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Defects related self-diffusion in a two-dimensional dusty plasma crystal

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Abstract

Single-particle motion and self-diffusion in a two-dimensional dusty plasma are investigated by molecular dynamic simulation. The velocity autocorrelation function indicates that the single-particle motion is strongly coupled to the collective motion in the dusty plasma when the coupling parameter is high enough. The point defects play an important role in the particle self-diffusion process. A simple point defect motion model is developed to explain the mechanism of self-diffusion and estimate the self-diffusion coefficient in the dusty plasma. The value of the self-diffusion coefficient calculated by using the model is in agreement with the result obtained from mean square displacement for a two-dimensional dusty plasma crystal.

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1. Introduction

The dynamical behaviour of dusty plasma has recently attracted the special attention of the scientists studying dusty plasma [1–13]. The transport coefficients such as thermal conductivity, viscosity and self-diffusion in dusty plasma are investigated. Salin and Caillol [1] calculate the thermal conductivity, shear viscosity and bulk viscosity in an equilibrium one-component plasma (OCP) by molecular dynamic (MD) computations. Donko and Nyiri [2] obtain the thermal conductivity and shear viscosity for a non-equilibrium one-component plasma system. Ohta and Kremer [3, 14–16] calculate the self-diffusion coefficient in a Yukawa fluid by molecular dynamic simulation. Tankeshwar [6] proposes a simple model for the calculation of self-diffusion in a fluid. However, in a dusty plasma crystal with point defect, the self-diffusion has not been studied in detail by molecular dynamic simulation. The self-diffusion coefficient is one of the most fundamental dynamical parameters that reflects the nature of interparticle potentials and characterizes the thermodynamics of the system. The effect of a point defect on the self-diffusion process is important in the dusty plasma. In this paper, we intend to study the single-particle motion and self-diffusion in a two-dimensional (2D) dusty plasma crystal with point defects, and explain the mechanism of self-diffusion and estimate the self-diffusion coefficient in the dusty plasma.

We consider a dusty plasma system, a collection of identical particles of mass M and charge Q, immersed in a neutralizing background plasma. The interparticle interaction potential is assumed to be the screened Coulomb potential: $\phi(r) = (Q^2/4\pi\varepsilon_0 r)\exp(-r/\lambda_D)$, where r is the distance between two particles and λ_D is the screening length of the background plasma. The thermodynamics of the system can be characterized by two dimensionless parameters: $\kappa = a/\lambda_D$, i.e., the ratio of the average interparticle distance a to the screening length and the coupling parameter $\Gamma = Q^2/(4\pi\varepsilon_0 a k_B T)$, where T is the system temperature.

Our simulations were performed in a canonical ensemble; the Nosé–Hoover thermostat scheme [17] is used to keep the system at constant temperature. The calculations were performed on a system of 256 particles in a square box with periodic boundary conditions. The time step is $0.1\omega_{\mathrm{pd}}^{-1}$, where $\omega_{\mathrm{pd}} = \sqrt{Q^2/\varepsilon_0 M a^3}$ is the dusty plasma frequency. Usually, the initial runs last about 3×10^4 steps for equilibration, and in subsequent 2×10^4 time steps, the velocity autocorrelation function (VAF) and mean square displacement (MSD) are computed. In this paper, we use an experimentally related value of $\kappa = 1$.

The velocity autocorrelation function $Z(t)$ and mean square displacement $\langle r^2(t)\rangle$ are defined by

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

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

where $\langle\cdots\rangle$ indicates thermal average, N is the number of simulation particles and $\vec{r}_i(t)$ and $\vec{v}_i(t)$ are the position and velocity of the ith particle at time t, respectively.

The Fourier transformation of $Z(t)$ gives the spectrum function

$$\tilde{Z}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} Z(t)\exp(-\mathrm{i}\omega t)\,\mathrm{d}t. \tag{3}$$

For a two-dimensional system, the particle self-diffusion coefficient can be calculated by

$$D = \lim_{t\to\infty}\frac{\langle r^2(t)\rangle}{4t}. \tag{4}$$

2. Simulation results

The single-particle motion of a many-body system is usually investigated by the VAF. Figure 1(*a*) shows the normalized VAFs at different coupling parameters. Figure 1(*b*) shows the spectrum functions of the corresponding VAFs. In figure 1, one can see that at $\Gamma = 2.5$, the VAF rapidly decays to zero with very weak oscillation, and the spectrum function is only a broadened peak at zero frequency. This indicates that the single-particle motion is only thermal diffusion motion. When Γ increases to 10, VAF begins to exhibit decay oscillations; and a peak appears at the frequency of $0.98\omega_{\mathrm{pd}}$, indicating that the single-particle motion has a vibration mode in addition to the diffusion mode. With the increase of Γ, the oscillations become more and more evident. The oscillation frequency is close to the dusty plasma frequency

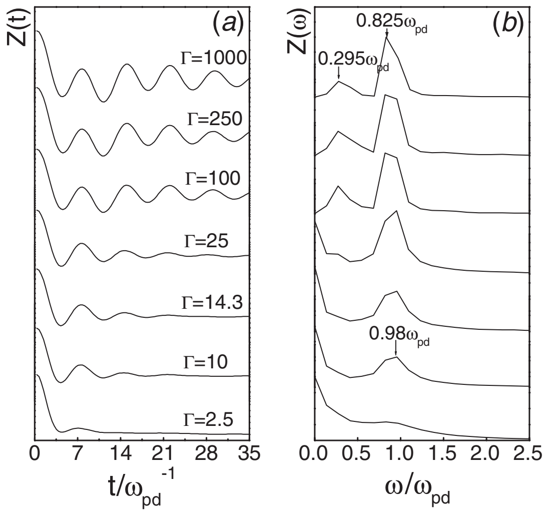

Figure 1. (*a*) The normalized VAFs at different coupling parameters. (*b*) The spectrum functions of the corresponding VAFs.

ω_{pd}, indicating that the single-particle motion is strongly coupled to the collective motion. At $\Gamma \geqslant 100$, the oscillation frequency shifts to $0.825\omega_{pd}$, and a new small peak appears at a lower frequency of $0.295\omega_{pd}$, meanwhile the diffusion peak at zero frequency disappears. The appearance of the low-frequency peak indicates that a new motion mode is involved in this case. Usually, when Γ increases to 100, the dusty plasma begins to freeze. When the dusty plasma freezes to a solid, a transverse collective mode will be excited. Schmidt [12] and Ohta *et al* [3, 13] have investigated the transverse excitation in a strongly coupled one-component plasma with molecular dynamics simulation, and the broad low-frequency peak is due to the appearance of transverse collective modes. In the above simulations, the sample is composed of 256 particles. As is known for particle systems with other potentials, the numerical results depend on the simulation particle number N [18]. In order to observe the dependence of the oscillation frequency on the finite size of the sample (namely, the particle number N), the simulations are performed again with $N = 625$ and 900, respectively, for several Γ values. For example, when $\Gamma = 1000$ and $\Gamma = 100$, the corresponding high oscillation frequency peaks appear at $0.825\omega_{pd}$, $0.826\omega_{pd}$ and $0.826\omega_{pd}$ for the cases of $N = 256$, 625 and 900, respectively, whereas the low-frequency peaks are always located at $0.295\omega_{pd}$ for the three cases. From the above results, one can see that the oscillation frequencies do not depend obviously on the simulation particle number N in the calculation accuracy, so in order to save computer time the particle number $N = 256$ is sufficient for the simulations. In the following simulations, the samples are all composed of 256 simulation particles.

In order to study self-diffusion in the two-dimensional dusty plasma, MSDs are investigated for different coupling parameters for a long time $t \sim 2200\omega_{pd}^{-1}$. Figure 2 shows the MSDs for different coupling parameters. In figure 2, one can see that with increasing coupling parameter, the MSD obviously decreases. When $\Gamma = 100$, 200 and 300, there are two relaxation time scales. On the time scale of $t < 250\omega_{pd}^{-1}$, the MSD shows ballistic behaviour with $\langle r^2(t)\rangle \propto t^2$, and on the time scale of $t \geqslant 250\omega_{pd}^{-1}$, the MSD shows diffusive behaviour with $\langle r^2(t)\rangle \propto t$. When $\Gamma = 1000$, the MSD increases linearly with time. When $\Gamma = 5000$, the MSD almost does not increase with time and exhibits an oscillatory character. These results for the cases of $\Gamma = 100$, 200, 300 and 1000, as shown in figures 3 and 4, are

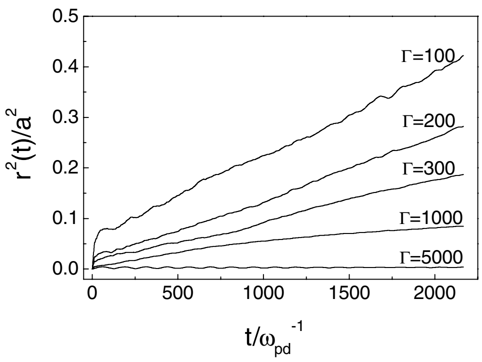

Figure 2. The MSDs with time at different coupling parameters.

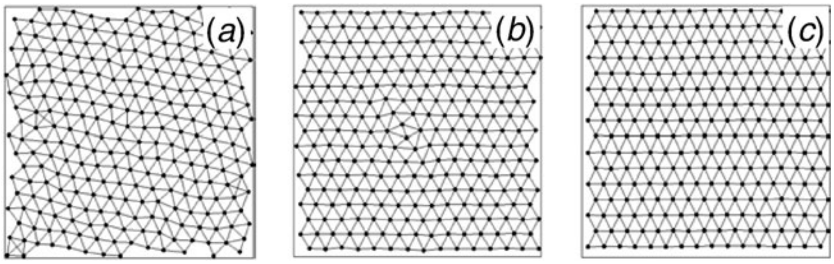

Figure 3. Particle locations and nearest-neighbour bonds at (*a*) $\Gamma = 100$, (*b*) $\Gamma = 1000$ and (*c*) $\Gamma = 5000$, respectively.

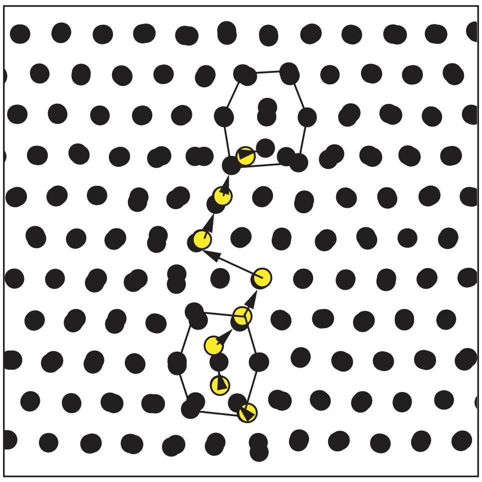

Figure 4. Particle configurations for two moments, where the hexagons indicate the point defects, the grey circles denote the moved particles and the arrows indicate the directions of motion of the moved particles.

due to the fact that the point defects exist and continually move from one location to another in the dusty plasma, and the particles are affected greatly by the point defect motion, so the particles also move from one place to another, and the particle MSDs increase gradually with

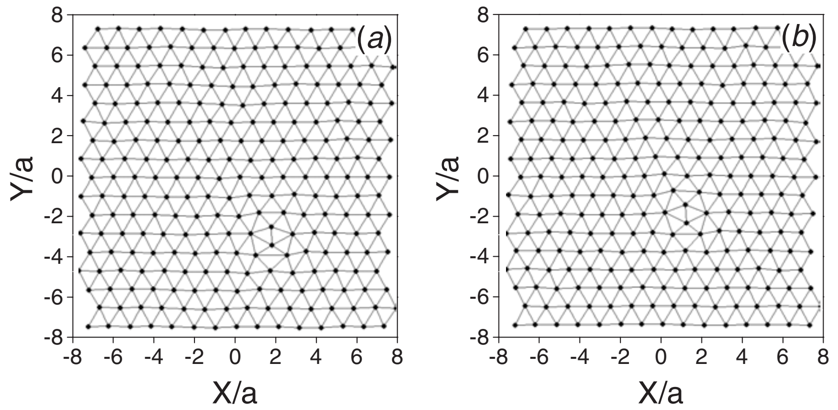

Figure 5. Particle locations and nearest-neighbour bonds for two moments (*a*) $t_1 = 0$ and (*b*) $t_2 = 106.2\omega_{pd}^{-1}$, respectively, with $\Gamma = 1000$.

time. For the case of $\Gamma = 5000$, there is no point defect in the crystal, and the crystal is a perfect lattice, where every particle is confined near its equilibrium position and vibrates around this position, and the particle MSD almost does not increase with time and exhibits an oscillatory character. Otherwise, in the crystal with $\Gamma = 1000$, the number of point defects is much less than in the cases of $\Gamma = 100$, 200 and 300, so the MSD for $\Gamma = 1000$ is also much lower than in the other cases. From the above discussion, one can conclude that the point defects really play an important role in the self-diffusion process for the two-dimensional dusty plasma. Otherwise, for the lower coupling parameters, such as $\Gamma = 100$, 200 and 300, the two relaxation time scales are due to the fact that at short time $t < 250\omega_{pd}^{-1}$, the dynamics of the particle is essentially that of a free particle, and shows a ballistic behaviour with $\langle r^2(t)\rangle \propto t^2$ [8, 16]. During the time $t < 250\omega_{pd}^{-1}$, the particles have moved a substantial distance relative to their nearest neighbours and to move farther must escape from the cage formed by their neighbours [16, 19]. At relatively high temperature, namely lower Γ value, the rearrangement of the neighbours is rapid and the ballistic regime directly becomes a diffusive regime for the time $t \geqslant 250\omega_{pd}^{-1}$ with $\langle r^2(t)\rangle \propto t$ [16]. In conclusion, for the short time $t < 250\omega_{pd}^{-1}$, the particle shows a caged-particle motion with $\langle r^2(t)\rangle \propto t^2$, and in the time $t \geqslant 250\omega_{pd}^{-1}$, the particle motion shows a diffusive behaviour with $\langle r^2(t)\rangle \propto t$.

In figure 2, one can see that with increasing coupling parameter, the slope of the MSD for time $t \to \infty$, i.e. the self-diffusion coefficient D (equation (4)) is obviously reduced. This result is related to the effect of point defects on the particle self-diffusion process. We can establish a simple point defect motion model to explain the mechanism of self-diffusion and estimate the self-diffusion coefficient in the dusty plasma. In the model, for example with $\Gamma = 1000$, the whole simulation region is a square with area $LxLy = (16 \times 16)a^2$ (here a is the mean interparticle distance). In figure 3(*b*), the size of the point defect is assumed to be $(2 \times 2)a^2$. The point defect continuously moves from one location to another, as shown in figure 4, and the motion of the point defect seems like a random walk motion, so we can assume that the track of the point defect finally covers the whole of the simulation region of the crystal during time $t = (16a/\upsilon)(16a/2a) = 128a^2/\upsilon$, where υ is the point defect motion velocity. If we assume the displacement of every particle to be λa during the point defect motion time t, then the particle self-diffusion coefficient can be calculated by $D = (\lambda a)^2/4t$ for the two-dimensional dusty plasma. The point defect motion velocity υ can be estimated from the particle configurations for two moments as is shown in figure 5. The point defects are located at positions ($x_1 = 1.696a$, $y_1 = -2.934a$) and ($x_2 = 1.143a$, $y_2 = -1.898a$), respectively, for the two moments, so the point defect displacement is $\Delta d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} = 1.17a$ during the time interval $\Delta t = t_2 - t_1 = 106.2\omega_{pd}^{-1}$. Therefore, the point defect motion velocity $\upsilon = \Delta d/\Delta t = 1.17a\big/106.2\omega_{pd}^{-1} = 0.011a\big/\omega_{pd}^{-1}$. From figure 4, we assume the particle average displacement to be $\lambda a = 0.3a$ during time t, so the self-diffusion coefficient $D = (\lambda a)^2/4t = (0.3a)^2/(4 \times 128a^2/\upsilon) \approx 1.9 \times 10^{-6}a^2\big/\omega_{pd}^{-1}$. This value is in agreement with the result $D \approx 2.0 \times 10^{-6}a^2\big/\omega_{pd}^{-1}$ obtained from MSD (figure 2 and equation (4)) for the case of $\Gamma = 1000$. From the above, one can see that the point defect plays an important role in the particle self-diffusion process, and the point defect motion model is effective in estimating the self-diffusion coefficient for the two-dimensional dusty plasma crystal with point defects.

3. Conclusions

We have investigated the dynamic behaviour of dusty plasma by molecular dynamic simulation. The velocity autocorrelation functions show that the single-particle motion is strongly coupled to the collective modes in the dusty plasma when the coupling parameter is high enough, and the lower frequency peak is due to the coupling between the single-particle motion and transverse collective modes. With increasing coupling parameter, the particle mean square displacement and self-diffusion coefficient are obviously reduced. The point defects play an important role in the particle self-diffusion process. A simple point defect motion model is proposed for explaining the mechanism of self-diffusion and estimating the self-diffusion coefficient in the two-dimensional dusty plasma crystal. The value of the self-diffusion coefficient calculated by using the motion model is in agreement with the result obtained from the particle mean square displacement for the two-dimensional dusty plasma crystal with $\Gamma = 1000$.

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