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Structure and phase transition of a two-dimensional dusty plasma*

Liu Bin(刘 斌), Liu Yan-Hong(刘艳红)†, Chen Yan-Ping(陈雁萍),
Yang Si-Ze(杨思泽), and Wang Long(王 龙)

Institute of Physics, Chinese Academy of Sciences, Beijing 100080, *China*

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The structure and phase transition of a two-dimensional (2D) dusty plasma have been investigated in detail by molecular dynamics simulation. Pair correlation function, static structure factor, mean square displacement, and bond angle correlation function have been calculated to characterize the structural properties. The variation of internal energy, shear modulus, particle trajectories and structural properties with temperature has been monitored to study the phase transition of the 2D dusty plasma system. The simulation results are in favour of a two-step continuous transition for this kind of plasma.

Keywords: dusty plasma, phase transition, molecular dynamics simulation
PACC: 5240K, 5225

1. Introduction

A dusty plasma is an ionized gas containing small particles of solid matter, which are usually charged negatively by collecting electrons and ions from a plasma. Dusty plasmas are of interest in astrophysics, space physics, industrial plasma processing, and laboratory basic plasma physics.[1,2] Astronomers and space physicists were the first to study this topic because our solar system is full of dusty plasmas such as planetary rings, comet tails, and nebulae. Scientists using industrial plasma processing discovered that particles suspended in a plasma are the major cause of costly wafer contamination during semiconductor manufacturing. Basic plasma physics researchers use dusty plasmas to investigate topics such as waves, instabilities, strongly coupled plasmas, and Coulomb crystallization.

A dusty plasma is a strong-coupled system in which particles are highly charged so that the Coulomb interaction energy between the particles can be far greater than their kinetic energies. It exhibits interesting phenomena such as the formation of a liquid or solid structure when the coupling is sufficiently strong.[3,4] In the laboratory research, dusty plasma crystals have recently been produced experimentally and their structural and dynamic behaviours were studied in many laboratories.[5,6]

Dusty plasmas provide another model system for crystalline structures to study phase transitions in condensed matter, for example, the two-dimensional (2D) melting is one of the fundamental problems in condensed matter physics.[7] Compared with other model systems such as the 2D electron system on the surface of liquid helium and colloidal suspensions, in a dusty plasma crystal the individual particles are easily observable and the dusty-plasma system will change according to the variations of discharge conditions within a few seconds, in contrast to the relaxation times of many hours for colloidal suspensions.[8−10]

The nature of the melting transition in a 2D system has been a matter of hot controversy in the past years. Kosterlitz, Thouless, Halperin, Nelson, and Young (KTHNY) suggested that 2D solids might melt by a transition sequence involving two continuous transitions separated by a novel nearest-neighbour-bond-orientational ordered fluid—the hexatic phase.[11−14] Competing theories predict that the transition is of the usual first-order type observed in a three-dimensional (3D) system.[15]

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†E-mail: yhliu@aphy.iphy.ac.cn

melting transition of the plasma crystal. Experimental investigations showed the melting transition from a solid-state structure to a fluid or even gas-like state in the dusty plasma crystal consisting of only two layers.[10] Plasma crystal melting due to particles heated by ion streaming motion in the sheath is shown to exhibit a non-equilibrium two-step phase transition.[16] Langevin molecular dynamics (MD) simulations show that the bilayer crystal with point defects and uncorrected dislocations exhibits a two-step melting.[17] However, the information of the phase transitions in a 2D dusty plasma is very limited, and the structural properties and phase transition of the 2D dusty plasma crystal have not been studied in detail by means of molecular dynamics (MD) simulation, so further effort is required. In this paper, we study the structural properties and phase transition in a 2D dusty plasma by constant temperature MD simulation.[18]

2.Model and method

In the simulation, the dusty plasma was modelled as a collection of identical dust particles dispersed in a neutral background. The pair interaction potential is $\phi(r) = (Q/4\pi\varepsilon_0 r)\exp(-r/\lambda_{\rm D})$, where Q is the charge of the particle, r denotes the distance between two particles, and $\lambda_{\rm D}$ is the Debye length of the background plasma. The thermodynamics of the system can be characterized by two dimensionless parameters: $\kappa = a/\lambda_{\rm D}$ and $\Gamma = Q^2/4\pi\varepsilon_0 aT$, where a is the mean interparticle distance, T is the temperature of the system in energy units.

It should be pointed out that the simulation is different from usual experiment in several aspects. First, we use periodic boundary condition to make the system infinite, compared with a finite cluster up to thousands of dust particles in an experiment. Second, in our experiment, an external electrostatic potential, which usually has a parabolic shape, is required to keep the particles together. Third, in the experiment the particles are subjected to gas drag forces and random forces from the neutral gas and various electrostatic fluctuations. It is the random forces that heat the particles to a specific temperature, compared with a thermostat used to keep the system at constant temperature in the simulation here. However, we think these differences will not affect the significance of the basic information from the simulation of structure and phase transition of a 2D dusty plasma system.

In this research, we use constant temperature MD to simulate the structural properties and phase transition in a 2D dusty plasma. In the simulation, constant temperature is achieved by coupling the system to a heat bath with the desired temperature. The Nosé–Hoover thermostat scheme is used to keep the system at constant temperature.[19] Calculations were performed in a system with 256 particles in a 2D square box under periodic boundary conditions. The structural properties of the dusty plasma are investigated over a wide range of coupling parameters from the initial configuration of a square lattice. The time step is $0.1\omega_0^{-1}$, where $\omega_0 = \sqrt{Q^2/4\pi\varepsilon_0 Ma^3}$ (M is the mass of a dusty particle). At each coupling parameter, the initial run lasts 3×10^4 steps for equilibrium, and in subsequent 2×10^4 time steps, the structural properties of the system are measured by calculating the pair correlation function $g(r)$, static structure factor $S(q)$, mean square displacement (MSD), and bond angle correlation function $G_6(r)$. The internal energy, shear modulus and the particle trajectories are also investigated during the heating and cooling processes. In this paper, we use an experiment related value of κ=1.

(A) Pair correlation function

The structural order of a condense system can be characterized by the pair correlation function $g(r)$, defined as,

$$g(r) = (S/N)N(r, \Delta)2\pi r\Delta, \tag{1}$$

where S is the area of the simulated region, N is the number of simulation particles, and $N(r, \Delta)$ indicates the number of particles located between $r - \Delta/2$ and $r + \Delta/2(\Delta = 0.1a$, where a is the mean interparticle distance).

(B) Static structure factor

The structural order of a solid or liquid can also be described by a static structure factor, which is defined as

$$S(q) = (1/N)\left\langle \sum_{j,k} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_{jk}) \right\rangle, \tag{2}$$

where $q = |\boldsymbol{q}| = |\boldsymbol{k}a|$ is the reduced wavenumber. $\boldsymbol{r}_{jk} = \boldsymbol{r}_j - \boldsymbol{r}_k$ is the reduced distance between two particles located at $\boldsymbol{r}_j$ and $\boldsymbol{r}_k$.

(C) Mean square displacement

A simple way to distinguish a solid from a liquid is to examine the particle mean square displacement

(MSD), which is defined as follows,

$$< R^2(t) >= \left\langle (1/N)\sum_{i=1}^{N}(\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0))^2 \right\rangle, \quad (3)$$

where $< \cdots >$ indicates thermal average, N is the number of simulation particles, and $\boldsymbol{r}_i(t)$ indicates the position of the ith particle at time t. For a 2D system, the mean square displacement is related to the self-diffusion constant by,

$$D = \lim_{t\to\infty} \langle R^2(t)\rangle / 4t. \quad (4)$$

(D) Bond angle correlation function

A 2D solid shows a long-range-bond-orientational order and a quasi-long-range positional order, compared with the fluid, which is characterized by a short-range exponentially decaying order in both position and bond angle. For a triangular lattice, the bond angle correlation function $G_6(r)$ is defined as

$$G_6(r) = \langle \mathrm{e}^{\mathrm{i}6[\theta(r)-\theta(0)]} \rangle, \quad (5)$$

where $\theta(r)$ is the angle made by a bond between a particle at r and its nearest neighbours with respect to an arbitrary fixed axis.

(E) Shear modulus

Another characteristic feature of a solid is that it has finite shear modulus. In our simulation, the shear modulus is estimated based upon the fact that, for a small wavenumber q, the transverse wave frequency $\omega_t(q)$ is related to the shear modulus by

$$\omega_t^2(q) = \mu q^2 / M n_d, \quad (6)$$

where n_d is the dust density and M is the particle mass. The relationship of $\omega_t(q) \sim q$ is numerically obtained by the spectrum of transverse current correlation function

$$C_t(q,t) = (1/2N)\langle [\boldsymbol{q}\times\boldsymbol{j}_q(t)]\cdot[\boldsymbol{q}\times\boldsymbol{j}_{-q}(0)]\rangle, \quad (7)$$

$$\tilde{C}_t(q,\omega) = \int_0^\infty \mathrm{e}^{\mathrm{i}\omega t} C_t(q,t)\mathrm{d}t. \quad (8)$$

The current $\boldsymbol{j}_q(t) = \sum_{m=1}^{N} \boldsymbol{\nu}_m(t)\mathrm{e}^{\mathrm{i}q\cdot r_m(t)}$, where $\boldsymbol{\nu}_m(t)$ and $\boldsymbol{r}_m(t)$ are the reduced velocity and position vector of the mth particle at time t, respectively.

3. Simulation results

3.1. Structural properties of a 2D dusty plasma

The structural properties of a 2D dusty plasma were studied in a wide range of coupling parameters, from the regime of liquid to solid. From the pair correlation function, static structure factor and mean square displacement, we can characterize the structure of the dusty plasma system.

The mean square displacement is shown in Fig.1 as a function of time, at different coupling parameters and $\kappa = 1$. When Γ=2.5, MSD gradually increases with time. This is evidently the feature of a liquid. With increasing Γ, MSD decreases considerably. When $\Gamma \geq 100$, the MSD approaches a constant at a large time scale. This means that the motion of each particle is confined to its equilibrium position. This is the feature of a solid, where an atom vibrates around its equilibrium position. From the MSD and Eq.(4) we can obtain the self-diffusion constant. Figure 2 shows the self-diffusion constant D as a function of Γ. In the regime of Γ=10.0–100.0, D decreases rapidly with Γ, indicating the transition of the structure.

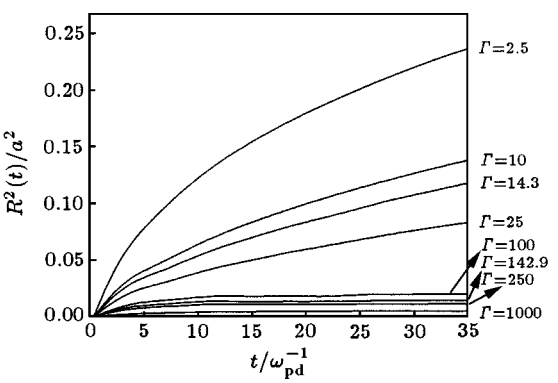


Fig.1. The mean square displacement (MSD) at different coupling parameters.

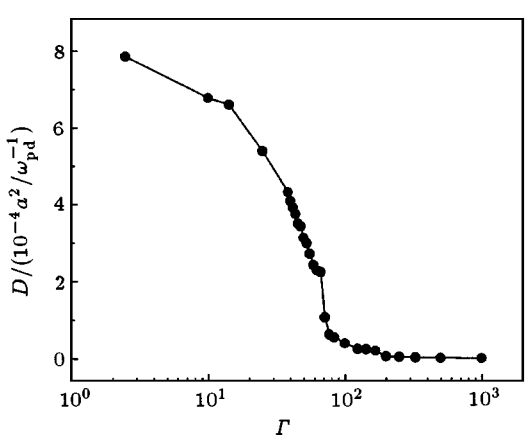


Fig.2. The variation of self-diffusion constant D with coupling parameter.

The pair correlation function $g(r)$ is shown in Fig.3, for different coupling parameters. Numbers marked with the arrows indicate the number of particle obtained by integrating $g(r)$ in successive shell. It is evident that each particle has six nearest neighbours. From Fig.3, we see that with increasing coupling parameter: (1) The height of the first peak increases and the peak width decreases; at Γ=2.5, $g(r)$ is almost constant when the distance is greater than one interparticle distance; at Γ=25, several peaks appear, indicating that the particles are distributed in specific shells around any test particle, and each particle has six nearest neighbours, 12 next neighbours and 18 next–next neighbours, hence the structure is similar to that of a liquid; at Γ=100, there appears a shoulder on each peak but the first one, and the third peak becomes higher than the second peak. We can note that in Fig.2 there is also a large drop in self-diffusion constant at this coupling parameter; (2) Oscillations in peaks increase, indicating the appearing of structural order; (3) At a sufficiently high coupling parameter, all peaks but the first one split; at Γ=1000 the $g(r)$ shows a very typical crystalline structure, and each particle has neighbours of 6–4–8–12–6,..., in successive shells.

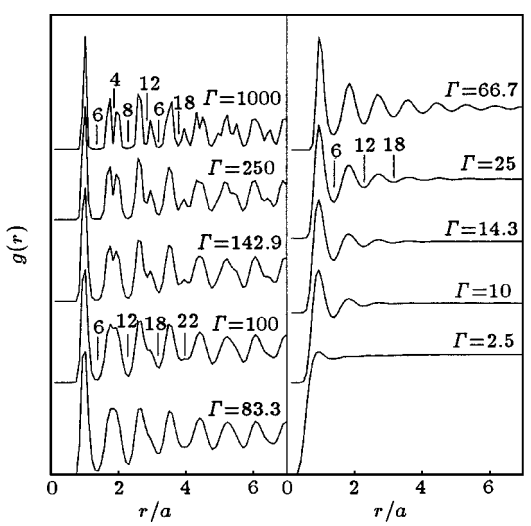


Fig.3. The pair correlation function $g(r)$ at different coupling parameters, the numbers marked with arrows indicate the number of particle in successive shells.

The static structure factor is shown in Fig.4 for different coupling parameters. According to Hansen–Verlet freezing criterion, the first peak of the static structure factor encodes the information of long-range ordering and consistently achieves a height of 2.85 when a 3D system reaches freezing. The corresponding value in a 2D system is 4.0. From Fig.4, at Γ=142.9 the height of the first peak is 4.02, indicating that the dusty plasma has frozen.

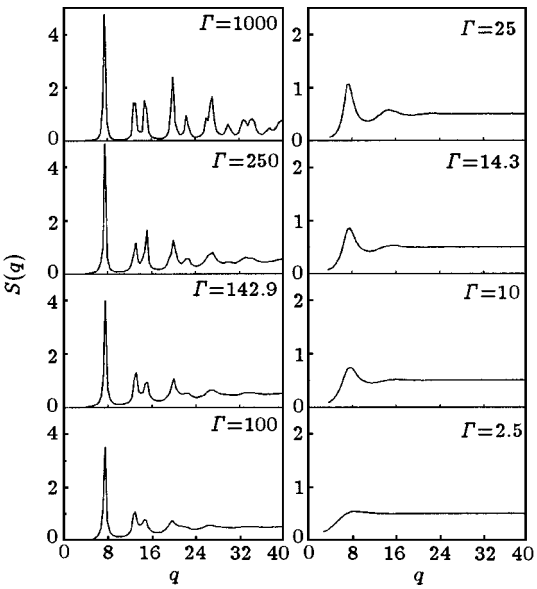


Fig.4. The static structure factor $S(q)$ at different coupling parameters.

From the MSD, $g(r)$, and $S(q)$ above, we conclude that: (1) At small coupling parameters, the dusty particle has a larger diffusion motion. (2) At a larger Γ, there appears a liquid structure. (3) When Γ=100, the particle diffusion decreases greatly, but an ordered structure is still absent. (4) When $\Gamma \geq 142.9$, an ordered structure appears.

The bond angle correlation function $G_6(r)$ is shown in Fig.5, for different Γ. At Γ=1000, $G_6(r)$ tends to 0.85, a long-range bond angle order is clearly presented. At Γ=100, when the liquid is nearly freezing, the $G_6(r)$ decays much slower, and there is a non-zero tail even at $r = 10a$ (here a is the mean interparticle distance). At Γ=40, when the system is obviously in the liquid region, $G_6(r)$ tends exponentially to zero.

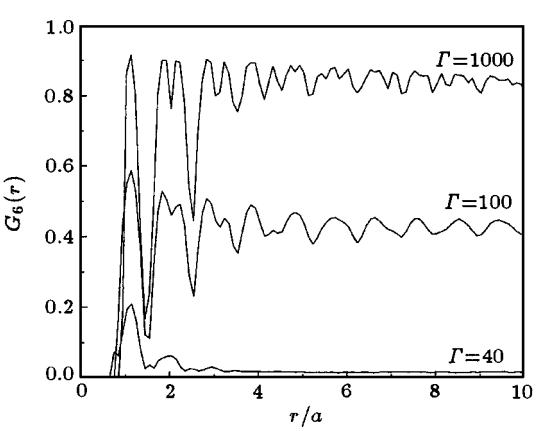


Fig.5. The bond angle correlation function $G_6(r)$ for different coupling parameters.

3.2. Melting and freezing transition

In this section, the phase transition of a 2D dusty plasma is investigated during the processes of heating and cooling. We will try to answer the questions: (a) At what value of Γ does a 2D plasma crystal melt? (b) Is the transition a first-order or a higher-order one?

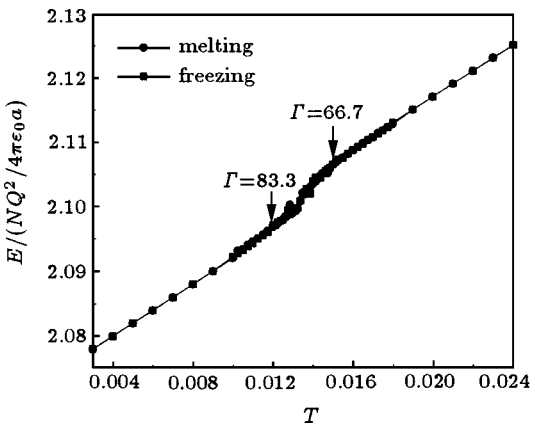


Fig.6. The variation of internal energy with reduced temperature during the melting and freezing processes.

We use the reduced dust temperature $T(=\Gamma^{-1})$ as the variable for investigating the phase transition. During the melting/freezing process, the temperature is changed within the range of T=0.001–0.025, usually with a temperature step of 0.001. At each temperature, the initial run lasts about 3×10^4 steps for equilibrium, and subsequently 2×10^4 time steps, and then the internal energy (E), bond angle correction function $G_6(r)$, shear modulus and particle motion trajectory are investigated.

The internal energy is shown in Fig.6 as a function of the reduced temperature, during the melting and freezing processes. The slope of the melting curve changes at temperatures of 0.012 and 0.015 (i.e. Γ=83.3 and Γ=66.7). In order to obtain the detail of the internal energy change, a temperature step of 0.00025 is taken between T=0.01 and 0.018, and even 0.000125 between T=0.012 and 0.015. From the pair correlation function shown in Fig.3, we have noted that the peak split disappears and the third peak becomes lower than the second peak at T=0.012 (i.e. Γ=83.3). This indicates that the feature of solid structure disappears. From Fig.6, it is also seen that the data points for the melting and freezing processes overlap very well, and show a little difference only in the phase transition region (i.e. T=0.012–0.015). No temperature hysteresis is observed during the melting and freezing processes, compared with the first-order melting transition of a solid. This probably encourages one to conjecture that the phase transition is not of first-order, and should be of high-order. But it is not necessary so because it is also difficult to observe the hysteresis for a weak first-order transition or a finite size system employed in a numerical simulation.

The bond angle correlation function is shown in Fig.7 for the cases immediately before and after the melting, i.e. at Γ=83.3 and 66.7. The bond angle correlation function decays slowly with r at Γ=83.3 (i.e. T=0.012), obeying the law of $r^{-0.25}$; and the bond angle correlation still exists even at $r = 10a$. According to KTHNY theory, the $G_6(r)$ in the hexatic phase should decay as $r^{-\eta}$ with $\eta \leq 0.25$, as compared with the ordinary liquid phase where it decays exponentially.[7] So, our result seems consistent with the existence of a hexatic phase at T=0.012. From Figs.3 and 7, it is evident that an isotropic liquid phase forms at T=0.015. Therefore, our simulation seems consistent with the result that solid-hexatic and hexatic-fluid transitions occur at temperatures of 0.012 and 0.015, respectively.

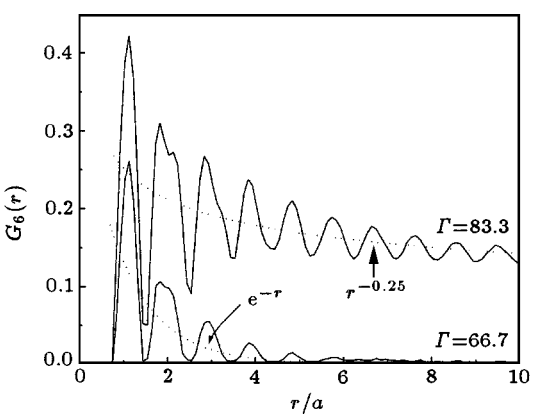


Fig.7. The bond angle correlation functions at Γ=83.3 and 66.7. Exponential and power law fits are also plotted for comparison.

The shear modulus μ is shown in Fig.8 as a function of the reduced temperature during the heating process. At each temperature, we first calculate the transverse current correlation function from the particle positions and velocities. Next, we plot the dispersion curve of transverse waves. Finally, from Eq.(6) we obtain the shear modulus at the specific temperature. From Fig.8, it is noted that the shear modulus decreases rapidly at T=0.012, and abruptly to zero at $T \geq 0.015$. As we know, finite modulus is a distinguished feature of solids. So from the drop of the shear modulus, we can conclude that the dusty plasma

crystal begins to melt at T=0.012, and becomes an isotropic liquid at T=0.015.

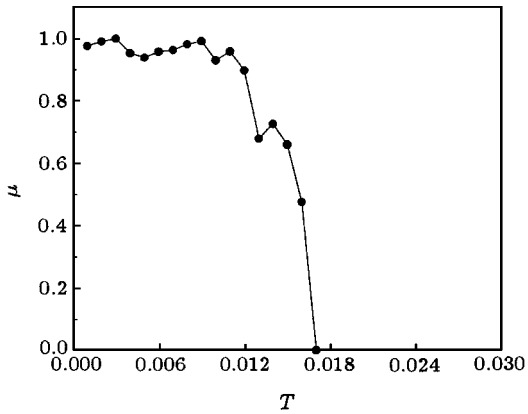


Fig.8. The variation of shear modulus with temperature during the melting process.

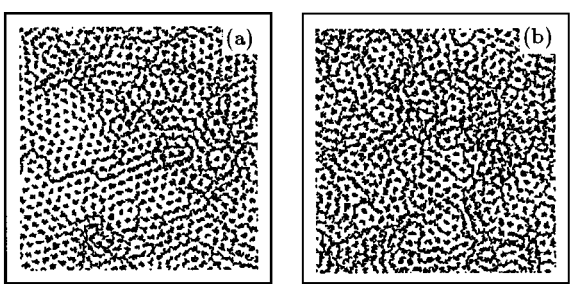


Fig.9. The particle motion trajectories at temperatures of (a) T=0.012 and (b) T=0.015.

Phase coexistence is a basic feature in first-order transition, so we can trace the trajectories of dusty particles in the transition region. In these simulations, the particle number is taken to be 1024 in order to simulate a larger size. Figure 9 shows the particle trajectories at temperatures of 0.012 and 0.015. From Fig.9, one can see that there are some stream lines at T=0.012 and 0.015, and they are so many that there is not any structural order present. We thus cannot gain any information of phase coexistence from these simulations.

4. Conclusions

In summary, the structure and phase transition of a 2D dusty plasma system have been investigated by means of MD simulation in this paper. The structural order of the 2D dusty plasma is characterized by pair correlation function, static structure factor, mean square displacement and bond angle correlation function. The internal energy, bond angle correlation function, shear modulus and the particle motion trajectories are also computed during the melting and/or freezing processes. The results show that the dusty plasma system can be solid, liquid and even gas-like state with decreasing coupling parameter. During the melting process, the solid-hexatic and hexatic-liquid transition seems to occur at temperatures of 0.012 and 0.015 (i.e. Γ=83.3 and Γ=66.7). The temperature hysteresis has not been observed during the melting and freezing processes, and no phase coexistence is presented. Based upon the information described above, the phase transition of the 2D dusty plasma seems in favour of a two-step continuous transition (solid-hexatic and hexatic-liquid).

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