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# Effects of charge and mass variations on the structure in 2D one-component and two-component dusty plasmas*

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**Abstract**

Using molecular dynamics simulation, we calculate the mean square displacement, the pair correlation function, the velocity autocorrelation function and the spectrum function of a two-dimensional (2D) charged dust system. Results show that the critical coupling constant $\Gamma^*$ for the phase transition from a liquid-like state to a solid-like state decreases with increasing charge and mass of particles in the one-component system. A scaling relation between $\Gamma^*$ and $\mu$ ($\Gamma^* \propto \mu^{-1.72\pm0.07}$) is given, where $\mu$ represents the quantities of charge and mass. In the system with two species of particles, the coagulation process is found to be delayed by the presence of one species, and $\Gamma^*$ is closer to that of the 'smaller' particles species, which has the smaller charge and mass.

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## 1. Introduction

In the past years, dusty plasma has attracted great interest due to its wide applications in space, environment, and laboratory plasmas [1–3]. Dusty plasma is a strong-coupled system [4] in which the charged dust particles interact with each other through a Coulomb potential. When the coupling is sufficiently strong, the system exhibits interesting phenomena such as the formation of a liquid-like or solid-like state. Recent investigation on the dusty plasma [5–18] provides an insight to the behaviour of the strong-coupled system. In experiment, Thomas *et al* and Melzer *et al* [5–6] have reported the formation of a liquid-like or solid-like structure in different laboratory conditions, and a two-dimensional dusty plasma lattice in a radio-frequency discharge was observed [7]. At the same time, molecular dynamical

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(MD) simulation turns out to be another important method for investigating dusty plasma, which could foretell some results of experiments. Schmidt *et al* and Kalman *et al* [8–9] have simulated the wave dispersion of the dusty plasma. For different temperature, Liu *et al* [10] have investigated the dynamical and structural properties of the system. Most of the above researches are confined to the fixed charge and mass of dust particles. However, recent experiments reported that the charge and mass of dust particles are not constant. Nejoh [11] has showed that dust charge varies with electrostatic potential, electron and ion density, electron and ion temperature. The investigation on the effects of particle's mass and charge on phase transition is still open and will bring new insight on the plasma physics.

In this paper, we consider a two-dimensional dusty plasma which contains many charged dust particles immersed in a neutral background, and we intend to investigate the effects of charge and mass on the phase transition. For simplification, we choose a point charge model and assume the charge varies in proportion to the mass in the system. In this paper, two kinds of the system are considered: one contains single species and the other contains two species. It is found that the critical $\Gamma^*$ for the phase transition from liquid-like to solid-like state deceases with increasing the charge and mass in a one-component system. The correlation function between the critical $\Gamma^*$ and $\mu$ ($\Gamma^* \propto \mu^{-1.72\pm0.07}$) is given, where $\mu$ denotes the particle's charge and mass. In the system with two species of particles, the coagulation process is found to be strongly dependent on the particles with smaller $\mu$. The manuscript is constructed as follows. In section 2, we give a detailed account of the physical model used in our calculation. The simulation results of one-component and two-component systems are presented in sections 3 and 4, respectively. Conclusions are given in section 5.

## 2. Model and molecular dynamical simulation

The Coulomb potential energy or screened Yukawa potential energy of the system is written as

$$\phi(r) = \frac{Q_i Q_j}{r} \mathrm{e}^{-\kappa r}, \tag{1}$$

where the subscripts $i$ and $j$ indicate two different particles in the system. $r$ is the distance between two particles' centroid. Normally, the thermodynamics of the screened coulomb system is characterized by two dimensionless parameters: coupling constant $\Gamma = Q_i Q_j/(4\pi\varepsilon_0 a k_B T)$ which is the ratio of the interparticle Coulomb potential energy to the kinetic energy, and screening constant $\kappa = a/\lambda_D$ which indicates the screening strength. Here $T$ is the system temperature, $a = 1/\sqrt{n}$ denotes the mean interparticle distance, $n$ is the concentration of particles and $\lambda_D$ is the screening length. The force acting on the dust particle $i$ can be written as

$$F_i(t) = -Q_i \sum_{j\neq i} \nabla_i \phi(r_{ij}), \tag{2}$$

and the interparticle spacing between particles $i$ and $j$ is $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

In the simulation, we consider a canonical system using a Verlet arithmetic method of molecular dynamic simulation, where a Nosé-Hoover thermostat scheme [12] is applied to achieve the constant temperature in the system. The simulation is performed in a system with 400 particles in a 2D square box of side $L = 20a$ under periodic boundary conditions. Units are applied, length is in the unit of the mean interparticle distance $a$, energy is in the unit of $U_0 = Q_0^2/4\pi\epsilon_0 a$ and time $t$ is in the unit of $t_0 = \sqrt{4\pi\epsilon_0 M_0 a^3/Q_0^2} = \sqrt{4\pi}\omega_{pd_0}^{-1}$ ($\omega_{pd}$ is the plasma frequency), where $Q_0$ and $M_0$ is in the normalized potential energy $U_0$. In

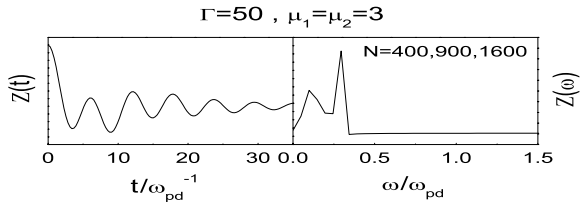


**Figure 1.** The velocity autocorrelation function varies with the time and simulating particle number $N$ at $\mu_1 = \mu_2 = 3$, $\Gamma = 50$.

each computing, the time step is $0.03\omega_{pd}^{-1}$ and the initial run lasts $5 \times 10^4$ steps for achieving the system equilibrium, and the subsequent $3 \times 10^4$ steps for calculating the characteristic functions. Normally, a mean square displacement (MSD) $\langle r^2(t)\rangle$, a pair correlation function $g(r)$, a velocity auto correlation function (VACF) $Z(t)$ with its corresponding spectrum function $Z(\omega)$ are the good tools for analysing the system's structural and dynamical properties. These equations can be expressed as follows [13, 14]:

$$g(r) = \frac{S}{N}\frac{N(r,\Delta)}{2\pi r\Delta}, \tag{3}$$

$$\langle r^2(t)\rangle = \left\langle \frac{1}{N}\sum_{i=1}^{N}(\vec{r}_i(t) - \vec{r}_i(0))^2 \right\rangle, \tag{4}$$

$$Z(t) = \frac{\left\langle \sum_{i=1}^{N} \vec{v}_i(t)\cdot\vec{v}_i(0)\right\rangle}{\left\langle \sum_{i=1}^{N} \vec{v}_i(0)\cdot\vec{v}_i(0)\right\rangle}, \tag{5}$$

$$Z(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} Z(t)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t. \tag{6}$$

Here $N$ is the number of simulation particles, $S$ denotes the area of the simulation region, $N(r,\Delta)$ means the number of particles located between $r-\Delta/2$ and $r+\Delta/2(\Delta = 0.1a)$, $\langle\cdots\rangle$ is the thermal average, $\vec{r}_i(t)$ and $\vec{v}_i(t)$ are the position and velocity of the particle $i$ at time $t$. We define a parameter to simplify the symbol

$$\mu_i = Q_i/Q_0 = M_i/M_0, \tag{7}$$

where the dimensionless $\mu_i$ represents the particles with different charge and mass and $i$ denotes the particles species. We choose $\kappa = 1$ to represent the real experimental condition.

In order to see how the simulation accuracy depends on the particle number, we run the simulation with 900 particles and 1600 particles as well. From figure 1, the oscillation frequency in the frequency window does not depend on the particle number. Among the cases of $N = 400, 900, 1600$, the high oscillation frequency peaks appear at $0.296\omega_{pd}$, and the low oscillation frequency peaks appear at $0.098\omega_{pd}$. Therefore, we choose 400 particles as the simulating objects to save the computing time. We use the potential energy $U = Q_i Q_j/4\pi\varepsilon_0 a$ to normalize $\Gamma$ so as to $\Gamma = 1/T$, which is an input constant relating the system temperature. For lower $\Gamma$, the particles are more active, and the random force from the heat bath is limited, so the fluctuation of the kinetic energy is large. For larger $\Gamma$ ($>= 30$), the fluctuation is quite small (below 4%). In figure 2, we present the maximal fluctuation of kinetic energy of the dusty plasma in a big time window. We adjust the random force from the heat bath

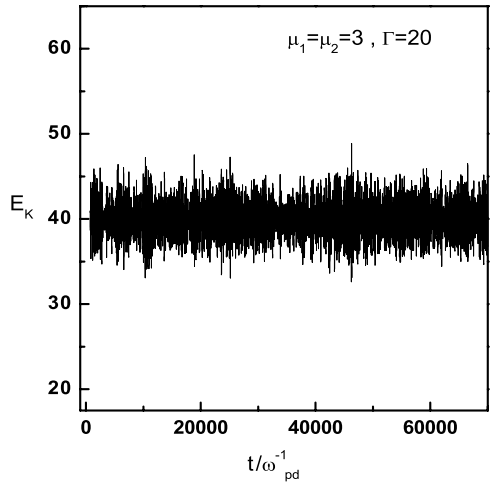


**Figure 2.** Kinetic energy varies with time in the one-component systems at $\mu_1 = \mu_2 = 3$, $\Gamma = 20$.

before computing the characteristic functions and each case is tested to guarantee the constant temperature.

## 3. The one-component system

The one-component dusty plasma is a basic model. In this system, the charged dusty particles are identical. All the particles have the same charge and mass, $Q_i = Q_j = Q$, $M_i = M_j = M$. Here, we intend to investigate the effects of $Q$ and $M$ on the phase transition from the liquid-like to solid-like states. The simulation is performed with the charge and mass parameter $\mu$ ranging from 1 to 10 and the coupling constant $\Gamma$ from 2.5 to 200. The phase transition can be observed through a MSD and $g(r)$. When the MSD keeps constant for a long time and a shoulder appears on each peak except the first one of $g(r)$, meanwhile, the third peak becomes higher than the second peak [13, 15], it means that the system coagulates. The two characteristic functions determine the critical $\Gamma^*$ for phase transition together; also the phase transition can be confirmed by the observation of the particle's structural change.

In figure 3, at a given $\mu$, the MSD increases with time at low $\Gamma$ (it is liquid or gas character) and decreases clearly with increasing $\Gamma$. When $\Gamma$ is higher than a critical value $\Gamma^*$, the MSD keeps a constant value at a large time scale $\left(t > 13\omega_{pd}^{-1}\right)$. The feature means that the system has a phase transition from the liquid-like to solid-like states. From figures 3(*a*)–(*d*), the shape of the MSD also indicates a phase transition from liquid to solid with increasing $\mu$ at a given $\Gamma$, and the critical coupling constant $\Gamma^*$ decreases with increasing $\mu$. For example, $\mu = 1$, $\Gamma^* = 140$; $\mu = 2$, $\Gamma^* = 50$; $\mu = 3$, $\Gamma^* = 20$; $\mu = 4$, $\Gamma^* = 10$. With increasing the quantity of mass, the inertia of particles is increased, and the particle activity is reduced in the canonical system. Simultaneously, with increasing the charge quantity, the particles will undergo higher static-electric potential energy $U_\mu = \mu^2 U_0$. The dusty particles are restricted in a smaller region to make a small movement. Therefore, the MSD reaches a constant value at a lower $\Gamma^*$, which means the system turns into a solid-like state earlier. The same results could be obtained through analysing the pair correlation function in figure 4. A phase transition occurs at different $\Gamma^*$ for a given $\mu$, where the numbers marked with arrows

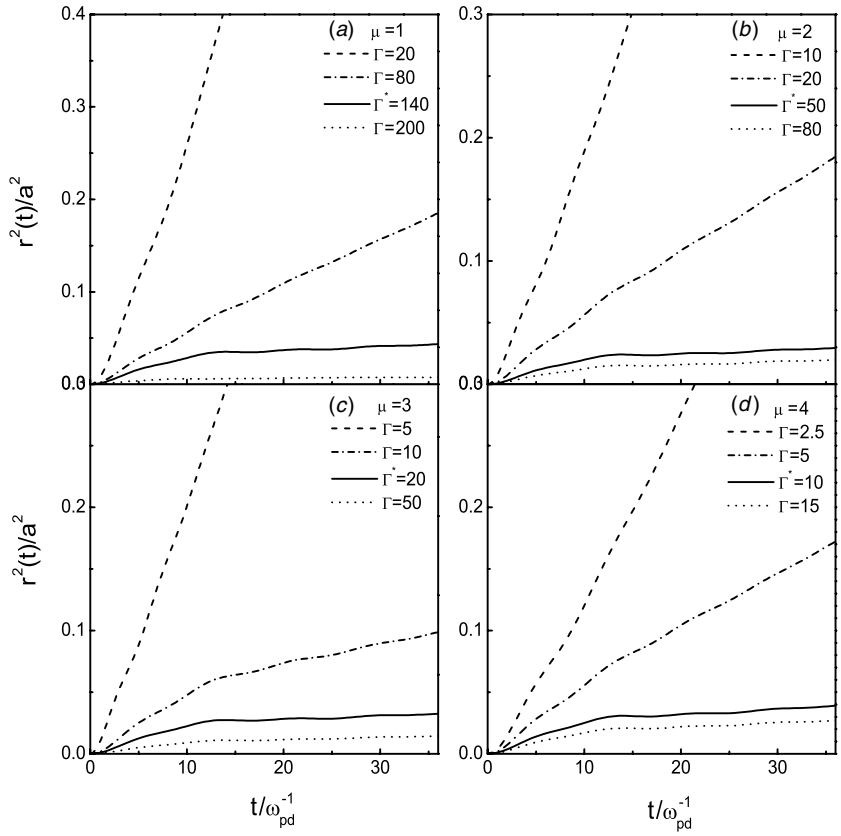


**Figure 3.** MSD varies with time at different Γ and $\mu$ in a 2D dusty plasma system composed of one component. (*a*) $\mu = 1$, (*b*) $\mu = 2$, (*c*) $\mu = 3$, (*d*) $\mu = 4$.

represent the number of particles in successive shells. The upper parts in figures 4(*a*)–(*d*) show a liquid character, where the neighbour number in a shell structure likes the liquid-like structure (6-12-18). The lower parts show a solid character, since a shoulder on each peak appears except the first one, and the third peak is higher than the second one, and the tested dusty particle has neighbours of a shell structure (6-5-6-12-5). One could also see that the configuration of 2D dusty plasma changes from non-ordering to ordering with increasing Γ at a given $\mu$, where the hexagon in figure 4 indicates the system is in a crystal-like state, and the critical value of $\Gamma^*$ decreases with increasing $\mu$.

In a many-body system, the velocity autocorrelation function is a good tool to describe the dynamical character. In figure 5, the oscillation of VACF strengthens with increasing Γ or $\mu$ at a given $\mu$ or Γ, respectively, and the period of oscillation becomes shorter corresponding to the larger frequency in $Z(\omega)$. $Z(\omega)$ in higher frequency domain is close to that of the plasma frequency, which means the motion of a single-dusty particle couples strongly with the collective motion of particles. When Γ is higher than a certain value at a given $\mu$, a new peak appears in a low-frequency domain, which indicates a new oscillatory mode. Schmidt [8] and Ohta *et al* [19, 20] have investigated the transverse wave and proved the low frequency related to the transverse collective mode. So we can know that the system tends to be a solid

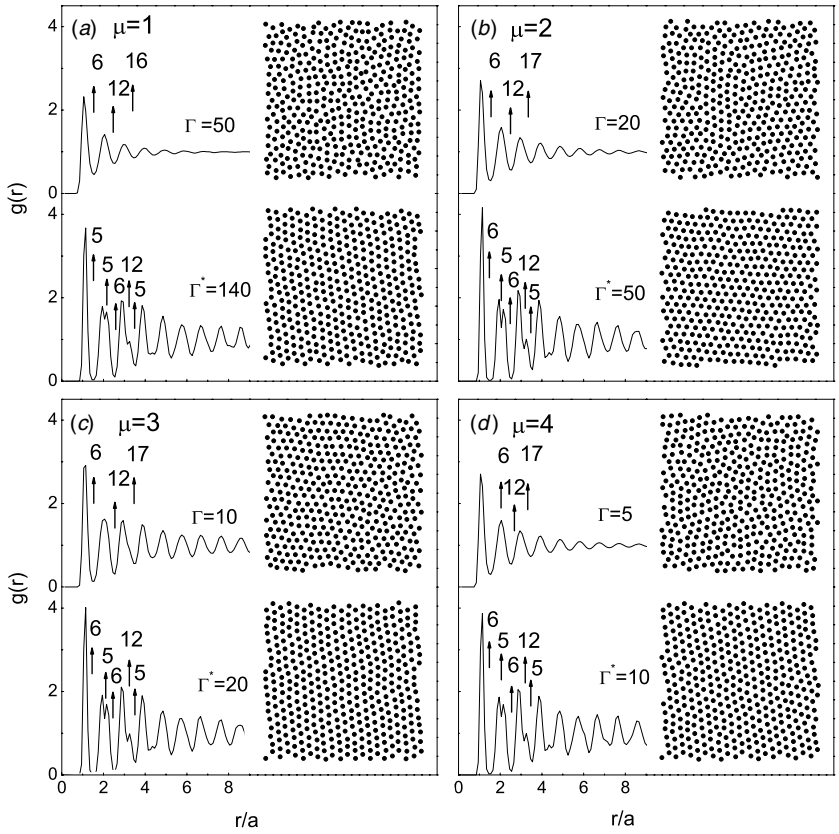


**Figure 4.** The pair correlation function $g(r)$ varies $r/a$ at different $\mu$ and $\Gamma$ in a one-component 2D dusty plasma. (*a*) $\mu = 1$, (*b*) $\mu = 2$, (*c*) $\mu = 3$, (*d*) $\mu = 4$.

state with increasing $\Gamma$ or $\mu$, and the low-frequency peak is corresponding to the transverse wave mode.

According to the above characteristic functions, we get a relation curve approximately between $\Gamma^*$ and $\mu$ for a two-dimensional one-component system in figure 6. One can see that the critical coupling constant $\Gamma^*$ quickly decreases with increasing the mass and charge parameter $\mu$. The correlation curve can be fitted by a function: $\Gamma^* \propto \mu^{-1.72\pm0.07}$. Since $\mu_i = Q_i/Q_0 = M_i/M_0$, the interparticle potential energy is $U \propto \mu^2$ and the charge influences the coagulation process more.

## 4. The two-component system

A two-dimensional one-component dusty plasma is the basic model, so a lot of work has been done on it. But in a real system, there are often different kinds of particles under a certain condition. Therefore, the research on many-species-particle system needs to be done. In this section, we investigate the structural properties of a two-component system, where $\mu_1 \neq \mu_2$. In the simulation, the mass and charge parameter of each kind of particles $\mu_{i(i=1,2)}$ ranges from 1 to 7 and the coupling constant $\Gamma$ ranges from 10 to 200. For simplification, we call one kind of particles with $\mu_1$ particle1 and the other kind of particles with $\mu_2$ particle2.

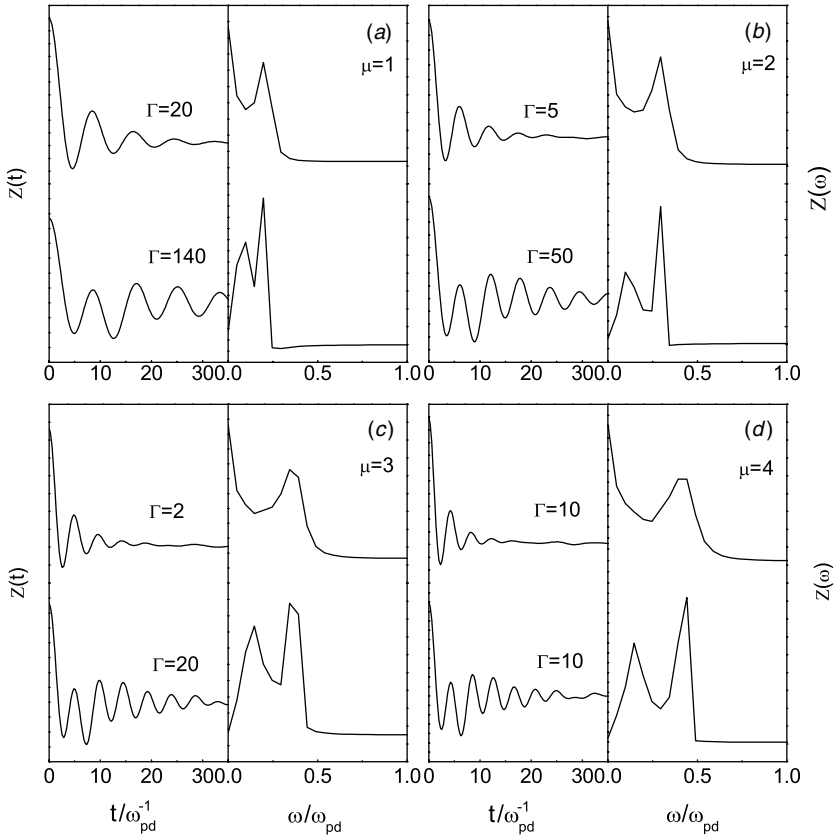


**Figure 5.** The velocity autocorrelation function with corresponding fourier transition varies with time and frequency at different $\Gamma$ and $\mu$ in one component system. (*a*) $\mu = 1$, (*b*) $\mu = 2$, (*c*) $\mu = 3$, (*d*) $\mu = 4$.

In figure 7, the MSD varies with time (where $\omega_{pd} \propto (\mu_1\mu_2/M^*)^{1/2}$, $M^* = M_1M_2/(M_1 + M_2)$ [21]) at a different coupling constant $\Gamma$ for a different charge and mass parameter ratio ($\mu_1 : \mu_2$). It is shown that $\mu_2$ is fixed and the MSD decreases with increasing $\mu_1$ at a given $\Gamma$ in figure 7(*a*). The MSD decreases with increasing $\Gamma$ at a given ratio $\mu_1 : \mu_2$ in figure 7(*b*) and keeps constant at a large time scale when $\Gamma$ is higher than a certain value (for example $\mu_1 : \mu_2 = 2 : 1$, $\Gamma^* = 110$), which means the system is in a solid state. Therefore, the temperature is the main reason to cause phase transition in a 2D two-component dusty plasma. The critical coupling constant value is located between $\Gamma_1^*$ and $\Gamma_2^*$ ($\Gamma_i^*$ is the critical $\Gamma$ of the one-component system containing only particle1 or particle2, respectively), and $\Gamma^*$ is closer to the $\Gamma_i^*$ of smaller $\mu$. Especially for the system with the ratio $\mu_1 : \mu_2$ far away from 1, the particles with small $\mu$ strongly affect the phase transition, which can be seen in figure 7(*c*). The phenomenon is not difficult to explain. The particles with large charge and mass quantities are confined in high static-electric potential energy, thus the system is easy to coagulate and the critical coupling constant is low. But when the system also contains the other kind of particles with smaller charge and mass quantities, this kind of particles can be treated as 'impurities' and will delay the coagulation process. So $\Gamma^*$ of the two-component system is higher than that of the one-component system containing identical particles with

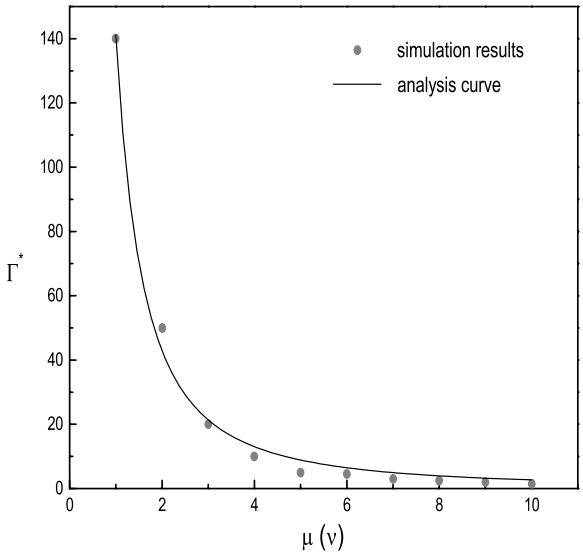


**Figure 6.** The critical coupling constant Γ* varies $\mu$ in 2D dusty plasma composed of one component.

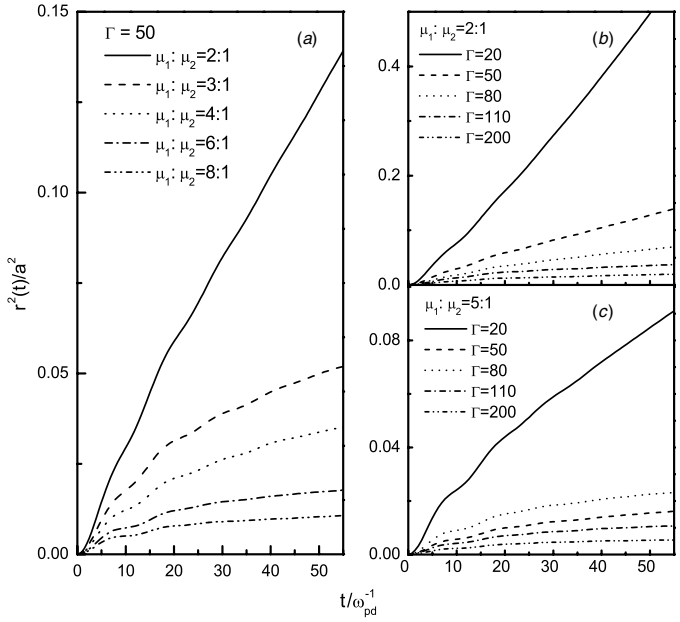


**Figure 7.** MSD varies with time at different Γ for kinds of particles.

large charge and mass quantities. On the other hand, the number of 'impurities' is so large that Γ* of the whole system is close to the critical coupling constant of the one-component system containing the 'smaller' kind of particles. These 'impurities' not only strongly delay the coagulating progress but also affect the configuration of a system. Figure 8 shows that the

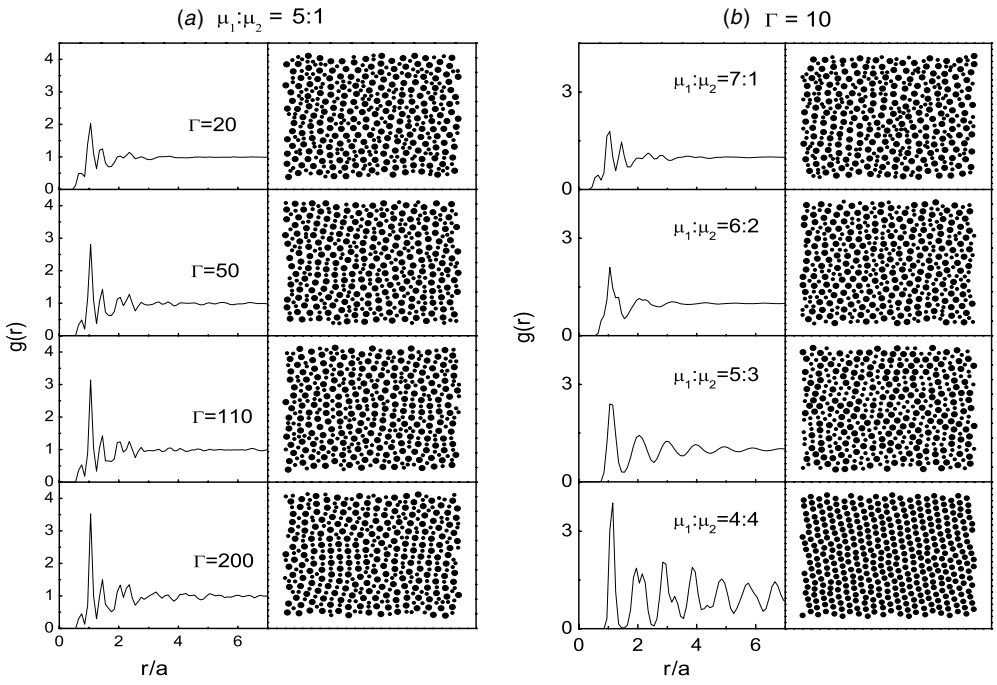


**Figure 8.** $g(r)$ varies with $r$ at different $\Gamma$ for kinds of particles.

shape of $g(r)$ is not like that of the one-component normal system, and the hexagon is not formed, especially for the system with the ratio $\mu_1 : \mu_2$ far away from 1 (figure 8($a$)). When the two kinds of particles have similar $\mu$ (for example $\mu_1 : \mu_2 = 5 : 3$ in figure 8($b$)), $g(r)$ is close to the normal shape with the ordered configuration. Therefore, the particles with a small charge and mass parameter would strongly affect the structural properties and the phase transition in a two-dimensional two-component dusty plasma.

## 5. Conclusions

In summary, we investigate the dynamical and structural properties of two-dimensional one-component and two-component dusty plasmas by using the molecular dynamics method. It is found that the critical coupling constant $\Gamma^*$ for phase transition from the liquid-like to solid-like states decreases with increasing the mass and charge quantities of particles in a one-component system. A correlation function between the critical $\Gamma^*$ and the charge and mass parameter $\mu$ is obtained: $\Gamma^* \propto \mu^{-1.72\pm0.07}$. In the system with two species of particles, the coagulation process is found to be delayed by the particles with smaller $\mu$, and the critical $\Gamma^*$ is closer to that of the one-component system containing the smaller $\mu$ particles.

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