Granular Species Segregation under Vertical Tapping: Effects of Size, Density, Friction, and Shaking Amplitude

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We present extensive molecular dynamics simulations on species segregation in a granular mixture subject to vertical taps. We discuss how grain properties, e.g., size, density, friction, as well as shaking properties, e.g., amplitude and frequency, affect such a phenomenon. Both the Brazil nut effect (larger particles on the top, BN) and the reverse Brazil nut effect (larger particles on the bottom, RBN) are found and we derive the system comprehensive "segregation diagram" and the BN to RBN crossover line. We also discuss the role of friction and show that particles which differ only for their frictional properties segregate in states depending on the tapping acceleration and frequency.

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Granular materials are systems of many particles interacting via short ranged repulsive and dissipative forces, both normal and tangential to the surface of contact. They are characterized by an energy scale mgd (of a grain of mass m and linear size d in the gravitational field g) which is many orders of magnitude larger than the thermal energy k_BT, and are thus named "nonthermal" systems. These characteristics make difficult the understanding of the large variety of counterintuitive phenomena granular materials exhibit, which are of great interest both for their industrial relevance and for the theoretical challenges posed to physicist and engineers.

Particularly the phenomenon of size segregation under vertical vibrations [1], which we consider here, has emerged as a real conundrum. Contrary to intuition, an originally disordered mixture when subject to vertical vibrations tends to order: large particles typically rise to the top, as small particles percolate into their voids during shaking [1–4] or move to the bottom due to convection mechanisms [5–7], giving rise to the so-called "Brazil nut effect" (BN). Differences in particle density also affect size separation [see references in [8]] and reverse-BN (RBN), with small grains above, can be observed, too [9,10]. The picture where grain sizes and weights are the parameters explaining segregation is found, however, to be too simple [9–20] and a full scenario is still missing.

In correspondence with some existing experiments [21–23], here we consider segregation phenomena in molecular dynamics simulations of tap dynamics: grains confined in a box are shaken and after each shake fully dissipate their kinetic energy before being shaken again. A picture of our model system is given in the left panel of Fig. 1 showing the final BN configuration reached by an initially disordered mixture shaken with an amplitude $\Gamma = A\omega^2/g = 1$ (where ω is the shake frequency, A its amplitude, and g gravity acceleration, see below). An example of the role of the external drive on segregation can be appreciated by comparison with the right panel of Fig. 1 showing the final RBN configuration reached by the same mixture when shaken at $\Gamma = 3$.

We show below how grain properties, e.g., size, density, friction, as well as the external forcing, e.g., shaking amplitude and frequency, affect the process and derive for the first time a comprehensive nontrivial "segregation diagram." The richness of such a diagram is not captured by current theoretical approaches [9,12,19] and calls for new theoretical and experimental investigations.

Simulations.—We make soft-core molecular dynamics simulations of a system of $N_l = 240$ large grains of diameter $D_l = 1$ cm and density $\rho_l = 1.9\ \mathrm{g\,cm^{-3}}$, and N_s small grains with diameter D_s and the density ρ_s. We vary D_s and ρ_s and chose the number N_s in such a way that the

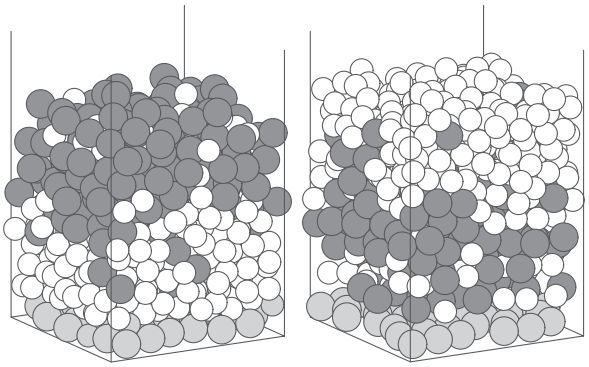

FIG. 1. We show a mixture of $N_l = 240$ large particles of diameter $D_l = 1$ cm and density $\rho_l = 1.9\ \mathrm{g\,cm^{-3}}$ (dark gray particles) and $N_s = 360$ small particles of diameter $D_s = 0.8$ cm and density $\rho_s = 1.27\ \mathrm{g\,cm^{-3}}$ (white particles). It is contained in a box (whose base is made of other immobile grains, light gray particles, see text) and is subject to vertical taps with normalized amplitude Γ. The pictures show two configurations at rest attained at stationarity: interestingly, when shaken with $\Gamma = 1$ (left) the system goes into a BN configuration and when $\Gamma = 3$ (right) it goes in a RBN configuration.

two species occupy a comparable volume, $N_l D_l^3 \simeq N_s D_s^3$. The particles are enclosed in a box with a square basis of side length $L = 7$ cm (see Fig. 1) with periodic boundary conditions in the horizontal directions, so that convection is avoided. In order to prevent crystallization some particles are randomly glued on the container basis (in such a way that no further particle can touch the bottom of the container).

Two grains interact when in contact via a normal and a tangential force. The normal force is given by the so-called linear spring-dashpot model, while the tangential interaction is implemented by keeping track of the elastic shear displacement throughout the lifetime of a contact [24]. The model and the values of its parameters have been described in [25], with the value of the viscous coefficient of the normal interaction such that the restitution coefficient is $e = 0.8$. In most of our simulation the static friction coefficients are equal for the two species, $\mu_{ll} = \mu_{ls} = \mu_{ss} = 0.4$ (μ_{ij} is the friction coefficient in the interaction between a grain of type i and a grain of type j, and $\mu_{ij} = \mu_{ji}$), but we will also consider the case $\mu_{ll} \neq \mu_{ss}$ to investigate the role of friction in the segregation process.

The system, starting from a random configuration, is subject to a tap dynamics up to reach a stationary state. Each tap consists of one oscillation of the container basis with amplitude A and frequency ω, i.e., the bottom of the box moves with $z(t) = A\cos(2\pi\omega t)$. We checked that both A and ω are important to select the final segregation state (Γ is not the only relevant parameter) and consider here the case where $\omega = 30$ Hz and A is varied. A tap is followed by a relaxation time where the system comes to rest. A grain is considered to be at rest if its kinetic energy becomes smaller than $10^{-5} mgd$, where $1 mgd$ is the energy required to rise it of a distance equal to its diameter. All measures are taken when the system is at rest and in the stationary part of the tap dynamics. Actually, it is known that for small values of Γ the system dynamics has strong "glassy" features [26,27] and thus the states attained can be very far from stationarity. Here we are away from that region.

The degree of separation of the binary mixture in the stationary state is quantified by the usual vertical segregation parameter

$$\Delta h = 2\frac{h_s - h_l}{h_s + h_l}, \qquad (1)$$

where h_p is the average height of particles of species $p = l, s$ [$h_p = (1/N_p)\sum_{i=1}^{N_p} z_i$, here z_i is the height of particle i with respect to the container basis at rest]. We prepare the system in a random initial state characterized by $\Delta h \simeq 0$ via a Monte Carlo procedure. When subject to a tap dynamics the mixture evolves and the segregation parameter changes until a stationary state is reached.

Results.—We first describe the dependence of the segregation parameter, Δh, on the diameter ratio D_l/D_s and on the density ratio ρ_l/ρ_s of the two components for $\Gamma = 2$. Figure 2 shows Δh as a function of D_l/D_s for different values of the density ratio (left panel) and Δh as a function of ρ_l/ρ_s for different values of the size ratio (right panel). As expected, when the diameter ratio grows BN states are favored with respect to RBN states, even though such an effect is mitigated by increasing the density ratio ρ_l/ρ_s which shifts the BN to RBN crossover to higher values of D_l/D_s.

Such a size and density ratio dependence might seem to result from two simple competing effects. The first one is a "percolation" effect [4] according to which it is easier for the smaller particles to percolate through the voids between larger grains and, thus, reach the bottom of the container. The percolation effect becomes stronger as the size ratio between the components increases, and therefore should describe the size dependence found in Fig. 2 (left panel). The second effect is buoyancy, according to which the system tends to minimize gravitational energy, and therefore the species with higher mass density is pushed to the bottom of the container. This should describe the density dependence of Fig. 2 (right panel).

We find, however, that the properties of the external forcing have an essential role in selecting the final segregation state and the overall scenario appears to be richer: percolation/buoyancy effects changes with the intensity of vibration Γ (see Fig. 1). In Fig. 3 we plot the dependence of the segregation parameter, Δh, on Γ for given values of D_l/D_s and ρ_l/ρ_s: unexpectedly, a stronger shaking enhances RBN; i.e., as Γ increases Δh increases, too. A similar qualitative result was observed also in experiments with a continuous shaking dynamics [21].

Figure 4 summarizes these findings in a "segregation diagram" in the $(\rho_l/\rho_s, D_l/D_s, \Gamma)$ space. As expected, the BN effect is favored when D_l/D_s is large and RBN when

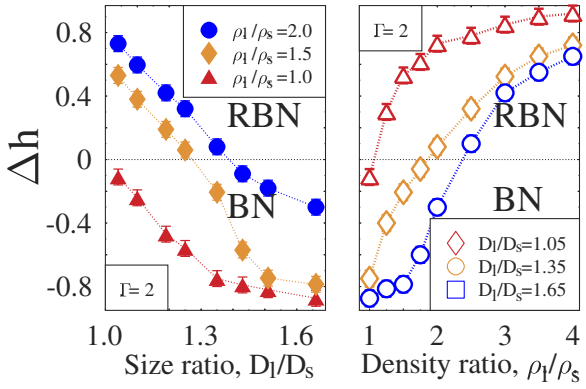

FIG. 2 (color online). The left panel shows the segregation parameter Δh as a function of the diameter ratio D_l/D_s of the mixture components, for $\Gamma = 2$ and $\rho_l/\rho_s = 1, 1.5, 2$. By increasing D_l/D_s the system crosses from RBN configurations (i.e., $\Delta h > 0$) to BN (i.e., $\Delta h < 0$). The right panel shows Δh as a function of the density ratio ρ_l/ρ_s for $\Gamma = 2$ and $D_l/D_s = 1.05, 1.35, 1.65$. By increasing ρ_l/ρ_s the system moves from RBN to BN, as the crossover point (where $\Delta h = 0$) turns out to depend on the size ratio D_l/D_s.

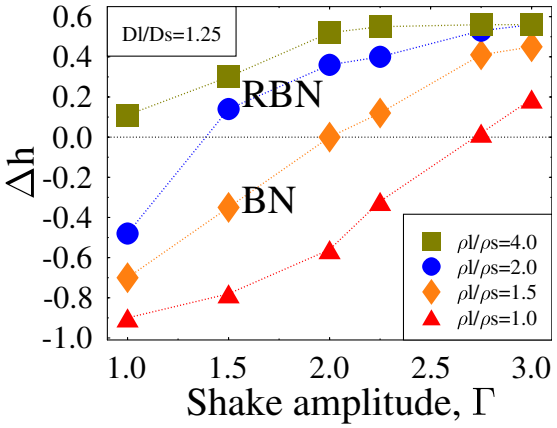

FIG. 3 (color online). Δh is plotted as a function of the adimensional vibrational acceleration Γ, in a mixture where $D_l/D_s = 1.25$, for the shown values of the density ratio ρ_l/ρ_s. As Γ increases the system moves from a BN to a RBN configuration.

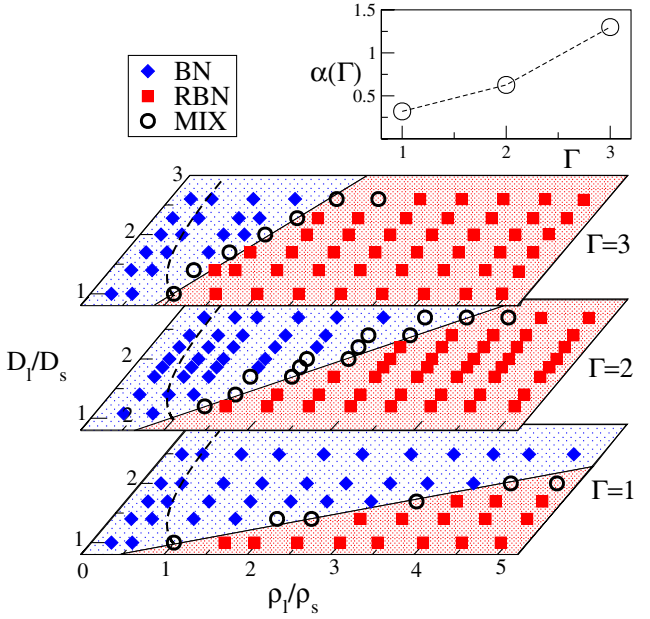

FIG. 4 (color online). The "segregation diagram" of the mixture in the $(\rho_l/\rho_s, D_l/D_s, \Gamma)$ space. The plot shows the regimes where the reverse (RBN) and the usual Brazil nut effect (BN) occur. Empty circles are the points where Δh is zero, within 10%, and named "mix" in the caption. The solid line separating the areas is given by Eq. (2). The dashed line is the crossover line proposed in Ref. [9] Inset: dependence on the adimensional acceleration Γ of the coefficient α of Eq. (2).

ρ_l/ρ_s grows. The BN to RBN crossover region is dependent on Γ: we approximate the BN to RBN crossover line $D_l/D_s = f(\rho_l/\rho_s, \Gamma)$ around $\rho_l/\rho_s \simeq 1$ with a linear function (continuous line in the figure):

$$\frac{D_l}{D_s} \simeq 1 + \alpha(\Gamma)\left(\frac{\rho_l}{\rho_s} - 1\right), \tag{2}$$

where the angular coefficient $\alpha(\Gamma)$, shown in the inset of Fig. 4, grows monotonically with Γ. Since $\alpha(\Gamma) > 0$, the present results, corresponding to grains with equal friction properties (see below for a different case), point out that RBN configurations can be found only if $\rho_l/\rho_s > 1$: i.e., by changing D_l/D_s there is no way to find RBN when $\rho_l/\rho_s < 1$. In this perspective our simulations may explain why in the "original" Brazil nut effect observed during the transportation of nuts of different size (but otherwise similar) the larger ones are systematically found to rise to the surface. The diagram of Fig. 4 appears to be in good agreement with the general features of known experiments as those of Ref. [21] [even though it is still unclear whether the phenomena of segregation under tapping, here considered, and under continuous shaking, as in [21], are qualitatively similar] and can help clarifying experimental results.

In Fig. 4 we also plot the BN to RBN crossover line found by the theory of Ref. [9] (dashed line): such a theory, approximating the granular mixture under vibration as a thermal system, predicts the right qualitative behavior as a function of ρ_l/ρ_s, but it does not capture the right D_l/D_s dependence. More elaborated models assuming lack of equipartition between the species, as in kinetic theories [12] or some simulations [14], or the existence of more than one configurational temperature, as in a statistical mechanics theory of the mixture [16,17], may be able to improve on this aspect.

Another parameter relevant to segregation is friction [15,28] which we now consider in order to extend the diagram of Fig. 4. We take grains with equal sizes and weights, but different friction coefficients; this is an interesting situation difficult to be experimentally accessed as real grains which differ in frictional properties usually also differ in other properties (such as mass, Young modulus, etc., ...). We study a mixture of $N_1 = N_2 = 300$ grains of diameter $D_1 = D_2 = 1$ cm and density $\rho_1 = \rho_2 = 1.9\ \mathrm{g\,cm^{-3}}$ with friction coefficients $\mu_{11} = 0.4$, $\mu_{22} \in \{0.05, 0.01, 0.2, 0.4, 0.6, 0.8\}$, and $\mu_{12} = \min(\mu_{11}, \mu_{12})$, as in [15]. As the two components only differ for their friction, the segregation parameter is now defined as $\Delta h = 2(h_2 - h_1)/(h_2 + h_1)$. This mixture indeed segregates: Fig. 5 shows that the species with higher friction coefficient always rise to the top, as the degree of segregation depends on the shaking intensity. This can be explained by considering that grains with smaller friction can more easily percolate to the bottom of the container.

Conclusions.—Our molecular dynamics simulations are not affected by the presence of air, humidity, and (due to the periodic boundary conditions) convection, and should be therefore considered as an ideal, even though comprehensive, experiment, well robust to changes in the MD model [24]. We found that both grain properties, such as diameters, densities and friction, and external driving properties, such as amplitude and frequency of shaking, are important to select the system final segregation state. We

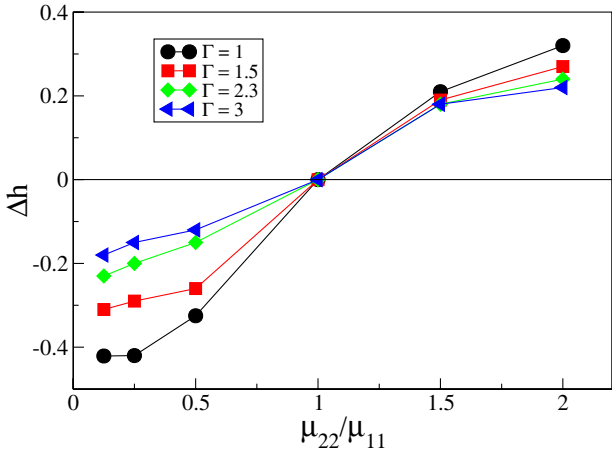

FIG. 5 (color online). The segregation parameter Δh is shown as a function of the ratio between the static friction coefficient μ_{22}/μ_{11} of a mixture of grains which differ only for their frictional properties. Particles with higher friction coefficient are always found on the top of the container, although the degree of segregation depends on Γ.

determined the "segregation diagram" in the three parameters space (D_l/D_s, ρ_l/ρ_s, Γ) and derived the BN to RBN crossover line $D_l/D_s = f(\rho_l/\rho_s, \Gamma)$. In particular, in our model system, a mixture of grains only differing in sizes always segregates in a BN configuration, explaining why in the original "Brazil nut" problem large grains always sit at the top. We also discussed how segregation is influenced by grains friction by showing, for instance, that in a mixture of particles differing only for their surface friction by increasing Γ the smoother grains tend to rise to the top, a result easy to be experimentally checked. As our results are in agreement with known experiments and can help their clearer interpretation, our comprehensive "segregation diagram" is not explained by current theories and necessitates further theoretical and experimental investigations.

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