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Shear-induced particle diffusion in inelastic hard sphere fluids

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A large-scale numerical simulation of a system of inelastic, rough, hard spheres of volume fraction $\phi_S = 0.565$, starting from a disordered configuration in a Couette geometry, shows a transition to a layered state, which possesses long-range orientation order, after long run times. This phase transition is shown to cause a dramatic decay of the long-time transverse self-diffusion coefficient of particles. As the solid volume fraction is increased to 0.58, the dimensionless transverse self-diffusion coefficient decays further, approaching a value of order 10^{-5}, which indicates structural arrest. [S1063-651X(98)50811-2]

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In a sheared granular flow, grains do not move along streamlines but instead exhibit fluctuating motions due to encounters with their neighboring grains. Hence, the grains within the assembly are continually losing information concerning their relative positions due to shearing. This loss of information characterizes the diffusive motion of the grains. Recently, computer simulations have been used to develop a better understanding of diffusion processes in unbounded dense granular shear flows [1]. This attempt led to a conjecture that a rapidly flowing monosized granular material is a diffusive system except at large solids concentrations. It was reported that at a volume fraction $\phi_c \approx 0.56$, the grains appeared to be trapped in a microstructure and prohibited from moving relative to their neighbors. This behavior, which characterizes a crystalline system, has not been observed in experiments of rapid granular flows between parallel rough boundaries [2]. In contrast, clear experiment evidence [2] exists for the movement of the particles in directions transverse to the bulk motion at even higher solid concentrations than those examined in the previous simulations [1].

Diffusion processes are of considerable importance in dense granular flows occurring in common industrial systems, for which the significance of interactions between the grains and the boundaries on the flow dynamics is obvious. Hence, it is important to examine whether a transition volume fraction, ϕ_c, exists for a confined dense granular flow of monosized particles. To this end, three-dimensional computer simulations of the flow of a system of dense, rough, inelastic, optically bidisperse hard spheres, with 4296 interior particles that are the same in terms of size and interaction, but have different colors, are carried out in a Couette geometry. Since a color label plays no role in the particle dynamics, the algorithm presented in a previous study [3] can be used to create the particles trajectories in a rectangular periodic computational box (with the lengths of the three sides of the box equal to $L_x = 1$, $L_y = 1$, and $L_z = 0.497$). The reader is referred there for more details, including a geometrical description of the problem. The walls are comprised of 400 hemispherical massive particles (with the same diameter as the interior particles) positioned at $Z = \pm L_z/2$, and no periodic boundary conditions are assumed in the directions normal to the walls.

In contrast to the previous simulations [1] in which the particles were initially organized in a triangular prismatic packing, the initial disordered hard-sphere configuration is created using the technique described by Clarke and Wiley [4]. For the present simulations, an initial set of random overlapping spheres is chosen. Then the individual spheres are moved randomly until the overlaps are removed. On one side of the labeling plane, $Z = 0$, the particles are dark in color, whereas on the other side the particles are light in color. The snapshot of the initial configuration of dark colored particles, projected onto the plane normal to the shear flow in the x direction (which is the yz plane in this work), is shown in Fig. 1(a).

A shear flow is applied to the aforementioned system of hard-dissipative spheres, by increasing average shear rate from zero to $\gamma = 2U/L_z \approx 4\ \mathrm{s}^{-1}$. Here U represents the velocity of one of the walls. Dissipation induced by particle-particle collisions is modeled using a coefficient of restitution, $e = 0.84$, as well as a surface friction coefficient, $\mu = 0.41$ [5]. The values of the dissipation parameters are chosen to be close to those used in the previous simulations [1].

For sufficiently long run times, the system eventually reaches an equilibration state in which the amount of energy supplied by shearing is balanced by that lost due to dissipative collisions as well as frictional interactions. In order to monitor the evolution of the system toward a state of equilibration, the instantaneous values of dimensionless normal stress exerted by the particles on the bottom wall [6] are recorded. The manner in which the dimensionless normal stress, P^*, of the aforementioned system varies with dimensionless time, $t^* = tU/L_z$, is illustrated in Fig. 2. The decay of the absolute value of mean dimensionless normal stress, $|\overline{P^*}|$, appears to be almost exponential for $t^* < 200$. There is, however, a significant decrease of $|\overline{P^*}|$ at about $t^* \approx 200$, which is clear evidence of a phase transition.

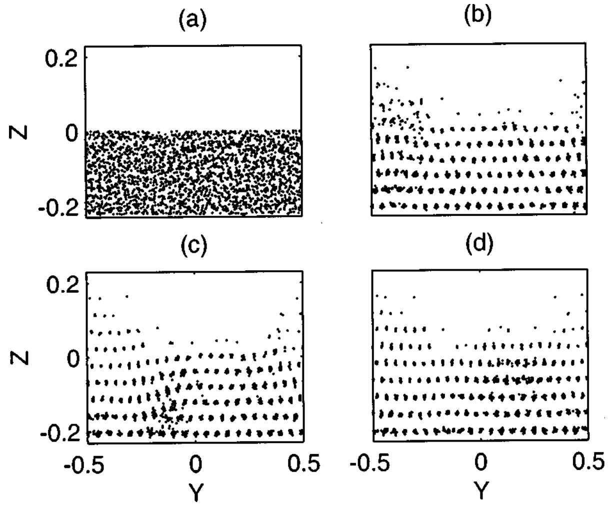

FIG. 1. (a) Snapshot of the initial configuration of dark colored particles in the computational box projected on the *yz* plane. (b) The configuration projected on the *yz* plane at $t^*\approx 55$. (c) The configuration at $t^*\approx 159$. (d) The final configuration at $t^*\approx 250$.

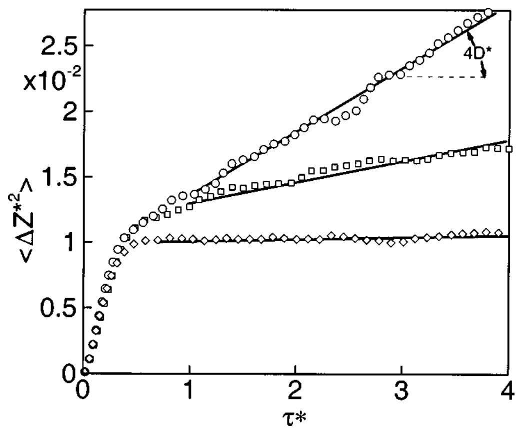

FIG. 3. Dimensionless square transversal displacement, $\langle \Delta Z^{*2}\rangle = \langle \Delta Z^2/(2R)^2\rangle$, as a function of dimensionless time, $\tau^* = \tau U/L_z$, for $L_z/(2R)\approx 10.25$. The circles, squares, and diamonds represent $\langle \Delta Z^{*2}\rangle$ at $t^*\approx 55$, 159, and 245, respectively. The solid lines are linear fits through the data for $\tau^*>1$.The dimensionless long time transverse self-diffusion coefficients for cases represented by the circles, squares, and diamonds are $D^* = D/[2(2R)^2 U/L_z]\approx 1.2\times 10^{-3}$, 4×10^{-4}, and 4×10^{-5}, respectively. The values of the dissipation parameters, solid volume fraction, and shear rate are found in Fig. 2.

Time evolution of lateral movements of dark colored particles, shown in Fig. 1, clearly indicate that at average shear rate $\overline{\gamma}\approx 4\ \mathrm{s}^{-1}$, a shearing, monosized granular flow of solid volume fraction $\phi_s = 0.565$, could be a diffusive system. This observation leads to the question whether the absence of particle diffusive motion in the unbounded rapid monosized granular flow simulations of Campbell [1] could be caused by remnants of the initial lattice configuration for spheres.

In attempting to quantify the diffusional movements of particles illustrated in Fig. 1, variations of the mean square displacement $\langle \Delta Z^{*2}\rangle = N^{-1}\Sigma_{i=1}^{N}\langle [Z_i^*(t^*+\tau^*) - Z_i^*(t^*)]^2\rangle$ with the argument $\tau^* = \tau U/L_z$ at different dimensionless time t^* are shown in Fig. 3. At long τ^*, deviation from the free diffusion regime [7] becomes apparent with $\langle \Delta Z^{*2}\rangle$ behaving almost linearly in τ^*. This indicates that the dynamics has reached a new diffusion regime for which the diffusion coefficient can be calculated using Einstein relation [8]. This property of the system, which is called the long-time transverse self-diffusion coefficient, reflects the cooperative effects of long-range spatial correlations. Here, $Z_i^*(t^*) = Z_i(t^*)/(2R)$represents the position of particle i in the z direction at dimensionless time t^*, which is normalized by the particle diameter, N is the number of particles in the computational box, t is time, τ^* shows that the samples are taken at time interval τ apart, and the angle brackets indicate the ensemble average. For the sake of brevity, further information concerning the particle diffusivity in the x and y directions will be given elsewhere.

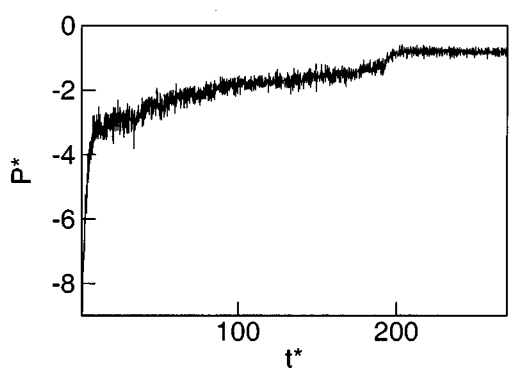

FIG. 2. Dimensionless normal stress, $P^* = P/[4\rho_p R^2(2U/L_z)^2]$, exerted by the particles on the bottom wall as a function of dimensionless time t^* at $\phi_s\approx 0.565$ for the coefficient of restitution $e=0.84$, the surface friction coefficient $\mu = 0.41$, and $\gamma = 4\ \mathrm{s}^{-1}$. Here, P represents the normal stress and ρ_p is the material density.

Considering variations of the dimensionless normal stress with dimensionless time, shown in Fig. 2, there is clear indication of an ordering phase transition at about $t^*\approx 200$. In an ordered system the changes of geometry of a cage formed by the nearest neighbors of a particle due to fluctuations become infrequent. This could result in a dramatic decay of the long-time transverse self-diffusion coefficient. Using the results given in Fig. 3, it can be readily shown that the dimensionless long-time transverse self-diffusion coefficient, $D^* = D/[(2R)^2 2U/L_z]$, decreases by an order of magnitude due to the phase change at $t^*\approx 200$.

At this point it would be desirable to have a knowledge of the instantaneous values of the dimensionless velocity component in the z direction, $V_z^* = V_z/U$. Following the approach proposed by Bakshi and Stephanopoulos [9] an approximate continuous function for V_z^* in terms of the Battle-Lemarie wavelets [10] is obtained using the simulations results. Figure 4 illustrates the contours of constant of V_z^*in the yz plane normal to the shear flow at $X^* = X/L_z = -0.28$and $t^*\approx 250$. Here, V_z is the velocity component in the z direction. The structure of velocity field, as shown in Fig. 4, indicates that clusters could exist in the computational box. However, further numerical work is required to provide a more realistic description of the movements of clusters in a rapidly flowing monosized granular material. It is worth mentioning that there is no periodic boundary conditions in the z-direction, therefore, V_z^* should be zero at $Z = \pm L_z/2$.

By examining the radial distribution function for the sample at $t^*\approx 250$, shown in Fig. 5, a peak at $r^* = r/R$

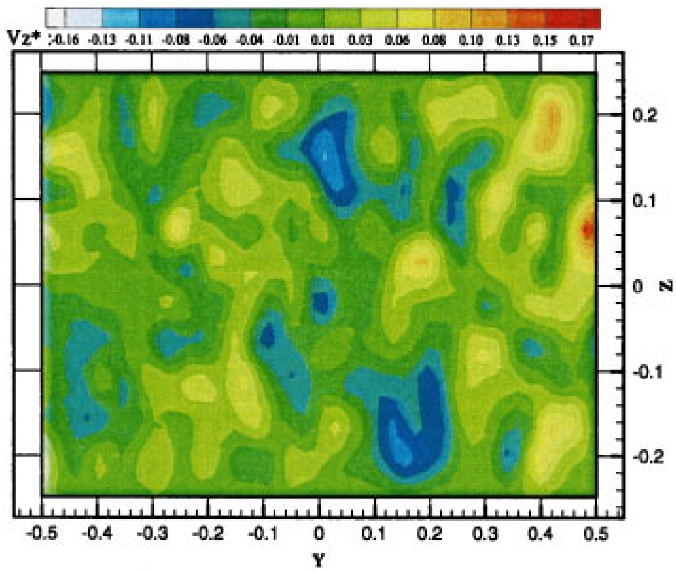

FIG. 4. (Color) Contours of constant dimensionless velocity component in the z direction, V_z^*, in the yz plane at $x^*=-0.28$ and $t^*=250$.

$\approx 2\sqrt{3}$ can be observed indicating the existence of ordered zone in the system. Here, R represents the particle radius. Therefore, it can be concluded that the initially disordered system has evolved to an ordered state in the presence of a shear flow. To clarify this further, the degree of translational order is tested by evaluating the translational order parameter, which is described by Fourier components ρ_k in the expansion of the mass density $\rho(\mathbf{r}_i)=\rho_0+\Sigma_k\rho_k\exp(j\mathbf{k}\cdot\mathbf{r}_i)$. Here, $\mathbf{k}$ is a reciprocal lattice vector and $\mathbf{r}_i$ is the position vector of the center of particle i. By choosing $\mathbf{k}=(2\pi/l)z$, it is found that ρ_k is 0.8 for $I=L_z/11$. This could be evidence of a layered state with only eleven layers. For $\mathbf{k}$ parallel to $-\mathbf{x}+\mathbf{y}-\mathbf{z}$ the value of ρ_k is found to be close to zero, indicating that the presence of the sliding fcc phase in the system can be ruled out. Here $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ represent unit vectors in the x, y, and z direction, respectively.

In the absence of cuboctahedral symmetry, an obvious question is whether a particle and its 12 nearest neighbors in the above-mentioned system prefer to adopt any orientational order. To answer this question a set of orientational order parameters [11], denoted by $Q_{lm}(\mathbf{R})\equiv Y_{lm}(\theta(\mathbf{R}),\phi(\mathbf{R}))$, is associated with each bond [12]. It is investigated whether their rotationally invariant combinations, $Q_l=[4\pi/(2l+1)\Sigma_{m=-1}^{l}|\overline{Q_{lm}}|^2]^{1/2}$, can ever become nonzero at $l=4$, 6, 8, and 10 for the final configuration at $t^*\approx 250$. Here, $\mathbf{R}$ represents the position of the bond midpoint, $Y_{lm}[\theta(\mathbf{R}),\phi\mathbf{R})]$ are spherical harmonics, $\theta(\mathbf{R})$ and $\phi(\mathbf{R})$ are the polar angles of the bond measured with respect to a fixed reference coordinate system, and the averaged quantity, $\overline{Q_{lm}}\equiv\langle Q_{lm}(\mathbf{R})\rangle$, is taken over the bonds joining particles in the sample with their near neighbors.

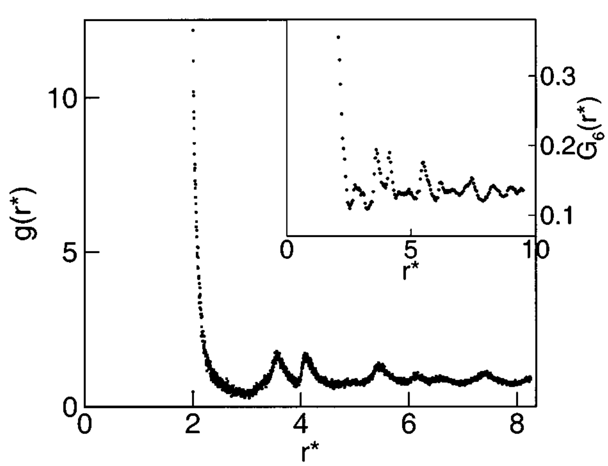

FIG. 5. Radial distribution function for the sample at $t^*\approx 250$. Inset: The bond-angle correlation function, $\overline{G}_6(r^*)$, vs dimensionless distances $r^*=r/R$ for the sample at $t^*\approx 250$.

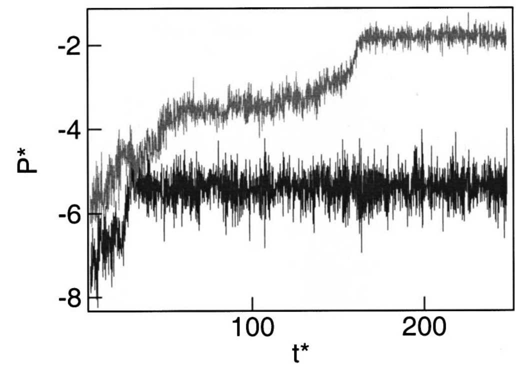

FIG. 6. Dimensionless normal stresses, $P^*=P/[4\rho_pR^2(2U/L_z)^2]$, exerted by the particles on the bottom wall as a function of dimensionless time t^* for the coefficient of restitution $e=0.93$, the surface friction coefficient $\mu=0.123$, and $\overline{\gamma}=4\ \mathrm{s}^{-1}$. Upper and lower curves represent the wall stresses at solid volume fractions $\phi_s\approx 0.565$, and $\phi_s\approx 0.582$, respectively.

It is found that the signal at $l=6$ is strong ($Q_6\approx 0.4$) suggesting extended correlations in the orientations of bonds, possibly with an icosahedral symmetry. However, the size of the $Q_8\approx 0.24$ suggests the symmetry of the bond-oriented states is not perfectly icosahedral and some cubic order may be present. This would be consistent with the presence of several icosahedral clusters in the sample. This may support the aforementioned conjecture concerning the presence of clusters in the sample. In this light, at a moderate average shear rate, a system of inelastic, rough, hard spheres of solid volume fraction $\phi_s=0.565$ could exhibit behavior similar to a layered icosahedrally oriented liquid.

More information regarding possible types of orientational order of the above-mentioned system can be obtained from the bond-angle correlation functions $\overline{G}_l$ [13]. Considering the value of $G_6(r^*)$ at large r^*, shown in Fig. 5, it can be concluded that the system behaves similar to an icosahedrally oriented liquid, possessing a degree of symmetry intermediate between those of a crystal and a liquid.

The amplitude of fluctuations in the wall stress at $t^*>200$, shown in Fig. 2, is much smaller than that recorded in the tests of Savage and Sayed [14]. The gray colored curve in Fig. 6 illustrates that stronger fluctuations in the wall stress are obtained as compared to those in the previous case, shown in Fig. 2, by increasing the coefficient of restitution to $e=0.93$, and decreasing the surface friction coefficient to $\mu=0.123$. The fluctuations appear to be closer to those in the annular shear cell tests of Savage and Sayed [14]. Higher fluctuations resulting from lower dissipations of the system, leads to an increase in the transverse self-diffusion coefficients, as shown in Fig. 7. However, the results obtained are

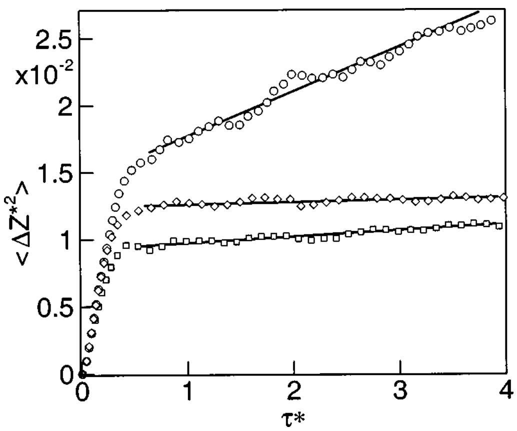

FIG. 7. Variations of $\langle \Delta Z^{*2} \rangle$ with the dimensionless time τ^*. The circles, squares, represent $\langle \Delta Z^{*2} \rangle$ at the solid volume fraction of $\phi_s \approx 0.565$ at $t^* \approx 159$, and 245, respectively, whereas the diamonds represent $\langle \Delta Z^{*2} \rangle$ at the solid volume fraction of $\phi_s \approx 0.582$ at $t^* \approx 200$. The solid lines are linear fits through the data for $\tau^* > 1$. The calculated value of D^* for the cases represented by the circles, squares, and diamonds are 8 $\times 10^{-4}$, 10^{-4}, and 10^{-5}, respectively. The values of the dissipation parameters and the shear rate are found in Fig. 6.

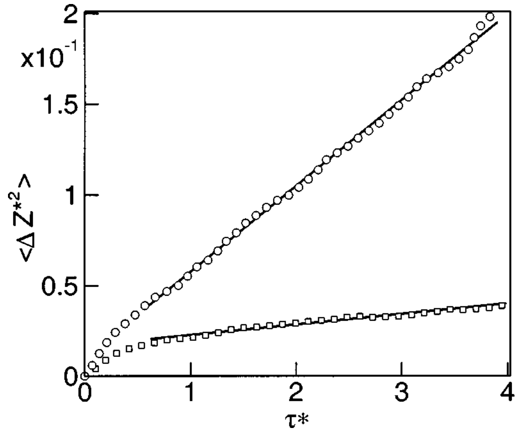

FIG. 8. Variations of $\langle \Delta Z^{*2} \rangle$ with the dimensionless time τ^*. The circles represent $\langle \Delta Z^{*2} \rangle$ of the system comprised of smooth, inelastic particles with the coefficient of restitution $e = 0.93$, whereas the squares represent that of the rough, inelastic particles with the dissipation parameters $\mu = 0.123$ and $e = 0.93$. The calculated values of D^* for the cases represented by the circles and squares are 1.2×10^{-2} and 1.5×10^{-3}, respectively.

much smaller than those measured by Natarajan, Hunt, and Taylor [2] in gravity-driven channel flows of granular materials.

In order to further examine the effect of particle roughness on the diffusivity, variations of the mean square displacement $\langle \Delta Z^{*2} \rangle$ with τ^* for systems of smooth and rough particles at solid volume fraction of $\phi_s \approx 0.565$, are plotted in Fig. 8. The samples are taken at $t^* \approx 40$ which is close to the average dimensionless residence time of particles in experiments of Hunt and co-workers [2]. The calculated dimensionless long-time transverse self-diffusion coefficient for the system comprised of smooth particles is $D^* \approx 1.2 \times 10^{-2}$, which is an order of magnitude higher than that for the system of rough particles. The above-mentioned value for the system of smooth particles is close to those measured by Natarajan, Hunt, and Taylor at moderate shear rates. This observation supports Menon and Durian [15] statement that the dynamics of grains in a dense granular flow are dominated by collisions rather than sliding contact.

It should be noted that at the higher solid volume fraction of $\phi_s \approx 0.582$, the transition time to an ordered state is quite short for a system of rough particles, as shown in Fig. 7. Moreover, the dimensionless long time transverse self-diffusion coefficient approaches to a value of $D^* \approx 10^{-5}$ indicating a nearly frozen structure.

In summary, simulations of a system of sheared, dense, monosized granular material indicate that the system could be diffusive at solid volume factions even higher than 0.56. In fact, it is shown that the calculated dimensionless transverse long-time self-diffusion coefficient for a dense system ($\phi_s \approx 0.565$) comprised of smooth particles is close to that previously reported for a dense gravity-driven channel flow in which the average residence time of particles was rather short. However, at long run times, a phase transition is seen to occur for systems of rough particles, which causes a sharp drop in the transverse long-time self-diffusion coefficient of the particles. The system is found to behave like an icosahedrally oriented liquid. Evidence also exists for the occurrence of clustering, which will be examined more critically in a future study.

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