Dynamically Shielded Dust Simulation of Phase Transition in Dusty Plasmas

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We report on analytical and simulation studies of microphysical processes that trigger phase transitions in a dusty plasma subject to ion streaming. For pressures below the critical pressure $P_c$ for condensation, the grains acquire a large random kinetic energy and form a weakly coupled fluid. If $P$ is increased to greater than $P_c$, the grains lose their kinetic energy and reach a strongly coupled crystalline state. The dust heating in the fluid phase is due to an ion-dust two-stream instability, which is stabilized at $P > P_c$ by the combined effect of ion-neutral and dust-neutral collisions. If the pressure is decreased from the crystalline state to below the critical pressure $P_m$ for melting, transverse phonons are destabilized by ion streaming, which destroys the short range ordering of the dust grains and triggers melting. It is found that $P_m < P_c$. For $P_m < P < P_c$ mixed phase states can exist.

1. Introduction
Dust grains immersed in plasma discharges acquire a large negative charge and settle into a dust cloud at the edge of the sheath. In this region, the plasma ions stream toward the electrode at a velocity $u \sim c_s \sqrt{(T_e/m)}$. It is found experimentally that at sufficiently high gas pressure $P$, the random kinetic energy of the grains is damped by gas friction, and the grains are strongly coupled and self-organize into a crystalline configuration [1-3]. For lower pressures a very different behavior is seen. Despite the dissipation of grain kinetic energy to gas friction, the dust grains reach a steady-state kinetic temperature $T_d$ which is much larger than the temperature of any other component in the plasma. $T_d$ is so large that the dust acts like a fluid [1-3].

We have used the dynamically shielded dust (DSD) model [4-6] to simulate these physical processes. We find that the known experimental features are nicely reproduced in the simulations, that additional features are revealed, and that the simulations are particularly suitable for critically examining the phenomena and developing physics-based models. In both the experiments and the simulations, the grains typically line up directly behind each other along the streaming direction, but transverse to the streaming form a hexagonal lattice [1–3]. It has been understood for some time that this is because the ion flow creates an electrostatic wake downstream of each grain, and there are positively charged points in the wake structure behind each grain which attract other grains. However, there are other features that have not been understood. For example, there has been no satisfactory explanation of the grain heating mechanism that leads to such a large $T_d$ at low pressure. In addition, the simulations reveal features of the evolution that were later observed in experiments.

2. Dynamically shielded interaction and the DSD simulation model
We first briefly describe the physics on which the DSD model is based. A dusty plasma consists of electrons, positive ions and negatively-charged dust grains, all interacting with each other electrically and mechanically. However, it is possible to faithfully represent the system as consisting of only one type of particle, dust grains, with the ions and electrons appearing only as a dielectric medium which mediates the interaction between grains. This representation simplifies the theory enormously, and in a simulation model it completely eliminates the electron and ion time scales, which are many orders of magnitude faster than the dust time scales of interest. The basis for this reduction is the realization that the dust grains may be strongly coupled to each other, but the electrons and ions are only weakly coupled to the grains. The typical kinetic energy of an electron is of course of order $T_e$. In a discharge, usually $T_e$ is much larger than the ion temperature $T_i$, but nonetheless the typical ion kinetic energy is also of order $T_e$, since the ions are streaming at velocity of order $c_s$. The potential at a grain surface is of the order of $-T_e$, and falls off faster than $r^{-1}$. Since the grain radius $a$ is normally much smaller than the mean spatial separation between ions or electrons, at any given time very few ions and electrons are close to a grain. Except for these few, the interaction potential energy between ions and grains, or electrons and grains, is small compared to the typical kinetic energy of an ion or electron. Thus it is quite accurate to treat the plasma by linear response theory [7,8]. Accordingly, the interaction between grain $j$ located at $r_j$ and another grain located at $r$ is given by the dynamically-shielded Coulomb potential

$$\phi(r) = \int d^3k \sum_j e^{ik(r-r_j)} \phi_j(k), \quad (1a)$$
where

\[ \phi_j(k) = \frac{-Ze}{2\pi^2k^2D(k, -k \cdot \mathbf{u} + iv)} \tag{1b} \]

and \( D(k, \omega) \) is the plasma dielectric given by

\[ D(k, \omega) = 1 + \frac{1}{k^2\lambda_0^2} \int \frac{d^3v}{k^3} \frac{k \cdot \nabla \phi_j(v)}{\omega - k \cdot v + iv} \int \frac{d^3v}{k^3} \frac{\nabla \phi_j(v)}{\omega - k \cdot v + iv} \tag{1c} \]

Here \(-Ze|e|\) is the charge on the \( j \)th dust grain, \( \lambda_{De} \) is the electron Debye length, \( f_{i0} \) is the ambient ion distribution function, \( \nu_i \) is the ion-neutral collision frequency, and \( v_i \) is the ion-neutral collision frequency. Equations (1) represent the complete linear response of the plasma ions and the warm electrons, including wakefields, ion-neutral collisions, and Landau damping. Note that the electron thermal speed is invariably much higher than their streaming speed, and hence their contribution to the dielectric (1c) reduces to Debye shielding, as represented by the second term on the right hand side. Since the plasma response is linear, the force exerted on any particular grains by all of the other grains is given just by the linear superposition of dynamically shielded potentials of the form (1a). The representation (1) is thus a very great simplification in the theory, which is soundly based on the physics. The potential structures resulting from the solutions of Eq. (1) are very similar to full nonlinear solutions obtained from particle simulations [9,10].

The theoretical structure described above has been embodied in the DSD particle simulation model. The details of the simulation model were described earlier [4-6] and are not repeated here. Briefly, only the dust grains appear as simulation particles. Electrons and ions do not appear as particles but their contributions are included via the dynamically-shielded Coulomb interaction (1), which represents the interaction between grains [7,8]. In various versions of the code, we have used particle-in-cell (PIC) or molecular dynamics (MD) techniques, or some combination of the two, to compute the interaction force. We find that the known experimental features are reproduced in the simulations, additional features are revealed, and the simulations are particularly suitable for critically examining the phenomena and developing physics-based models. For example, in the pressure regime where the dust condenses into a crystal, simple hexagonal crystal structure is usually seen in the simulations, but other crystal structures also occur in parameter regimes where the confining forces are weak, or where the pressure is very high and therefore the wakefield nodes are weak. At low pressure, it has been known for some time that the grains acquire a very large random kinetic energy and behave like a fluid rather than a crystal, but the source of this dust heating has been a mystery. We have demonstrated that the grain heating at low pressure is due to ion-dust two-stream instability [5].

In addition, the simulations provide an explanation for the mixed phases that have been seen in experiments [2]. In Fig. 1 we plot the variation of \( T_d \) as \( P \) is continuously varied in the DSD simulation run. A marked difference is evident between the critical pressure \( P_m \) for the solid-to-fluid (melting) transition, which occurs as \( P \) is decreased, and the critical pressure \( P_c \) for the inverse fluid-to-solid (condensation or freezing) transition which occurs as \( P \) is increased. For \( P_m < P < P_c \), mixed phase states are seen. As we shall see, this hysteresis occurs because the instability which triggers melting is different from the instability which heats the dust in the fluid phase, and thereby inhibits freezing.

![Fig. 1. Hysteresis in DSD simulation model](image)

3. Fluid-to-solid transition (condensation)

At low pressure, the dust is subject to a two-stream instability with the ions. In situations of interest, it is easily seen that the phase velocity of the instability does not overlap either the ion or the dust velocity distribution, and therefore both species can be treated as cold. The dispersion relation simplifies to [5],

\[ 1 + \frac{1}{(k\lambda_{De})^2} - \frac{\omega_i^2}{\omega(\omega + iv_i)} - \frac{\omega_d^2}{\omega(\omega - k \cdot v)(\omega - k \cdot v + iv)} = 0 \tag{2} \]

where \( \omega_i \) and \( \omega_d \) are ion and dust plasma frequencies, \( \lambda_{De} \) is the electron Debye length, and \( v_d \) and \( v_i \) are dust- and ion-neutral collision frequencies. This instability is responsible for the high temperature of the dust at low pressure. Although the nonlinear evolution of the instability is not yet understood in detail, some features are clear. Because of collisions, the instability is convective in the dust frame. Therefore, the extent of dust heating increases with the dust cloud thickness. However, even thin dust clouds exhibit sufficient dust heating to maintain the dust in a fluid state. Even for dust homogeneously filling an infinite region, the instability saturates before reaching an amplitude sufficient for trapping. \( T_d \) ranges typically from several tens of eV in thin dust clouds to hundreds of eV in thick clouds.

We have shown [5] that at pressures above a critical pressure \( P_c \), the instability is stabilized by the combined effects of ion-neutral and dust-neutral collisions. Numerical solutions of Eq. (2), Fig. 1 of Ref [5], show that all modes are stable if both \( v_d/\omega_d \) and \( v_i/\omega_i \) are large enough. Since the ion-dust streaming instability is the heat source which keeps the dust in the weakly-coupled fluid phase,
its elimination is the trigger for condensation. It is found that the critical pressure \( P_c \), determined from the solution of Eq. (2) agrees quantitatively with the pressure at which simulations indicate the threshold for excitation of waves, and also with the pressure at which simulations show the fluid-to-solid phase transition. The results also agree with experimental determinations of the freezing pressure, to the qualitative extent compatible with uncertainties in the local experimental parameters. For further details we refer the reader to Refs. [4-6].

4. Solid-to-fluid transition (melting)

The basic physics underlying the melting transition has been elucidated in a series of papers by Melzer, Piel, V. and A. Schweigert, and collaborators [1,11], and by Melando [12]. In essence, instabilities of the crystal structure arise from the asymmetry of the dynamically screened Coulomb potential in the presence of flowing ions: upstream and to the side, the potential is similar to static Debye screening, and repels neighboring dust grains, but downstream there is an ion wake, which includes some points of positive charge accumulation. Neighboring dust grains are attracted to these points. While this feature is responsible for the ordering of the dust into crystals with grains lined up directly behind other grains, it also renders the resulting crystal susceptible to instabilities, essentially a form of ion streaming instability specific to the crystal phase.

In Refs [1,11], a phenomenological model for the asymmetric interaction between grains is constructed. The ion wake is represented as a single fictitious positively charged particle, rigidly attached behind each negative grain. The charge on the fictitious particle, and its separation from the grain, are fit to simulations of ion flow. Although this model is a reasonable heuristic representation of the actual physics, it does not provide analytic scalings for the dependence of the forces on physical parameters. Additionally, the two-parameter fit is sufficient to treat small excursions of the grains from their equilibrium crystal sites, but it is not apparent that it accurately represents the forces at large deviations from crystalline order.

We have been developing a first-principles analytic approach to the melting transition, which embodies the same physics that is present in the DSD simulation code. In addition, we are in the process of extending the work of Melzer et al, which concentrates on two-layer crystals, to many-layer crystals. In our work, the inter-grain potential is the dynamically shielded Coulomb interaction, and is given in k-space by Eq. (1b).

Crystal instabilities can be represented at various levels of detail. Both longitudinal and shear modes can be driven unstable, as well as obliquely propagating mixed modes, and indeed we believe that several types of modes are involved in the later stages of the melting process. However, experiments and DSD simulations indicate that the mode which initiates the melting process is a shear mode with propagation vector \( \mathbf{k} \) parallel to the ion streaming, i.e. a mode in which the horizontal grain layers slide rigidly resulting in a misalignment with respect to the adjoining layers. In the linear stage of such a mode, the equation of motion of a grain in the \( j^\text{th} \) layer, due to the forces exerted by the grains directly above and directly below, is

\[
\begin{align*}
\ddot{m}\vec{x}_j &= C^+ (\Delta x_{j+1} - \Delta x_j) + \\
&+ C^- (\Delta x_{j-1} - \Delta x_j) - m v_d \dot{x}_j,
\end{align*}
\]

where

\[
C^\pm = \left[ -\frac{\partial^2 \phi(x,z)}{\partial (\Delta x)^2} \right]_{\Delta x=0}.
\]

\( \phi(x,z) \) is the Fourier transform of Eq. (1b), \( d \) is the separation between grain layers, and \( \Delta x \) is the displacement of the grain from its equilibrium position in the x direction (transverse to the propagation direction z). It is straightforward to include next-nearest-neighbors in the same way. But the key point is that, unlike the situation in ordinary crystals, the force constants \( C^\pm \) are such that \( C^+ \neq C^- \). For a transverse mode in an infinite crystal, \( \Delta x \sim \exp[i(k_d\xi + \omega t)] \), Eq. (3) leads to a dispersion relation,

\[
\omega = -\frac{i v_d}{2} \left[ \mp \sqrt{\Delta} \right],
\]

\[
\Delta = 1 - \frac{4}{m v_d} \left[ (C^+ + C^-)(1 - \cos kd) - i(C^+ - C^-) \sin kd \right].
\]

Similar analyses can be performed for longitudinal phonons, and for crystals with free surfaces. Eq. (5) is similar to the dispersion relation for phonons in an ordinary crystal, except that here instability occurs because \( C^+ \neq C^- \). However the instability can be stabilized at high pressure due to the dust collisionality \( v_d \), which is visible explicitly in Eq. (5), and/or the ion collisionality \( v_i \), which appears as damping of the attractive wake force \( C^- \) through the dielectric \( D \) in Eq. (1b). The phonon streaming instability is in this sense similar to the two-stream instability that occurs in the fluid-dust phase. However, the stabilization pressure \( P_m \) for the phonon instability (i.e. the critical pressure for melting) is lower than the critical pressure \( P_c \) for Buneman instability (i.e. for freezing), as indicated by the DSD code results. Hence, there is a range of pressures where both the solid and fluid phases of the dust are stable, which allows a mixed-phase system to exist, as observed [2]. A detailed comparison of these results with simulation and experiments will be the subject of a future article.

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References


