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Non-equilibrium phase transitions in suspensions of oppositely driven inertial particles

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Abstract

The structural evolution of a two-specie suspension of inertial particles under opposite driving forces is investigated by molecular dynamics simulations. The effects of the driving force (F) and the total number density of the particles (ρ) on the final structure are explored. When F is increased under a high ρ, the system starts with a frozen phase, passes through an ordered phase characterized by two demixed lanes moving in opposite directions, and finally returns to a disorder phase. When ρ is increased under a low F, a novel *re-entrant* phase transition is found: more than two lanes parallel to the driving forces are observed first, followed by a disordered phase with different kinds of particles blocking each other, and then an ordered state with all particles separating into two demixed lanes. We comment on the possible mechanisms underlying these phase transitions in terms of the compromise between the directional driven motion and random thermal fluctuation.

Keywords: Phase transition; Lane; Inertial particle; Color field; Molecular dynamics (MD) simulation

1. Introduction

Non-equilibrium phenomena are ubiquitous in nature and usually characterized by rich scenario of phase transitions both in time and in space. In recent years many works have been done about such phase transitions in driven systems [1,2]. In particular, systems with two species of particles driven in opposite directions are studied [3–5]. Variations in the strength of the driving field and/or particle density are found to induce phase transitions from homogeneous particle distributions to spatially inhomogeneous structure. Typical examples are found in binary mixtures of "positively and negatively charged" colloidal particles driven by an external field, where the same charged particles will separate into several lanes if the intensity of driving field exceeds a critical value [6–8]. Such laning phenomenon of Brownian particles has also been observed in experiment recently [9]. The simulating results also reveal a reentrance effect in the lane formation [10], that is, for increasing particle density under a fixed strong driving field, there is first a transition towards lane formation which is followed by another transition back to a state with no lanes.

Lane formation has also been found in granular systems where particle inertia is considerable. It has been found in oppositely driving pedestrian zones that, at low number density, particles of the same species will form lanes parallel to the driving field, while at relatively high density, jamming will happen [11–14]. In particle sedimentation systems, adding neutrally buoyant particles to a monodisperse suspension is found to accelerate the settling speed of the heavier particles owing to their stratification [15], that is, homogeneous mixture would spontaneously develop remarkable local clustering and separation of the two species. Although this structure formation was further investigated for more general properties of the two particle species [16–20] and on the mechanism underlying this instability [21–23], the effect of driving force intensity on the phase transition in such systems have not been reported systematically. The intensity of the driving force in real pedestrian dynamics and the particle-fluid interactions in real sedimentations may have limited the parameter space explored.

In this work, we will consider an idealized model with a suspension of identical inertial particles driven by external

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fields in opposite directions, so as to establish a phase diagram of the structural changes in this system in a wider parameter space and compare it with non-inertial colloidal systems. The results may serve as a reference frame for studying the separation and grading of particles in real suspensions.

In fact, the model is similar to that used in the color field systems [24–26], except that the friction coefficient for energy dissipation is *constant*, rather than correlated to the driving field and the total kinetic energy by a thermostat [24–26]. It can also be understood as an idealization of dilute suspension of micro- or mini-particles in liquids where Brownian motion is less significant as compared to colloidal particles and the linear Stokesian drag law still holds. Of course, the suspension is much denser in our case, but choosing a constant friction coefficient allows us to separate its effect [27] and concentrate on the effect of driving force. It is also reported that ordered structure in driven systems is associated with small noise-to-field ratios [14]. In our simulation, all mechanical noise stems from particle interactions and no constraint is imposed except its dumping under a constant friction coefficient, the controlling factors in the system is thereby reduced, which facilitates a parametric study.

The paper is organized as follows. In Section 2, we will illustrate the particle model and the arrangements of the simulations in detail. The simulation results on the formation and evolution of the dynamical patterns and the phase diagram are described in Section 3, together with qualitative analysis on the physical mechanism behind. We conclude in Section 4.

2. Simulation method

We consider a 2D system containing equal numbers of A and B particles ($N_A = N_B = N/2$) in a square area S surrounded by periodic images of itself. We define the particle number density as $\rho = N/S$. The particles interact with a soft potential [24]

$$\phi_{ij}(r) = \varepsilon\left(\left(\sigma/r_{ij}\right)^{12} - \left(\sigma/r_{\mathrm{cut}}\right)^{12}\right) \quad \left(r_{ij} < r_{\mathrm{cut}}\right), \tag{1}$$

$$\phi_{ij}(r) = 0 \quad \left(r_{ij} \geq r_{\mathrm{cut}}\right). \tag{2}$$

where r is the inter-particle distance. Normalized values are used throughout this paper by choosing the characteristic energy of the pair potential ε, the particle exclusion diameter σ and particle mass m as the units of energy, length and mass, respectively. All simulations are performed for $S = 8100$, and $r_{\mathrm{cut}} = 1.5\sigma$.

We denote the location of particle j at time t by $\vec{r}_j(t)$ and its velocity $\frac{d\,\vec{r}_j(t)}{dt}$ by $\vec{v}_j(t)$. The equation of motion for particles reads

$$\frac{d\,\vec{v}_j}{dt} = -\vec{\nabla}_{\vec{r}} \sum_{k \neq j} \phi_{kj}(r) + F\,\vec{e}_j - \zeta\,\vec{v}_j. \tag{3}$$

The right hand side includes all forces acting on the particles, namely the inter-particle potential force, the constant driving forces and the friction force. The driving field is symmetric with $F = F_A = F_B > 0$. If particle j belongs to species "A", it is driven in the direction $\vec{e}_j = (1,0)$ and otherwise in the direction $\vec{e}_j = (-1,0)$. Except the applied directions of the driving field, the two types of particles have no difference.

As has been mentioned, when thermostat is used in some molecular dynamics simulations [24–26], the friction coefficient ζ is correlated to the intensity of the driving force and particle velocities by

$$\zeta = \sum_{j=1}^{N} F\,\vec{e}_j \cdot \vec{v}_j \Big/ \sum_{j=1}^{N} \vec{v}_j \cdot \vec{v}_j. \tag{4}$$

However, the physical process to realize this thermostat is not obvious. For instance, it is hard to image how ζ can decrease or even return to be negative when the direction of particle velocity diverts form the driving force. Therefore, it is not favorable for concentrating on the effects of F and ρ only, since the effect of ζ has to be introduced if such a thermostat is adopted. In this work, ζ is set to a constant of 2.0.

The equations of motion are solved by a Verlet scheme with an adaptive time step ensuring that no particle moves more than 0.001σ per step under the maximum theoretical velocity. No significant change is seen when finer time steps are used, and it is, therefore, small enough. We have also checked that the results are independent of the size of the simulated area. For every F, particles are initially distributed randomly. To relax the system, each particle is assigned a high random velocity initially which is annealed gradually to zero before the driving field is applied and then kept constant. Each simulation is conducted typically for 10,000 time units while the statistics is usually gathered in the last 5000 time units.

3. Simulation results and discussion

The evolution of the system under different combinations of F and ρ are systematically studies through molecular dynamics simulations. A general phase diagram for the steady states is then obtained. Four phases can be identified altogether, namely the freezing phase, the multiple-lane phase, the disorder phase and the two-lane phase, as will be detailed in Fig. 7 later. The phase transition scenario in this system is different from that in no-inertia colloid systems. For $\rho = 1.0$, with the continuous increase of F, the steady structure transforms from a two-lane state to a disorder state at a critical value, as will be detailed in Section 3.1. And for a given low F, the continuous increase of ρ leads to a reentrance phase transition: multiple-lane / disordered state / two-lane, as will be detailed in Section 3.2.

3.1. Under constant number density ($\rho = 1.0$)

The simulations are carried out for constant number density first, with $\rho = 1.0$, that is, $N_A = N_B = 4050$. Two threshold values of F can be identified for the phase transitions. For $F < F_1 = 1.5$, the system settles down to a macroscopically immobile state after a transient motion. Particles of different species are mixed and block each other (Fig. 1a). For $F_1 \leq F \leq F_2 = 10.0$, the binary mixture segregates into two demixed lanes moving collectively with the field (Fig. 1b). In this regime, although the interfaces between the two lanes are not perfectly smooth,