Bond-orientational order in sheared dense flows of inelastic hard spheres

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Three-dimensional bond-orientational order is studied using computer simulations with 4296 hard, monodisperse inelastic spheres flowing in a Couette geometry at a high shear rate. At an average volume fraction close to 0.6, a state with extended correlations in the orientations of particle clusters starts to develop for rough particles after sufficiently long run times. However, no clear evidence of crystallization is found in the system. Further tests of a sheared system comprised of smooth, inelastic spheres reveal crystallization consistent with the previous experimental observations. © *1998 American Institute of Physics.* [S0003-6951(98)00730-X]

Recent experimental findings for dense granular flows[1] support the speculation that in such systems both friction and collisional–translational interactions[2] between grains play significant roles. However, based on the conflicting evidence reported by Menon and Durian,[3] models based on only simple, inelastic collisions[4] could be appropriate for the study of the dynamics of granular media at high solid concentrations. In fact, the measurements[3] using diffusing-wave spectroscopy revealed that the hydrodynamics of grains were dominated by inelastic collisions rather than sliding contacts in the intermediate regime.[1] Moreover, in contrast to the observed crystallization in computer simulations,[5] the arrangement of the beads in the system of Menon and Durian[3] showed no evidence of density inhomogeneities or crystalline packing. In this light, the physical relevance of the observed nondiffusive behavior of a granular fluid at high concentrations[5] remains a topic of controversy.

The motivation for this work is, therefore, to devise computer experiments to explore the fundamental questions pertaining to the formation of long-range orientational order in complex systems[6] such as dense granular flows. To this end, shear-induced structural changes are investigated in a system, comprised of 4296 inelastic hard spheres, having an average volume fraction of $\bar{\phi}_s \approx 0.6$ in a Couette geometry as shown in Fig. 1. The initial random configuration of particles is obtained using the technique proposed by Clarke and Wiley.[7] Previous observations of a similar system at a lower density[8] revealed that the crystallization process may be initiated at a layer adjacent to the walls where a regular pattern, such as those employed by Natarajan, Hunt, and Taylor,[1] is used. Since crystallization due to boundaries is not of interest in the present study, the use of regular boundaries is avoided.

The classical algorithm of Alder[9] is used to create hard-sphere trajectories in a periodic box shown in Fig. 1. The algorithm is slightly modified to introduce dissipation in instantaneous binary collisions between neighboring particles through a coefficient of restitution e, as well as a surface friction coefficient, μ. There are, however, no periodic boundary conditions in the directions normal to the walls.

Using the values of the coefficient of restitution and the surface friction coefficient suggested by Drake[10] for cellulose acetate spheres in a glass-walled chute, it has been observed that the contact value of the radial distribution function increases dramatically and the shearing motion ceases after only a very short run time. The observations by Natarajan, Hunt, and Taylor[1] at an average concentration close to that of the present study are not consistent with the above-mentioned behavior. Therefore, the use of high values for the surface friction coefficient,[5] namely $\mu = 0.5$, to model particle dissipation in a sheared granular flow is questionable. This observation supports the point by Menon and Durian[3] that the hydrodynamics of grains are dominated by inelastic collisions rather than sliding contacts even in dense slow flows. In order to reduce dissipation, while still taking into account the effects caused by surface roughness, the simulations are carried out using the idealized sticking–sliding collision model of Lun and Bent[11] with the following collision

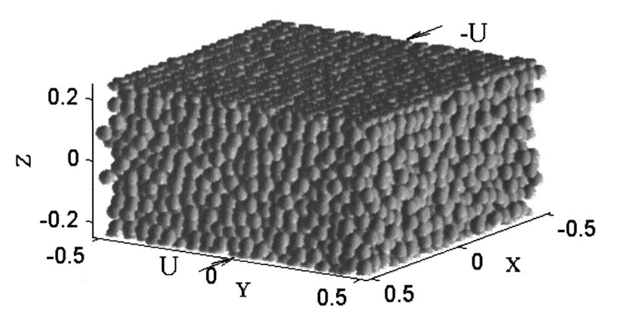

FIG. 1. Sketch of the periodic cell for the dense Couette flow of monodisperse spheres. The hemispheres of the top and bottom walls move at average velocity U in opposite directions along the x direction.

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