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Brownian Dynamics Simulations on Hard-sphere Colloidal Suspensions

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The soft-core system and the hard-sphere system [1] have been investigated mainly by Molecular dynamics (MD) simulation. In this paper, we report the result of the Brownian dynamics (BD) simulation for the mono disperse hard-sphere suspensions.

The colloidal particles in a solvent undergo frequent random collisions with the solvent molecules, leading to Brownian motion. On time scales \( t \geq \tau_R = a^2 / D_0 \), the position \( \mathbf{X}_i \) of the particle \( i \) is then assumed to obey

\[
\frac{d}{dt}\mathbf{X}_i(t) = \mathbf{u}_i(t),
\]

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

\[
< \mathbf{u}_i(t) > = 0, \quad < \mathbf{u}_i(t)\mathbf{u}_j(t') > = 2D_0 \delta_{ij} \delta(t-t') \mathbf{1}.
\]

Here \( D_0 \) is a single particle diffusion coefficient, \( a \) is the radius of the particle, and the brackets indicate the average over an equilibrium ensemble.

The Brownian equation of motion (1) accounts for solvent friction, but ignores hydrodynamic interactions between colloidal particles. In this paper we discuss how neglect of the hydrodynamic interaction affects crystallization of hard spheres.

In our simulation, the particle number is 864 and the time interval of the Brownian motion \( \delta t \) is 0.005. During \( \delta t \), the velocity of the particles do not change except by the two-body elastic collisions. After \( \delta t \) the velocity of the all particles change according to Eq.(2). The simulation is done for different volume fractions \( \phi = 0.460, 0.510, \) and 0.560. As initial conditions, we start from (a) the ordered FCC packing and (b) the disordered Jodrey-Tory's (J-T) packing [2] with periodic boundary condition. The J-T packing makes the random configuration.

Figure 1 shows the log-log plot of the mean-square displacement \( M_2(t) = \frac{1}{N} \sum_{i=1}^{N} < (\mathbf{X}_i(t) - \mathbf{X}_i(0))^2 > \) versus time \( t \). At \( \phi = 0.460 \) \( M_2(t) \) reaches the final equilibrium state rapidly from both initial conditions (a) and (b). At higher

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FIGURE 1. The log-log plot of $M_2(t)$ versus the scaled time $D_0 t/a^2$ for $\phi = 0.460$, 0.510, and 0.560 (from top to bottom). The solid and dotted lines indicate the results in case(a) and case(b), respectively.

FIGURE 2. Radial distribution functions $g_r(r/a)$ versus the scaled distance $r/a$ at $t = 1000$ for $\phi = 0.460$, 0.510, and 0.560 (from bottom to top). The solid and dotted lines indicate the results in case(a) and case(b), respectively.
volume fractions, it is still changing differently in case (a) and (b) within our simulation times.

In Figure 2 the radial distribution functions $g_r(r/a)$ are shown for case (a) and case (b). Here we note that their shapes are still different from each other even at time $t = 1000$, except for $\phi = 0.460$.

In order to discuss the local order of the particles’ position, it is convenient to introduce the order parameter $P_m$ as the fraction of the total number of the particles which have $m$ nearest-neighbor particles. It is assumed that two particles whose distance $r$ is within $r_{\text{neib}} = 2.5a$ are the nearest-neighbor particles, where $g_r(r/a)$ has a strong first peak within $r_{\text{neib}}/a$ in the equilibrium state (see Figure 2). Especially, $P_{12}$ indicates the crystal order parameter in three dimensions [3].

Figure 3 shows the time dependence of the order parameters $P_{12}$.

In conclusion, our BD simulations demonstrate that even at higher volume fraction the suspension of hard spheres seem not to crystallize. We expect that this is mainly due to neglect of the hydrodynamic interactions between particles. We should then investigate it in more larger system for longer time.

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