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Shear-induced segregation of a granular mixture under horizontal oscillation

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Abstract

We study the segregation process of a granular mixture of discs on an horizontally oscillating tray by realistic molecular dynamics simulations. As found in the experiments, we observe the initially disordered mixture to segregate via the formation of stripes perpendicular to the driving direction. The segregation process turns out to be the result of a dynamical instability very similar to the Kelvin–Helmholtz instability observed in fluid mechanics, and it is not due to the depletion potential, i.e., to the effective potential existing between two big particles in a bath of smaller ones, but rather to a dynamical process whose nature is discussed.

Introduction

A granular medium consisting of a collection of dry, cohesionless, identical particles exhibits a wide range of complex behaviours. Despite the simplicity of the constituent particles no reliable mathematical models exist for most of these collective phenomena. Of particular interest is the counterintuitive phenomenon of species segregation [1]. When subject to an external perturbation, such as vertical or horizontal oscillations, an initially disordered binary mixture of grains (which may differ in size, mass, frictional properties) often segregates into its components. Depending on the driving conditions, different mechanisms, such as percolation [2–4], inertia [5], convection [6], or even purely thermodynamical effects [7], have been shown to be responsible for the segregation process. Here we try to shed light on the phenomenon of species segregation of a binary mixture under horizontal shaking, which has been experimentally investigated by Mullin and co-workers [8–11], and recently further analysed in [12, 13]. In the experiments, a disordered monolayer of a binary mixture of grains of different properties, placed on a horizontal oscillating plate, is observed to evolve via the formation of alternating stripes of grains of different type perpendicular to the driving direction. The mechanism responsible for such a segregation process is still unclear. We investigate this phenomenon by means of soft-core molecular dynamics simulations (also known as discrete element methods) of a mixture of discs which lie on a oscillating tray (i.e., in two dimensions) with periodic boundary conditions in the x-direction (the oscillating direction) and hard walls in the other. The 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 [14]. The simulations parameters are chosen to model experimental conditions similar to those investigated by Mullin and coworkers [8–11].

We show that the segregation process is due to a dynamical instability of the interface between grains of different type, not to a thermodynamic process related to the depletion force as conjectured in the earliest works [8, 9]. As far as we know, this is the first time that a dynamical instability is shown to be responsible for the segregation of a granular mixture, and that a clear connection between segregation, pattern formation and dynamical instabilities is established. Our results call both for an experimental validation and for an analysis of stability type via continuum equations for granular mixtures.

The paper is organized as follows. Section 1 describes the numerical methods used to model the system. Section 2 shows how the segregation process depends on the area fraction of the two species, and on the parameters governing the dynamics. Here it is also shown that the depletion force is not big enough to play a crucial role on the dynamics of the system. Section 3 describes the dynamics of a mixture when the initial state is made of two stripes of grains of different type parallel to the driving direction, making clear the dynamical instability that appears to be responsible for the segregation process. Finally, some conclusions are drawn.

1. Numerical methods

We perform soft-core molecular dynamics simulations of a two-dimensional granular media taking into account grain–grain and grain–tray interactions [14]. 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 [15, 16]. In two dimensions this reduces to the linear spring-dashpot model,

$$\mathbf{f}_n = k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_n m_{\mathrm{eff}} \mathbf{v}_{nij}, \tag{1}$$

where k_n and γ_n are the elastic and viscoelastic constants, and $m_{\mathrm{eff}} = m_i m_j/(m_i + m_j)$ is the effective mass. We follow the realistic simulations of [14, 11] and model the interaction with the tray via a viscous force

$$\mathbf{f}_{\mathrm{t}} = -\mu_i (\mathbf{v}_i - \mathbf{v}_{\mathrm{tray}}), \tag{2}$$

where $\mathbf{v}_{\mathrm{tray}}(t) = 2\pi A\nu \sin(\nu t)\mathbf{x}$ is the velocity of the tray and $\mathbf{v}_i$ the velocity of the disc i, plus a white noise force $\boldsymbol{\xi}(t)$ with

$$\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t')\rangle = 2\Gamma\delta(t - t'). \tag{3}$$

We solve the equations of motion by a Verlet algorithm with an integration time-step of 6 μs. For the grain–grain interaction, we use the value $k_n = 2 \times 10^5$ g cm^2 s^{-2} and γ_n chosen, for each kind of grains, such that the restitution coefficient is given: $e = 0.8$ [16]. The two components of our mixture have mass $M_{\mathrm{b}} = 1$ g and $M_{\mathrm{s}} = 0.03$ g, and viscous coefficient $\mu_{\mathrm{b}} = 0.28$ g s^{-1} and $\mu_{\mathrm{s}} = 0.34$ g s^{-1}. The white noise has $\Gamma = 0.2$ g^2 cm^2 s^{-3}. Apart from a simple rescaling of masses and lengths, these values are those of [11] (and given in private communications), and are taken from direct measurements on the experimental system. The heavier grains of our mixture have diameter $D_{\mathrm{b}} = 1$ cm. We consider the lighter grain diameter D_{s} first to be Gaussian distributed with mean value 0.7 cm and 17% polydispersity, and then to be $D_s = D_b = 1$ cm. We use a tray of width $L_y = 20$ cm and length $L_x = 40$ cm or $L_x = 320$ cm. Our simulations refer to oscillations with amplitude $A = 1.2$ cm and frequency $\nu = 12$ Hz. The qualitative picture we discuss does not change if these values are changed; the dependence of our results on the values of some of these parameters is investigated in the next section and in [17].

2. Segregation under horizontal oscillation

The equation of motion for the horizontal coordinate x of a single grain placed on a tray oscillating with amplitude A and frequency ν along the x-direction is

$$M\ddot{x} = -\mu(\dot{x} - v_{\text{tray}}(t)), \tag{4}$$

where M is the mass of the grain, μ the coefficient of friction (of viscous type) between the tray and the grain, and $v_{\text{tray}}(t) = A\nu \sin(\nu t)$ is the tray velocity. The solution of this equation is

$$x(t) = -\frac{A}{1 + \tau^2\nu^2}[\cos(\nu t) + \tau\nu \sin(\nu t)], \tag{5}$$

with $\tau = M/\mu$. In our system the two species, having different relaxation times $\tau_b = M_b/\mu_b = 3.57$ s and $\tau_s = M_s/\mu_s = 0.09$ s, are thus forced to oscillate with different amplitudes and different phases. When N_s small grains and N_b large grains occupy an area fraction $\Phi = \Phi_s + \Phi_b$ sufficiently high, where

$$\Phi_s = N_s \frac{\pi}{4L_x L_y}\overline{D_s^2}, \qquad \Phi_b = N_b \frac{\pi}{4L_x L_y} D_b^2, \tag{6}$$

and $\overline{D_s^2}$ is the mean value of the square of small grains diameter, grains of different type are not free to oscillate following equation (5), and they collide frequently. Consequently, the properties of the stationary state reached by the granular mixture under the oscillatory shaking dynamics depend on the area fraction Φ_b and Φ_s of the two species. This is illustrated in figure 1. Schematically, we can summarize the different stationary states reached by the system as follows:

M *Mixed*. At small area fractions the two species are mixed.

LS *Liquid stripes*. At higher area fractions the system segregates via the formation of stripes of particles of different species perpendicular to the driving direction. Each stripe appears to be in a liquid-like state.

CS *Crystalline stripes*. At further higher area fraction segregation via stripe formation is observed too, but stripes of big discs crystallize. Stripes of smaller discs never crystallize because of their polydispersity.

G *Glass*. At very high area fractions, as in the case $(\Phi_s, \Phi_b) = (0.18, 0.7)$, the system appears to be locked in a disordered state, which we call 'glass'.

The distinction between the phases LS and CS is made by the radial distribution function $g(r)$ of big discs [18, 17]. In the LS state the radial distribution function has a maximum at $r = D_s$ and a second maximum at $r = 2D_s$. In the CS state a new maximum at $r = \sqrt{3}D_s$ appears. We want to stress that transitions M $\rightarrow$ LS and LS $\rightarrow$ CS occur at different values of the area fraction, as experimentally observed [8, 9].

The observed transitions have been originally attributed to the depletion potential [9], a form of interaction well known in colloidal systems [19]. Two big spheres immersed in bath of smaller ones are subject to an effective potential, due to an entropical effect (the clustering of big spheres increases the free space available to the smaller ones, and consequently the entropy

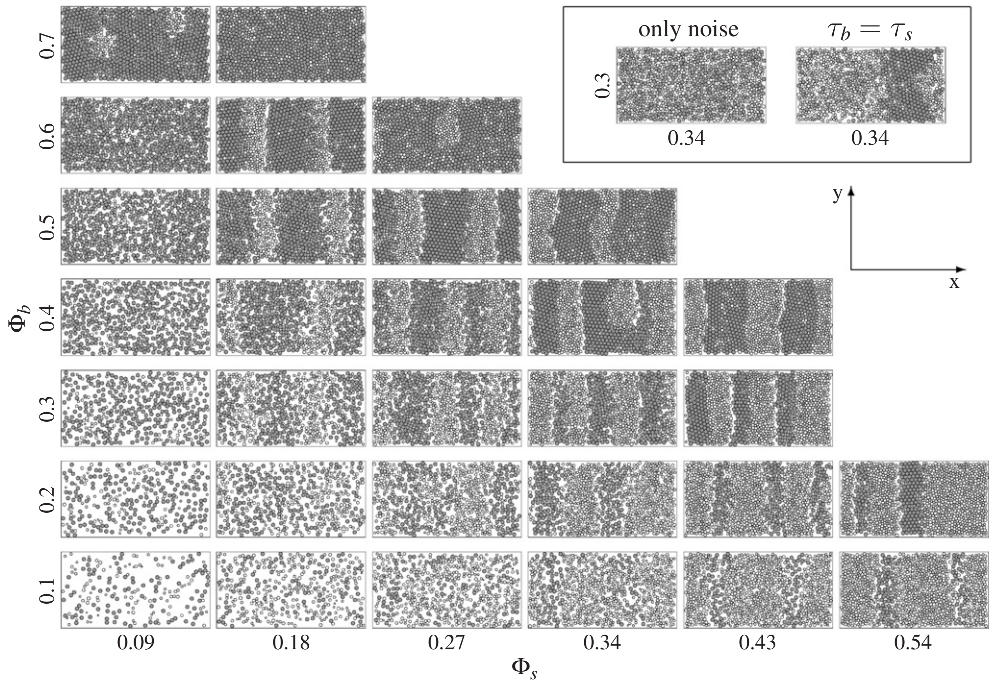

Figure 1. Main frame: stationary states reached by an initially disordered mixture of discs on a horizontally oscillating tray. The horizontal (vertical) axis represents the area fractions Φ_s (Φ_b) of the small polydisperse discs (big monodisperse) discs. At small area fraction the system remains in a disordered state. At higher area fraction the system segregates via the formation of stripes perpendicular to the driving direction. At further higher values of the area fraction stripes of big discs crystallize. Box: stationary states reached by the striped configuration corresponding to $(\Phi_s, \Phi_b) = (0.34, 0.3)$ after a change of the parameter governing the dynamics. In the inset named 'only noise' the amplitude of oscillation is set to zero, and the system evolves just because it is subject to a white noise force. In the inset named '$\tau_b = \tau_s$' the small grains' mass is changed such that the characteristic timescales of the two species become equal.

of the system), which is attractive at small distances. The strength of this potential, which is always proportional to the temperature, increases with the size ratio between the diameter of big and small spheres, and with the number of smaller spheres. In fact it is suggested [9] that the increase in the number of smaller discs leads to an attractive potential between big discs strong enough to induce phase separation. The anisotropy of the drive, in turn, was used to explain why the phase separation manifests via the formation of stripes. The interesting idea of using the depletion potential to explain transitions observed in mixtures of granular [9] in a thermodynamic-like fashion has been proved to be correct in different contexts [7, 20]. Here below we want to give evidence that, in the case of an horizontally oscillated granular mixture, this is not actually able to explain the observed phenomenon.

First, according to this picture, once the depletion potential disappears no segregation should be observed. Instead, as reported in the next section, we do observe segregation via stripe formation even in the case $D_s = D_b$, where no depletion force can be at work. According to the 'depletion picture', moreover, there should be just one critical value of the area fraction above which both stripe formation and crystallization occur, while in both experiments and simulations two different transitions are observed. In opposition to a thermodynamic interpretation we observe a dependence on the parameters governing the dynamics of the

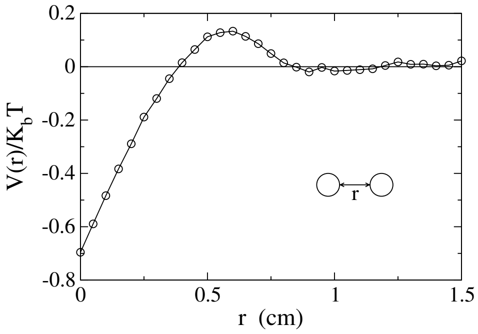

Figure 2. Depletion potential $V_b(r)/K_bT$ between two big discs in a bath of smaller discs plotted as a function of the distance r between the surfaces of the discs, as obtained by integration of the force. The potential has a maximum at $r \simeq D_s = 0.7$ cm. The area fraction of smaller discs is $\Phi_s = 0.6$. The minimum value of the depletion potential ($r = 0$) is such that $|V_b(0)/K_bT| < 1$; it is not big enough to contrast the randomizing action of the temperature. This result is in agreement with the fact that the depletion potential is much weaker in two than in three dimensions [23]. With higher values of the D_b/D_s ratio one may find $|V_b(0)/K_bT| > 1$.

system which is not explained by the depletion argument. As an example, here we illustrate that the state with three stripes reached by the system under the oscillatory dynamics when $(\Phi_s, \Phi_b) = (0.34, 0.3)$ (see figure 1) changes strongly in response to a variation of the parameters governing the dynamics of the system. We have considered two different cases (see figure 1, box). In the first case the amplitude of oscillation is set to zero. The system now evolves just because it is in contact with a heat bath and mix, as shown in the box of figure 1 ('only noise' case). It follows that the depletion force is not strong enough to induce phase separation in the absence of shaking. In the second case, the small grains' mass is changed such that the characteristic timescale of the two species becomes equal ('$\tau_b = \tau_s$' case). In this case the three stripes originally present in the system merge, implying that the formation of stripes is due to dynamics rather than to thermodynamics effects.

Finally, we have also conducted an explicit calculation of the depletion potential. We have made simulations in which two big particles are fixed at a distance $D_b + r$, while smaller discs are in contact with a heat bath at a temperature T. For every distance r we have measured the mean force acting between the big discs. Then, by integrating the force, we have calculated the depletion potential. The result is shown in figure 2 when the area fraction of smaller discs is $\Phi_s = 0.60$. Given the size ratio $D_b/D_s = 1.42$ of our mixture, we observe that $|V_b(0)/K_bT|$ is always smaller than 1, i.e. that the thermal energy is always bigger than the minimum of the depletion potential. Thus, in the cases we are considering, the depletion potential is not strong enough to induce phase separation.

We want also to comment on the role of the white noise force used in our simulations, which is introduced to model in a more realistic way the interaction between a disc and the tray. This interaction, in fact, may be considered of viscous type only at a first approximation, due to the roughness of the surfaces. The strength of the noise, that is, the value of the parameter Γ of equation (3), was chosen after a measure on the experimental system investigated by Mullin and coworkers [11]. We have verified that its value is unimportant so long as K_bT is smaller than the mean kinetic energy E_K of a big disc oscillating following equation (5),

$$E_K = \frac{1}{T}\left[\frac{1}{2}M_b\int_0^T \dot{x}(t)^2\right]. \qquad (7)$$

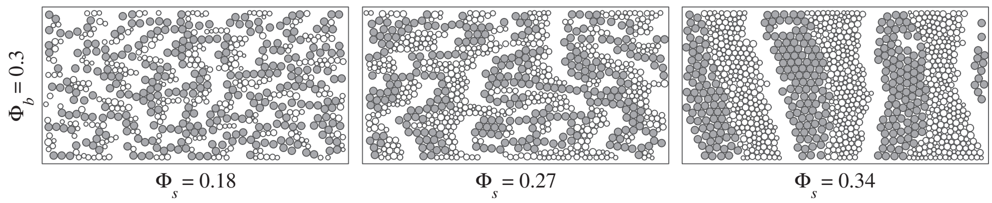

Figure 3. Stationary states reached by a mixture of big and small discs with area fraction $\Phi_\mathrm{b} = 0.3$ and $\Phi_\mathrm{s} = 0.18, 0.27$ and 0.34 under the oscillatory shaking dynamics in the *absence of noise*. A comparison with figure 1 shows that while in the presence of noise at area fraction $(\Phi_\mathrm{s}, \Phi_\mathrm{b}) = (0.18, 0.3)$ and $(0.27, 0.3)$ the system segregates via the formation of stripes, in the absence of noise the system gets trapped in states characterized by the presence of clusters of big discs elongated along the direction of oscillation. These clusters recall the segregation via line formation parallel to the direction of oscillation observed in [25]. At high area fraction $(\Phi_\mathrm{s}, \Phi_\mathrm{b}) = (0.18, 0.34)$ stripe formation is observed both with and without noise.

When $K_\mathrm{b}T > E_\mathrm{K}$, the system remains in a disordered state. We have investigated the condition $K_\mathrm{b}T \ll E_\mathrm{K}$ in the special case $K_\mathrm{b}T = 0$. In this case, when the area fraction of the system is high enough, we still observe segregation via stripe formation (figure 3, in the case $\Phi_\mathrm{s} = 0.34$), as in the case of finite Γ with $K_\mathrm{b}T < E_\mathrm{K}$. However, at smaller values of the area fraction the system gets trapped in states characterized by the formation of clusters of big discs elongated along the direction of oscillation (see figure 3, $\Phi_\mathrm{s} = 0.18$ and 0.27), in agreement with [25].

3. The instability mechanism

In order to understand the origin of the mechanism responsible for the segregation via stripe formation, which we have shown not to be related to the depletion potential, we have conducted another analysis. Here we report a simulation of a binary mixture under horizontal oscillation which differs from the previous one in two aspects. First, we set $D_\mathrm{s} = D_\mathrm{b} = 1$ cm, so that there is no depletion potential influencing the behaviour of the system. Second, we prepare the initial state with two stripes of particles of different type parallel to the driving direction (see figure 4). In this configuration one may expect particles of the two species to oscillate independently (following equation (2) with different relaxation times), and the initial configuration to be a stable one. Figure 4 shows that this is not the case. The oscillatory motion of the tray induces an oscillating shear velocity at the interface between the two species. This causes the interface to evolve via the formation of a modulation with a sine-like shape. As times goes on, the amplitude of the modulation grows until it breaks, giving rise to the striped pattern seen before. This suggest that the same instability mechanism is also responsible for the segregation via stripe formation in the case of an initially disordered mixture. In this case the instability takes place after the formation of microsurfaces due to the formation of local fluctuations of the density of the two species.

The instability mechanism shown in figure 4 is of the same type of that leading to the formation of ripples on a shoreline. In this case [21, 22], the formation of the pattern is due to the action of the sea, which oscillates back and forth. Gravity is then responsible for the stabilization of the pattern once a given size is reached, since it both associates an energy cost to the growing interface, and induces granular avalanches. It is difficult to study this instability process via hydrodynamic-like considerations, i.e. via a model for the Kelvin–Helmholtz instability with oscillating shear, because of the absence of gravity and surface

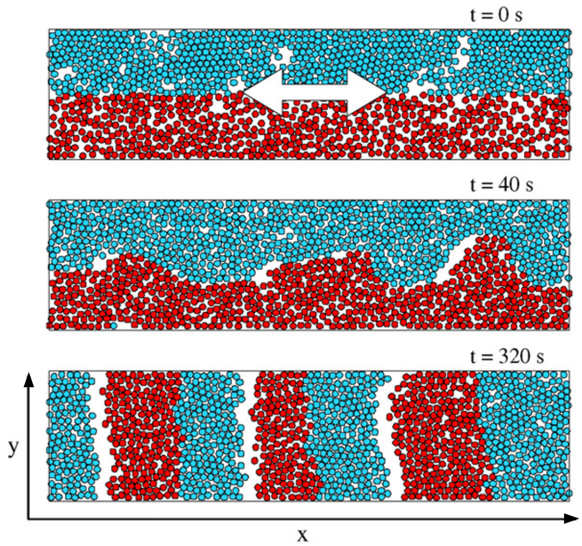

Figure 4. Evolution of a binary mixture of discs placed on a tray oscillating along the x-direction. Here we consider the case in which the diameters of particles of different species are equal. The pictures shows only 1/4 of the system length, which is of 320 D_b. The initial state ($t = 0$ s) is made of two stripes of particles of different species parallel to the driving direction. As times goes on, the flat interface between the two species evolves via the formation of a sine-like modulation ($t = 40$ s). Finally, the wavy interface between grains of different species breaks, leading to the formation of a striped pattern as seen before ($t = 320$ s).

(This figure is in colour only in the electronic version)

tension with which one usually defines the characteristic wavelength of the problem (the capillary length).

4. Conclusions

The phenomenon of species segregation of a granular mixture under horizontal oscillation is investigated via realistic molecular dynamics simulations. We have first studied how the final steady state depends on the area fraction of the two species. Then we have shown that the final steady state crucially depends on the parameters governing the dynamics, such as the friction coefficient and the amplitude of oscillation. This clarifies that the observed segregation phenomenon is not due to a spinodal decomposition associated with a first-order transition induced by the depletion potential, as initially conjectured [9]. An explicit calculation of the depletion potential confirms this result. Finally, we have studied the evolution, under the same oscillating drive, of a binary mixture prepared in a segregated state in which particles of different species form two stripes parallel to the driving direction. In this case, the system also evolves into a segregated state with stripes of particles of different type perpendicular to the driving direction. In this case, however, it is clear that the underlying mechanism is a shear instability of the initially flat interface between the two species, similar to the well known Kelvin–Helmholtz instability of two fluids under constant shear.

The dependence of the wavelength of the striped pattern on the parameter governing the oscillation (amplitude and frequency) is currently under investigation [17], and a simple heuristic model seems to be able to capture the origin of the shear instability [17, 24]. However, a reliable mathematical model able to quantitatively account for this surprising collective phenomenon of a granular medium is still lacking.

References

[1] Kudrolli A 2004 *Rep. Prog. Phys.* **67** 209
[2] Rosato A, Strandburg K J, Prinz F and Swendsen R H 1987 *Phys. Rev. Lett.* **58** 1038
[3] Bridgewater J 1976 *Powder Technol.* **15** 215
[4] Williams J C 1976 *Powder Technol.* **15** 245
[5] Shinbrot T and Muzzio F J 1998 *Phys. Rev. Lett.* **81** 4365
[6] Knight J B, Jaeger H M and Nagel S R 1993 *Phys. Rev. Lett.* **70** 3728
[7] Tarzia M, Fierro A, Nicodemi M and Coniglio A 2004 *Phys. Rev. Lett.* **93** 198002
[8] Mullin T 2000 *Phys. Rev. Lett.* **84** 4741
[9] Reis P M and Mullin T 2002 *Phys. Rev. Lett.* **89** 244301
[10] Reis P M, Ehrhardt G, Stephenson A and Mullin T 2004 *Europhys. Lett.* **66** 357
[11] Ehrhardt G, Stephenson A and Reis P M 2004 *Preprint* cond-mat/0403273
[12] Sánchez P, Swift M R and King P J 2004 *Phys. Rev. Lett.* **93** 184302
[13] Pooley C M and Yeomans J M 2004 *Phys. Rev. Lett.* **93** 118001
[14] Herrmann H J and Luding S 1998 *Contin. Mech. Thermodyn.* **10** 189–231
[15] Cundall P A and Strack O D L 1979 *Geotechnique* **29** 47–65
[16] Silbert L E, Ertas D, Grest G S, Halsey T C, Levine D and Plimpton S J 2001 *Phys. Rev.* E **64** 051302
[17] Pica Ciamarra M, Nicodemi M and Coniglio A 2005 in preparation
[18] Coniglio A, Fierro A, Herrmann H J and Nicodemi M (ed) 2004 *Unifying Concepts in Granular Media and Glasses* (Amsterdam: Elsevier)
[19] Asakura S and Oosawa F 1954 *J. Chem. Phys.* **22** 1255
[20] Bose M, Nott P R and Kumaran V 2004 *Europhys. Lett.* **68** 508
[21] Scherer M A, Melo F and Marder M 1999 *Phys. Fluids* **11** 58–67
[22] Stegner A and Wesfreid J E 1999 *Phys. Rev.* E **60** R3487
[23] Castañeda-Priego R, Rodríguez-López A and Méndez-Alcaraz J M 2003 *J. Phys.: Condens. Matter* **15** S3393
[24] Goldfarb D J, Glasser B J and Shinbrot T 2002 *Nature* **415** 302–5
[25] Chakrabarti J, Dzubiella J and Löwen H 2003 *Europhys. Lett.* **61** 415