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# Brownian Dynamics of Effective Diffusion Model on Hard-disk Colloidal Suspensions with Hydrodynamic Interactions

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Recently the nearly hard-sphere system has been investigated mainly by the computer simulation. In this paper, we report the result of the simulation for the monodisperse hard-disk suspensions of the interacting Brownian particles with effective diffusion due to the hydrodynamic interactions.

We simulate the suspensions in the following two cases:(A)with the hydrodynamic interaction through the effective diffusive field and (B)without the hydrodynamic interaction. In both cases, the particles can also make elastic collisions and the simulation is done in the two dimensional system with periodic boundary condition. The position vector  $\mathbf{X}_i$  of the particle  $i$  obeys the stochastic equation [1]

$$\frac{d}{dt}\mathbf{X}_i(t) = \mathbf{u}_i(t), \quad (1)$$

where  $\mathbf{u}_i(t)$  is a Gaussian, Markov random velocity with zero means and satisfies

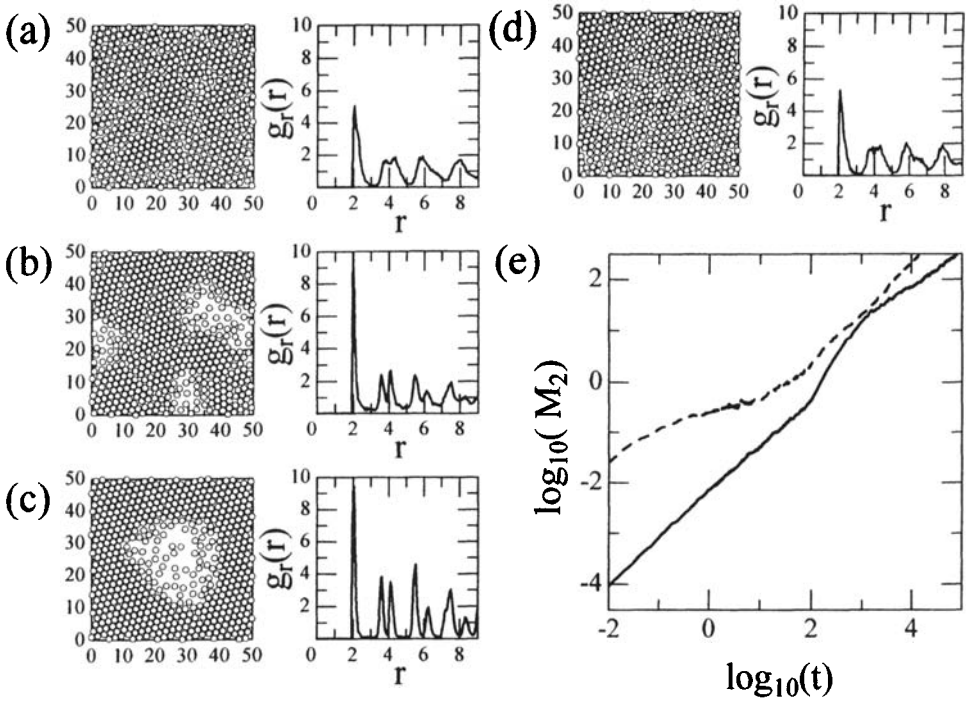
$$\langle \mathbf{u}_i(t)\mathbf{u}_j(t') \rangle = 2D_s(\Phi(\mathbf{X}_i(t), t) \delta_{ij} \delta(t-t') \mathbf{1}. \quad (2)$$

In case(A)  $D_s$  denotes the self-diffusion coefficient which depends on the local density of the particles  $\Phi(\mathbf{X}_i(t), t)$ . The most important feature of  $D_s$  is that it becomes zero as  $D_s \sim D_0 (1 - \Phi/\phi_g)^2$ , where  $D_0$  is a single particle diffusion coefficient, and the glass transition point  $\phi_g$  is assumed to be  $= 0.7589$  here. Here this dynamic anomaly results from the many-body correlation between particles due to the long-range hydrodynamic interaction [2]. In case(B), we have  $D_s(\Phi(\mathbf{X}_i)) = D_0$ .

Figures 1 (b)-(c) show the snapshots in case(A) during the process that the system goes to the equilibrium state from the initial condition(a) at mean density of the particles  $\phi = 0.720$ , while Figure 1 (d) shows the equilibrium state in case(B) starting from the initial condition(a). In case(A), the particles start to aggregate and the several voids are formed. Then, the larger voids seem to grow at the

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**FIGURE 1.** The differences between the case(A) and case(B) at mean density  $\phi = 0.720$ . (a)  $t = 0$ , (b)  $t = 300$ , (c)  $t = 45100$  in Case(A), (d)  $t = 10700$  in Case(B) and (e)  $\log_{10}(M_2)$  as the function of  $\log_{10}(t)$

expense of smaller voids, leading to one big void in the equilibrium state. On the other hand, there is no voids in case(B). Figures 1 (a)-(d) also show the radial distribution functions  $g_r(r)$  as the function of the distance between the particles  $r$ . In the equilibrium state of case(A), the second peak of  $g_r(r)$  shows the splitting characteristic of the crystalline state. In case(B), however, it only shows a broad peak, indicating a liquid state. Figure 1 (e) shows the log-log plot of the mean square displacement  $M_2 = \frac{1}{N} \sum_{i=1}^N \langle (\mathbf{X}_i(t) - \mathbf{X}_i(0))^2 \rangle$  versus dimensionless time  $t$ . In case(A), the crossover occurs because of the formation of the voids. In the equilibrium state, almost all particles are in the crystalline state. Only the particles inside of the void can move rapidly. In case(B), the crossover occurs because of the normal diffusion of the particles. All particles are moving randomly in the equilibrium liquid state [3].

We conclude that the long-range hydrodynamic interactions among particles are indispensable for the crystallization of the hard-disk particles.

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2. Tokuyama, M., and Oppenheim, I., *Physica A* **216**, 85 (1995).
3. Terada, Y., and Tokuyama M., in preparation.