Shear Instabilities in Granular Mixtures

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Dynamical instabilities in fluid mechanics are responsible for a variety of important common phenomena, such as waves on the sea surface or Taylor vortices in Couette flow. In granular media dynamical instabilities have just begun to be discovered. Here we show by means of molecular dynamics simulation the existence of a new dynamical instability of a granular mixture under oscillating horizontal shear, which leads to the formation of a striped pattern where the components are segregated. We investigate the properties of such a Kelvin-Helmholtz-like instability and show how it is connected to pattern formation in granular flow and segregation.

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A simple example of instabilities in fluid mechanics is the Kelvin-Helmholtz instability where a flat interface between two fluids flowing one past the other at different velocities is unstable, explaining, for instance, why waves on the sea surface form [1,2]. In athermal systems such as granular mixtures, where a hydrodynamiclike theory is not yet well established, the discovery of instabilities is a recent achievement [3–6]. By studying the evolution of two bands of different grains placed on a horizontally oscillating tray [see Fig. 1(a)], we discover a new dynamical instability. The instability appears as a growing wavy interface, which, at long times, leads to a pattern of alternating segregated stripes of grains, perpendicular to the driving direction. We suggest that this type of surface shear instability is the common mechanism for apparently different phenomena such as wave formation found in experiments on granular flow [6] and segregation processes [7] as observed in [8–11], initially explained in terms of a thermodynamic driven phase separation. In our simulations we determine the region of existence of the pattern formation–segregation process as a function of the area fractions of large and small grains, and we discuss the dependence of the pattern as a function of the amplitude and frequency of oscillation.

MD simulation model.—We perform molecular dynamics (MD) simulations (also known as discrete element methods) of a binary system of disks which lay on a tray (i.e., in two dimensions) with periodic boundary conditions in the x direction and hard walls in the other. Grains interact with the tray by a viscous force proportional to their relative velocity via a viscosity parameter μ different for the two species; when overlapping, grains interact via 2D Hertzian contact forces [12]. The simulations' details and parameters are chosen to model experimental conditions similar to those investigated by Mullin and coworkers [8,9,11,13].

Two grains with diameters D_i and D_j in positions $\mathbf{r}_i$ and $\mathbf{r}_j$ interact if overlapping, i.e., if $\delta_{ij} = [(D_i + D_j)/2 - |\mathbf{r}_i - \mathbf{r}_j|] > 0$. The interaction is given by a normal Hertz force with viscous dissipation [14,15]. In 2D this reduces to the linear spring-dashpot model, $\mathbf{f}_n = k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_n m_{\text{red}} \mathbf{v}_{nij}$, where k_n and γ_n are the elastic and viscoelastic constants, and $m_{\text{red}} = m_i m_j/(m_i + m_j)$ is the reduced mass. As in [13] we model the interaction with the tray via a viscous force $\mathbf{f}_t = -\mu(\mathbf{v} - \mathbf{v}_{\text{tray}})$, where $\mathbf{v}_{\text{tray}}(t) = 2\pi A \nu \sin(\nu t)\mathbf{x}$ is the velocity of the tray and $\mathbf{v}$ the velocity of the disk, plus a white noise force $\xi(t)$ with $\langle \xi(t)\xi(t') \rangle = 2\Gamma\delta(t - t')$, where $\Gamma = 0.2\ \text{g}^2\,\text{cm}^2\,\text{s}^{-3}$. The interaction between particles and walls is elastic. We solve the equations of motion by the Verlet algorithm with a time step of 6 μs. For the grain-grain interaction, we use the value $k_n = 2 \times 10^5\ \text{g}\,\text{cm}^2\,\text{s}^{-2}$ and γ_n chosen, for each kind of grains, such that the restitution coefficient is given: $e = 0.8$ [14]. The two components of our mixture (named b and s) have viscous coefficients $\mu_b = 0.28\ \text{g}\,\text{s}^{-1}$ and $\mu_s = 0.34\ \text{g}\,\text{s}^{-1}$. Apart from a simple rescaling of masses and lengths, these values are those of Ref. [13] (and have been given in private communications), and are taken from direct measurements on the experimental system in [8]. The size of the tray is $L_x = 320$ cm, $L_y = 16$ cm. The qualitative picture we discuss does not change if these values are changed.

Results.—We consider now a mixture of heavy grains, of mass $M_b = 1$ g and area fraction $\phi_b = 0.37$, and light grains, with $M_s = 0.03$ g and $\phi_s = 0.41$, all with the same diameter $D = 1$ cm, prepared in a horizontally fully segregated configuration [Fig. 1(a)]. The mixture is vibrated on a horizontal tray along the x direction with amplitude A and frequency ν. The characteristic time scale, $\tau_b = M_b/\mu_b$ and $\tau_s = M_s/\mu_s$, is different for the two species, and they are forced to oscillate with different amplitudes and phases, subject to an effective surface shear periodically varying in time. One may expect configurations in which the two different components form two stripes parallel to the driving direction [see Fig. 1(a)] to be stable, the two stripes oscillating independently with different amplitudes and phases. Instead, the initially flat interface between the two components is observed to

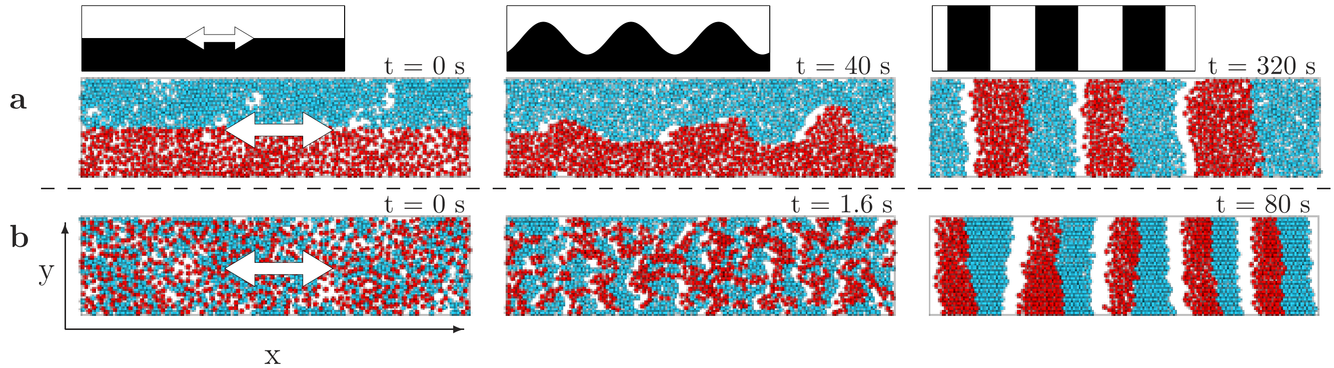

FIG. 1 (color online). Evolution of a binary mixture of heavy (red–dark gray) and light (blue–light gray) grains on a horizontal tray oscillating along the x direction with amplitude $A = 1.2$ cm and frequency $\nu = 12$ Hz (only a quarter of the system length is shown in each figure). (a) The system is initially prepared in a horizontally segregated configuration with a flat interface between the two species. Under shaking it develops a surface instability with a sinelike modulation of growing amplitude leading at long times to a state where segregated stripes perpendicular to the driving direction appear. The upper small panels show the corresponding evolution of the surface instability model Eqs. (1) in the presence of an oscillating shear $\Delta v(t) = 2\pi A\nu \sin(2\pi\nu t)$. (b) The same system is now initially prepared in a mixed state and then shaken. The formation of local fluctuations of the density of the two species (shown at $t = 1.6$ s) leads to microsurfaces generating the same instability mechanism as in (a).

evolve via the formation of a surface modulation which has a growing amplitude. Finally, this leads to a state where segregated stripes appear, perpendicular to the driving direction (at variance with known results in colloidal fluids [16]). This instability appears to be of the same kind as that observed in two fluid systems and in liquid-sand systems subject to horizontal oscillations under gravity, which is responsible for the ripples observed on the shoreline [17]. In these cases, however, because of gravity there is an energy cost associated with the growth of the interface, which therefore gets stabilized.

When the system starts from a disordered initial state, as shown in Fig. 1(b), the instability develops too. The formation of local fluctuations of the density of the two species creates microsurfaces which are forced to evolve according to the instability shown in Fig. 1(a). For instance, Fig. 1(b), at $t = 1.6$ s, shows the existence of clusters of particles of the same species elongated perpendicularly to the driving direction. As time goes on, these clusters merge, giving rise to the striped pattern of Fig. 1(b) ($t = 80$ s). It is apparent that the originally disordered system is ordered, i.e., segregated, by the dynamic instability. Figures 1(a) ($t = 320$ s) and 1(b) ($t = 80$ s) show that the wavelength of the final steady state depends on the initial conditions.

The segregation process shown in Fig. 1(a) reproduces that observed experimentally in [8,11]. In the present setup the grains' radii are equal, no "depletion" forces can be at work, and no "thermodynamic" coarsening phenomena can be considered responsible for this segregation process, as initially conjectured [11] by making an analogy with colloidal systems. Such a remark appears to be consistent with a scenario proposed by the use of modified Navier-Stokes equations [18]. Interestingly, segregation from a disordered initial state to a final striped one has also been observed in a two fluid system oscillated in the absence of gravity [19].

The above dynamical instabilities should manifest in the mixture also under different shearing protocols. To check this, we study now a different configuration where gravity induces granular flow, and thus a differential shear on the mixture components appears. The tray no longer oscillates, but it is inclined at an angle θ with respect to the horizontal by rotation around the y axis. The two species of grains attain different limit velocities (of the order of $v_b \simeq g\tau_b \sin\theta$ and $v_s \simeq g\tau_s \sin\theta$, with g the gravitational acceleration) and thus experience a differential shear. As shown in Fig. 2, under these conditions the initially flat interface between the mixture components changes also via Kelvin-Helmholtz-like instabilities. An unstable pattern forms and curl-like structures appear. This phenomenon, induced by surface dynamical instabilities, is very similar to those recently discovered in experiments on granular flows [6].

The results of Figs. 1 and 2 point out the essential role of shear induced surface instabilities in pattern formation and the connections with segregation transitions. Even though this is not a usual fluid, the complex nature of this phenomenon can be understood via schematic hydrodynamic-like considerations. On the two sides of the perturbed interface, flux lines are narrowed and widened as the pressure is, respectively, lowered and increased (Bernoulli law). The pressure gradient reinforces the perturbation of the interface, giving rise to positive feedback. Within such a perspective, the essential features of pattern formation observed in the two experiments of Figs. 1 and 2 are captured by a model originally proposed for the Kelvin-Helmholtz instability of granular flows [6]. The model describes the evolution of the velocity components, v_X and v_Y, of the system interface initially located at $Y(X) = 0$:

$$v_X = \Delta v(t) \tanh(Y), \qquad v_Y = c \sin(k_X X), \qquad (1)$$

where $\Delta v(t)$ is the relative bulk velocity between grains far on the two sides of the interface at time t, as k_X and c are

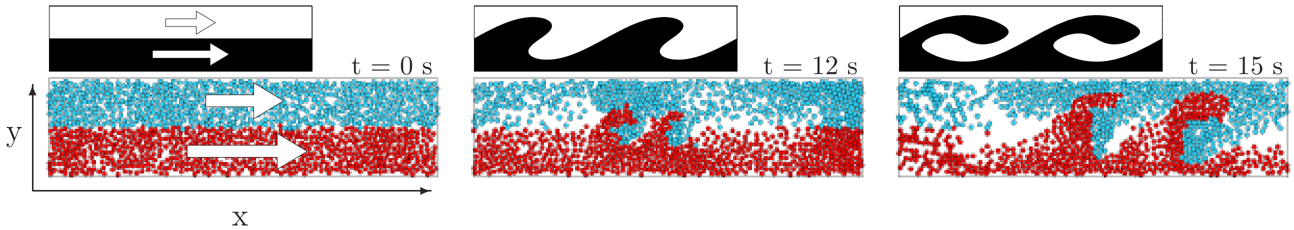

FIG. 2 (color online). Evolving interface in the same granular mixture as Fig. 1(a) flowing down a tray rotated at an angle $\theta = 12^\circ$ with respect to the horizontal around the y axis. The red (dark gray) grains are faster that the blue (light gray) ones. The upper small panels show the evolution, at corresponding times, of a Kelvin-Helmholtz-like surface dynamical instability modeled by Eqs. (1) in the presence of a constant shear $\Delta v(t) = \Delta v_0$, reproducing a pattern qualitatively similar to the one found in the main panels.

constant parameters (we consider the same values used in [6], i.e., $k_X = 5$, $c = 0.1$, but our results are robust to changes). The presence of a velocity gradient, $\Delta v(t)$, independent from its microscopic origin (different grains friction, different driving of the components, etc.), enhances shear and results in pattern formation. In the case of gravity induced deformations, $\Delta v(t) = \Delta v_0 \equiv v_b - v_s$ can be considered to be time independent since in the stationary regime the two limit velocities are given. In such a case, the model essentially coincides with the one introduced in [6] and describes well the qualitative features of the MD simulations of Fig. 2 (see upper panels). In the case of the vibrated horizontal tray, the relative bulk velocity is oscillating in time, and we fix $\Delta v(t) = 2\pi A\nu \sin(2\pi\nu t)$. This gives rise (see upper panels in Fig. 1(a)] to a growing interface with features very close to those observed in the simulations.

Pattern formation.—We show now under which conditions pattern formations occur and explain how the properties of the final state of the mixture, such as the emerging characteristic length scale of the stripes, λ, depend on both the dynamics control parameters and the relative concentration of the two components. This gives rise to a complex mixing or segregation diagram which we discuss in detail here for the case of the horizontally vibrated experiment. In order to make direct comparisons with experimental results on segregation observed by Mullin and co-workers [8,9,11,13], we consider now a binary mixture of large monodisperse disks, of diameter $D_b = 1$ cm, covering an area fraction ϕ_b, and small polydisperse disks [20], with average diameter $D_s = 0.7$ cm (with 17% polydispersity) and area fraction ϕ_s. Masses and frictional parameters are as given before.

The system starts from a mixed initial configuration as in Fig. 1(b). The nature of the state reached by the system under shaking at a late stage is crucially dependent on the area fraction of the two species: segregation in stripes is found only for high enough concentrations. This behavior, in the (ϕ_b, ϕ_s) plane, is summarized in the diagram of Fig. 3(a) showing the system "fluid" and "crystal" regions along with their segregation properties, for $\nu = 12$ Hz and $A = 1.2$ cm. Large grains are considered to be in a fluid configuration when their radial density distribution function, $g(r)$, shows a first peak at $r = D_b$ and a second one at $r = 2D_b$, and to be in a crystal configuration when a new peak at $r = \sqrt{3}D_b$ appears [11]. The system is in a "glassy" state [21] when on the longest of our observation time scales, the system is still far from stationarity.

Figure 3(a) shows that grains at small concentrations are mixed and in a fluid state. Segregation via stripes formation appears at higher concentrations. At even higher concentrations, large grains form stripes with a crystalline order, as smaller grains are always fluid for their polydispersity.

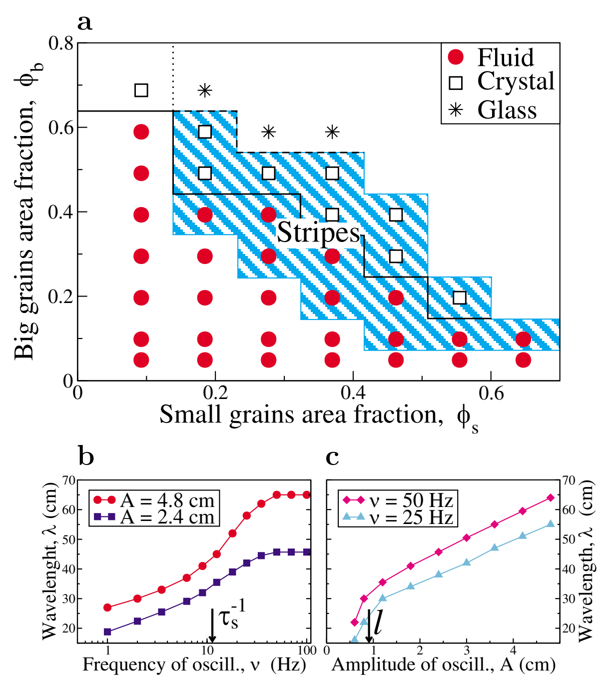

FIG. 3 (color online). (a) Ordering properties of the late stage configurations of the mixture as a function of the area fractions of the two components. The *shaded area* covers the region where segregation via stripes formation occurs. Circles, large grains are in a fluid state. Squares, large grains form a crystal. Stars, the system appears blocked in a glassy disordered configuration (see text). When stripes form their characteristic length scale, λ is a function of the frequency, ν, and of the amplitude, A, of the driving oscillations. This is shown, in the case $\phi_b = 0.30$ and $\phi_s = 0.28$, in (b) and (c).

Finally, at very high area fractions, the system is blocked in its starting disordered configuration (glassy region). For instance, by increasing ϕ_s at a fixed value of ϕ_b (say, $\phi_b \simeq 0.174$), we observe first a transition from a mixed fluid state to a segregated striped fluid and then a transition where the monodisperse phase crystallizes. The experiments of [11], where $\phi_b \simeq 0.174$, show the very same transitions found here at locations differing by 10%.

In the case $\phi_b = 0.30$ and $\phi_s = 0.28$, where stripes form, we describe their dependence on the dynamics control parameters in Figs. 3(b) and 3(c), showing that the length scale, λ, increases as a function of the shaking frequency, ν, and of the amplitude A. These results are to be compared, for instance, with those found in liquid-sand mixtures under oscillating flow, where ripples form with a wavelength depending on the amplitude of oscillation, but not on its frequency [22]. The dependence on ν can be schematically understood by comparison with the characteristic time scales $\tau_b = M_b/\mu_b$ and $\tau_s = M_s/\mu_s$ of the two species (here $\tau_b^{-1} = 0.28$ Hz and $\tau_s^{-1} = 11.3$ Hz): no sensitivity to ν is expected both when $\nu \gg \tau_b^{-1}, \tau_s^{-1}$, as grains remain almost at rest, and when $\nu \ll \tau_s^{-1}$, as grains oscillate with the tray. Analogously, the dependence on A is expected to be substantial when A is at least of the order of the mean grains separation length, $l = (4\phi_b/\pi D_b^2 + 4\phi_s/\pi D_s^2)^{-1/2}$, since under this condition grains strongly interact.

In conclusion, our simulations of a binary mixture under horizontal vibrations have revealed the existence of a new dynamical instability and shed light on the process of size segregation under oscillatory shear and its connections to pattern formation in granular flows. Within such a unifying framework, we derived the "phase diagram" of the mixing or segregation states of the mixture and its corresponding transitions. Finally, such hydrodynamiclike processes appear to be related to those known in thermal fluids and fluid-grain systems, ranging from Kelvin-Helmholtz instabilities to ripple formation in liquid-sand mixtures, even though interesting difference are found.

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