamics, the run is initialized with N_d (=1000) particles in the confining potential ϕ_{conf}. The particles interact among themselves via Yukawa potential and equilibrate to a desired temperature, which is controlled by using a Gaussian thermostat. The thermostart is removed after the desired equilibrium is acquired. In the afterglow phase of the discharge, when the anode voltage is switched off, particles move in a time varying inter-particle potential and plasma conditions. To simulate this phase, the confining potential is removed and the time evolution equations of n, T_e and the normalized dust charge Z_d $(= q_d/e)$ along with the equation of motion of particles are solved self consistently. In the afterglow phase, n changes due to losses on the walls of the plasma vessel and surface recombination on dust particles while changes in T_e are mostly due to collisions with background gas neutrals. The time scale of these changes is set mostly by the neutral gas pressure P_n. Since changes in n and T_e affect the inter particle potential through λ_d and q_d, it follows that the nature of the explosion and the maximum dust acceleration that can be obtained depends crucially on P_n. Therefore we have carried out simulations in both low pressure as well as high pressure regimes.

In order to describe the afterglow phase we adopt the zero-d model of Ivlev *et al* [4] which consists of the following equations for time evolution of plasma density, T_e and Z_d

$$\frac{dn}{dt} = -\frac{n}{\tau_D}; \frac{dT_e}{dt} = -\frac{T_e - T_n}{\tau_T} \tag{1}$$

where T_n is the temperature of the background neutral gas and is roughly equal to the ion temperature. τ_D and τ_T are given by

$$\tau_D^{-1} = \tau_W^{-1} + \tau_A^{-1}; \tau_T \approx \sqrt{\frac{m_i}{4m_e}} \frac{l_{en}}{v_{thi}\sqrt{\tilde{T}_e}} with \tag{2}$$

$$\tau_W \approx \frac{3\sqrt{\pi}\Lambda^2}{2\sqrt{2} l_{in} v_{thi}\left(1+\tilde{T}_e\right)}; \tau_A \approx \left(2\sqrt{2\pi} r_d^2 n_d v_{thi}\left(1+z\tilde{T}_e\right)\right)^{-1} \tag{3}$$

where $\tilde{T}_e = T_e/T_n > 1$, l_{en} and l_{in} are the electron-neutral and ion-neutral mean free paths and are roughly equal i.e., $l_{in} \approx l_{en} = (n_n\sigma)^{-1}$, n_n, n_d and r_d are the neutral gas density, dust particle density and the dust particle radius respectively, v_{thi} is the ion thermal speed, $z = Z_d e^2/r_d T_e$ and $\Lambda^{-2} = (\pi/H)^2 + (2.4/R)^2$, R and H being the radius and height of the plasma column respectively. The background gas pressure $P_n = n_n T_n$. The time evolution of Z_d is governed by

$$\frac{dZ_d}{dt} = -\frac{\left(Z_d - Z_d^{(eq)}\right)}{\tau_Z}; \tau_Z = \frac{\sqrt{2\pi}\lambda_{d0}^2}{v_{thi} r_d\left(1+z_{eq}\right)\tilde{n}}; Z_d^{(eq)} = z_{eq} r_d T_e/e^2 \tag{4}$$

where $\tilde{n} = n/n_0$, n_0 being initial plasma density and z_{eq} is given by

$$(n_e/n_i)\sqrt{\tilde{T}_e} e^{-z_{eq}} = \sqrt{m_e/m_i}\left(1+\tilde{T}_e z_{eq}\right) \tag{5}$$

Here $\lambda_{d0} = \left(\varepsilon_0 T_i/e^2 n_0\right)^{1/2}$, $n_e \approx n_i = n$ and n_0 is the plasma density in the confined phase just before the removal of the confining potential.Typically in complex plasma experiments, $\tau_Z \ll \tau_D, \tau_T$, hence the dust charge is always determined by solving Eq.(5) for z_{eq} and then using

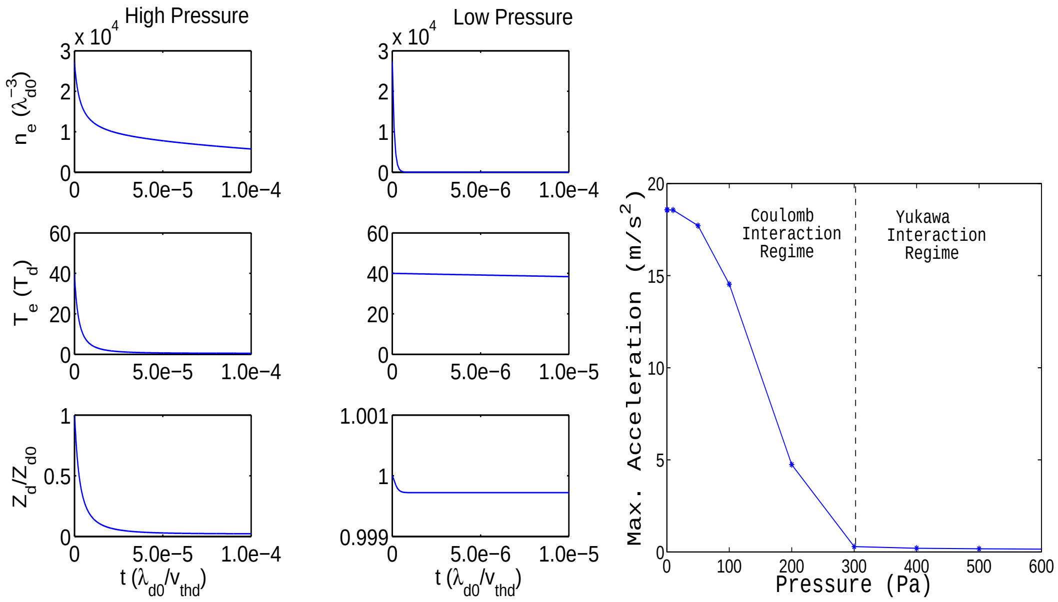

Figure 1: (a)Temporal decay of electron density, electron temperature and dust charge, in the afterglow phase, in high pressure $P_n = 500Pa$ (left column) and low pressure $P_n = 1.5Pa$(right column) regimes.(b) Max. dust acceleration vs gas pressure.

the relation $Z_d = Z_d^{(eq)} = z_{eq} r_d T_e/e^2$ to obtain the dust charge (z_{eq} is a weak function of T_e in Eq.(5)). The dust neutral collision frequency is small on the time scale of the cluster explosion. Now in the low gas pressure case, where $\tau_D < \tau_T$ the plasma density decays rapidly on a time scale set mostly by diffusive losses to the walls. While, in the absence of enough neutrals, T_e and Z_d decay on much longer time scale and thus remain close to their values in the confined phase just before the removal of the confining potential i.e., $T_e \approx T_{e0}$, $Z_d = Z_{d0}^{(eq)} = z_{eq} r_d T_{e0}/e^2$. The decay of plasma density removes the shielding between negatively charged dust particles in the afterglow phase, causing a *Coulomb* explosion of the cluster with full dust charge $Z_{d0}^{(eq)}$ ($\approx 10^4 e$) and thus maximum particle acceleration. In the high pressure case, T_e and hence Z_d decay rapidly in the afterglow phase (Eqs.(1), & (4)). On the other hand, because of the direct dependence of τ_W on n_n in Eq.(3), the plasma loss to the walls is slowed. Also due to the decay of electron temperature T_e, the recombination on particles surface also slows down. Due to these two factors the overall plasma density decay time scale is much longer than τ_T. Thus, in the high pressure regime, screening is preserved in the afterglow phase, causing a *Yukawa* explosion with reduced dust charge and thus smaller particle acceleration. The critical gas pressure for roll over between these two regimes is roughly given by the condition $\tau_D = \tau_T$.

In our MD simulation of cluster explosion, we solve the equation of motion of dust particles with a time varying inter-particle potential which is determined self consistently at each step by solving Eqs.(1) - (5) for n, T_e and Z_d in the afterglow phase. We have used the parameters of experiment in reference [1], in our simulations. In Fig.1(a) we show n, T_e and Z_d as a function of time in low and high neutral gas pressure regimes. The plots confirm that in the low pressure regime the density decay is much faster than the decay of T_e and Z_d, while in the high pressure regime T_e and Z_d decay much faster. In each run we evaluate the average acceleration of a dust particle at each time step. In the low pressure regime the acceleration increases as a function of time and attains a maximum value with plasma density decay and removal of shielding. We have carried out a series of runs to obtain the critical pressure for the transition from Yukawa explosion to Coulomb explosion. We show dust acceleration values for a range of neutral gas pressures in Fig.1(b) which clearly shows a transition at around $P_{nc} = 300Pa$. For neutral pressure of $\sim 1.5Pa$, we obtain an acceleration of $\sim 20\ m/s^2$ which is quite close to the observed value of $3g$ in Barkan and Merlino's experiment. At higher gas pressures our simulations show much weaker acceleration which is in agreement with the recent experimental observations of the afterglow phase of a complex plasma in the regime of $\sim$ 100 Pa by Filatova *et al* [5] and Merlino [6]. In this pressure regime the explosions are observed to be much weaker.

To summarize, we have simulated dust cluster explosion using a zero-d model for the afterglow phase of a complex plasma discharge. The nature of explosion and the magnitude of the dust acceleration are seen to depend critically on the pressure of the back ground neutral gas. A comparison of our simulation results with experimental observations shows that our simple model reproduces most of the essential qualitative features of a cluster explosion in various pressure regimes. Further work to include electron depltion is underway.

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