Vibrated Powders: A Microscopic Approach

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We present a microscopic model of a granular pile submitted to vibration, emphasizing the competing roles of collective and single-particle excitations which lead to specific characteristics of the resulting state. The effect of vibration on a powder is next investigated by a novel computer-simulation approach in three dimensions, which enables us to probe cooperative effects in the bulk; satisfying agreement with the predictions of the model is obtained.

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Although the physics of powders is now a burgeoning area of theoretical physics [1–7], there are correspondingly few reliable modern experiments [8–10] which seek to probe the most fundamental questions pertaining to these very complex systems. We have in earlier work [5], based on one of these experiments [9], investigated the phenomenon of granular relaxation in relation to the decay of the slope of a sandpile subjected to vibration.

It is well known that shaking and tapping a container of powder can either compress or dilate the powder, but theoretical evidence of this has so far not been forthcoming. We present for the first time a three-dimensional computer-simulation approach to relaxation in a vibrated powder where we focus, by analyzing cooperative dynamics in the powder, on the *effects* of vibration on the compactivity [2] (proportional to the inverse of the packing fraction) and structure of a three-dimensional pile. We will demonstrate that, within a single mode of vibration, both compression and dilation can result from different amplitude regimes, and we will probe this quantitatively by looking at the resulting volume packing fractions as well as configurational correlation functions. First, we outline the microscopic model [3] on which this work was based (a quantitative version of which is presented elsewhere [11]) and follow this by a description of the simulation techniques used to investigate it. Finally, we present and analyze our results.

In the model, a granular pile is represented by an assembly of potential wells [3], each representing a local cluster of grains, while the effect of vibration applied to the pile is modeled as being an effective noise H. If H is greater than the binding energy of the particles to their wells, then the grains are ejected, and move into neighboring wells: In terms of the real powder, this means that grains are ejected individually (*single-particle relaxation*) from their clusters. Conversely, if H is small relative to the binding energies of the particles, they are not ejected: This energy goes into the reorganization of the grains (*collective relaxation*) within their wells to minimize voids. The claim is [3] that for high intensities of vibration, the dominant process is single-particle relaxation, whereas collective relaxation dominates at low intensities. It will be realized [3] that while single-particle relaxation leads to a rapid decay of the slope, it will lead to a high compactivity and a rough surface. Equally, when collective relaxation dominates, the slope will relax slowly or not at all: On the other hand, slow collective reorganization of particles will lead to efficient void filling, i.e., to low compactivities and a smooth surface.

The motivation behind the simulation that follows is to probe, in three dimensions, the effects of the individual and collective particle dynamics on the *bulk* properties of the powder, the effect on the slope having been examined elsewhere [5]. We do this by examining the packing fraction and the correlation functions of the positions and displacements (which measure the range of cooperative effects) of the particles in the granular assembly, across a range of vibration amplitudes.

The simulation cell is an open-topped box with a square base of side L at height $z=0$, with periodic boundary conditions imposed at the vertical walls. Initially N monodisperse hard spheres are placed in the cell using a sequential random close-packing algorithm [12]. Incoming spheres start from large z with random lateral positions and follow compound trajectories, which are composed of vertical line segments and circular arcs corresponding to free-fall and nonslip rolling in contact with stationary spheres [12], until they reach stable positions where they are supported by the base or by three other stable spheres.

Stable configurations of monodisperse close-packed hard spheres formed by sequential deposition are characterized by a volume fraction $\phi=0.581\pm0.001$ [13] and a mean coordination $c=6.00\pm0.02$. They form the starting point for our shaking simulations in which the whole assembly is repeatedly and *cooperatively* repacked. Each repacking consists of a sequence of operations which we call a "shake cycle," which models the effects of a vibration cycle in the real powder.

The first phase of the cycle is a uniform vertical expansion of the sphere packing accompanied by random shifts of the spheres in a horizontal plane [5]. Sphere i, at height z_i, is raised to the new height $z_i'=(1+\varepsilon)z_i$, where ε is a measure of the amplitude of shaking. For each sphere noisy lateral displacements given by the transformation $x'=x+\xi_x$, $y'=y+\xi_y$, are accepted if they do not lead to overlapping sphere configurations. Here ξ_x and ξ_y are Gaussian random variables with zero mean and variance ε^2. The purpose of the expansion is to introduce a "free volume" of size ε between the spheres, so as to allow room for movement.

In the second phase of the cycle the whole system is reassembled by a series of displacements of the individual spheres. The displacements are chosen by a Monte Carlo procedure [14] with the proviso that overlaps are avoided: They occur preferentially in the downward direction. This represents a simple approximation to the many-particle dynamics of a falling assembly of spheres. This Monte Carlo process is terminated when the efficiency of making the moves falls below a threshold value, which is chosen to be 1%.

Finally, the sphere packing is "stabilized" by lowering all the spheres along compound paths as described above. The spheres are moved in turn, commencing with the lowest; however, the falling sphere may contact, and rest on, spheres which are still to be stabilized. This procedure allows the formation of complex structures, like bridges [3,5,15] and arches [8]; equivalent configurations *cannot* therefore be constructed by a purely sequential process. The stabilization phase does not significantly alter the final measured volume fraction of the packing, but is, however, responsible for forming all the particle contacts, and the formation of the contact networks [5] to be discussed later. *It is crucial to emphasize that phases two and three of our simulation together constitute the novel feature of our algorithm, as they enable us to probe the cooperative dynamics of a vibrated powder.*

We have performed simulations for $L=8$ sphere diameters, with $N \simeq 1000$, and $0.05<\varepsilon<1.5$. Checks have not revealed strong finite-size dependence for the results presented below. To reiterate our procedure: We start from the close-packed assembly with $\phi=0.581\pm0.001$, and subject the system to vibration. There is a transient regime, which we discuss below, and we take our data from well into the steady regime. Our chief conclusions (cf. Fig. 1) are that we observe a fall in the packing fraction for large ε, and, more interestingly, a *rise* in ϕ for small ε.

Thus, after each completed cycle the volume fraction and mean coordination number of the spheres are measured in the bulk of the packing to avoid end effects. In the transient regime, ϕ and c drift systematically. The length of the transient regime varies with the shaking amplitude from about two or three cycles when $\varepsilon>0.25$ to about fifty cycles when $\varepsilon=0.05$. These variations are a signal of the different microscopic processes which take place continually at large and small shaking amplitudes.

The results presented below are mean values taken from about fifty consecutive cycles in the steady regime. Figure 1 shows the variation of the volume fraction with the shake amplitude. For $\varepsilon>1.0$, the volume fraction is only weakly dependent on ε with $\phi \sim 0.55$. However, ϕ rises sharply as ε is reduced below $\varepsilon=1.0$. For $\varepsilon<0.2$ the shaken assembly adopts configurations which are more compact than those for sequentially deposited spheres. Our results in Fig. 1 show that the curve goes through a volume fraction of 0.581 (the appropriate value for static configurations generated by sequential packing under gravity) at $\varepsilon=0.2$. This is the point where it would be sensible to locate a transition in dynamic behavior. This transition is related in a complex way to the nature of bridge formation, and, as such, is a clear manifestation of the *change* in the collective behavior of the structures formed during the shaking process.

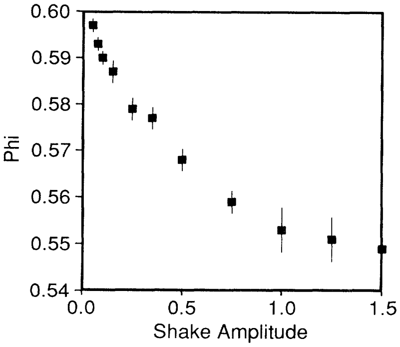

FIG. 1. Plot of volume fraction ϕ against amplitude of vibration ε.

We observe that the mean coordination number of the spheres in a shaken assembly (approximately 4.5) is substantially below that associated with a sequential deposit (approximately 6.0) reflecting the presence of bridges, arches, and other void-generating structures associated with shaking in the real assembly. This effect is, as expected, weaker for smaller amplitudes of shaking.

The pair distribution function $h(r)$ of the sphere separations r in the horizontal direction is illustrated by Fig. 2(a) for large and small shaking amplitudes. We observe that short-range order is stronger at the lower shaking amplitude where $h(r)$ has a prominent second peak; this indicates a significant second-neighbor shell.

We proceed now to establish the competing roles of single-particle and collective dynamics in terms of the correlations between the sphere displacements as a function of different amplitudes of vibration. In Fig. 2(b) we plot the correlation function $H(r)$ for the *vertical* displacements Δz_i (measured in the *horizontal* direction) of the spheres during one shake cycle:

$$H(r)=\langle \Delta z_i \Delta z_j \delta(t_{ij}-r)\Theta(|z_{ij}|-\tfrac{1}{2})\rangle/\langle|\Delta z_i|\rangle^2, \qquad (1)$$

where $z_{ij}=z_i-z_j$, $t_{ij}=\{(x_i-x_j)^2+(y_i-y_j)^2\}^{1/2}$, and $\Theta(x)$ is the complement of the Heaviside step function. We see that $H(r)$ decays rapidly to zero with increasing r: This represents the decay of longitudinal-displacement correlations measured in the transverse direction. The

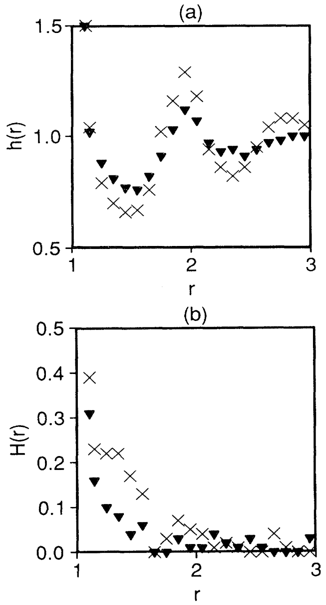

FIG. 2. Plot of correlation functions (a) $h(r)$ against r and (b) $H(r)$ against r. $h(r)$ is the pair-correlation function of particle positions, while $H(r)$ is the pair-correlation function of particle displacements in the transverse direction. The crosses correspond to $\varepsilon=0.05$, while the triangles correspond to $\varepsilon=1.0$. The peak heights in (a) (not shown for convenience of plotting) are $h(1)\sim6.35$ and 6.15 for $\varepsilon=0.05$ and 1.0, respectively.

data in Fig. 2(b) give an estimate for the horizontal range over which the spheres move collectively (a measure of the typical "cluster size" in the transverse direction) during a shake cycle. This range is approximately halved when the vibration amplitude is increased from $\varepsilon=0.05$ to 1.0. Our data suggest that the correlations of the *longitudinal* displacements [15] (not shown here) measured in the longitudinal direction are stronger than those measured in the transverse direction: This is because, as should be the case for any deposition under gravity, the motion of an individual particle is much more sensitive to the positions and motion of neighbors above or below it than it is to those alongside it. The correlation functions of the transverse components of the sphere displacements (not plotted here) are negative [15] at small separations. This is consistent with spheres sliding past each other as they are displaced in the x,y directions. Our results are consistent with the idea that collective reorganization of the spheres dominates during small-amplitude shaking and that the extent of these cooperative effects is many sphere volumes.

Two qualitatively different relaxation behaviors are illustrated in Fig. 3, which is a snapshot taken from a simulation with $L=3$. The small cluster of spheres in Fig. 3(a) is represented by its contact network in Fig. 3(b), where the contact network is formed from bonds placed between the centers of all pairs of touching spheres. The networks which result after the cluster of Fig. 3(a) undergoes a single shaking cycle with $\varepsilon=0.05$ and 1.0 are plotted in Figs. 3(c) and 3(d). We can see the result of a small shake by comparing Figs. 3(b) and 3(c)—the contact network deforms (as shown by differences in many bond orientations), while there are few topological changes. By contrast, after a large shake,

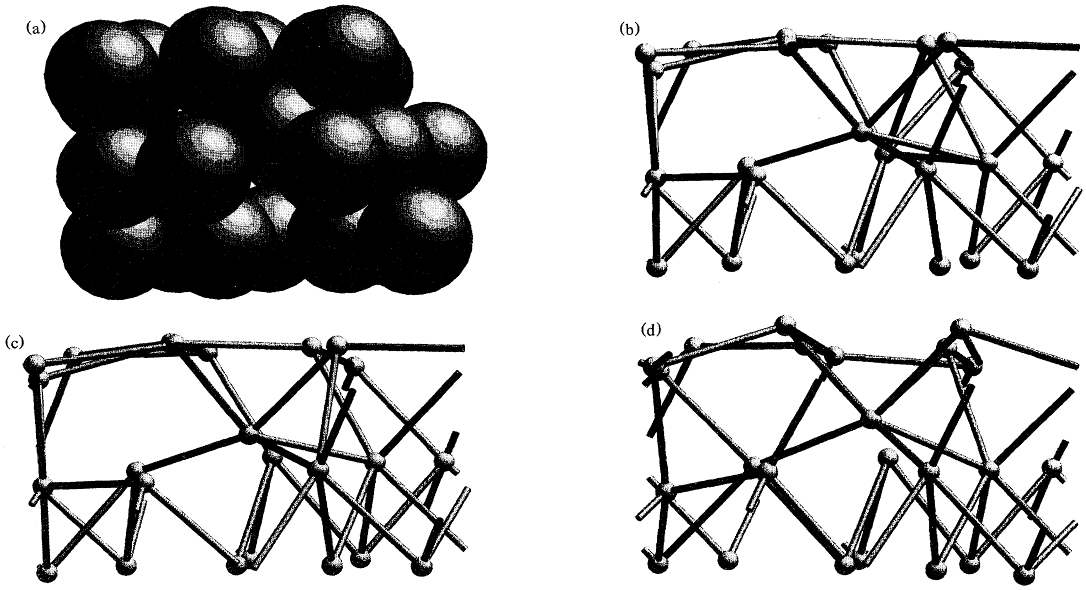

FIG. 3. (a) A random close packing of 24 spheres supported by a hard base. (b) The contact network corresponding to the packing in (a). (c) The contact network for the packing which results when a shake of amplitude $\varepsilon=0.05$ is applied to the cluster of (a). (d) The contact network for the packing which results when a shake of amplitude $\varepsilon=1.0$ is applied to the cluster of (a).

as seen from a comparison of Figs. 3(b) and 3(d), the network connectivity is substantially altered, i.e., there are several examples of bond creation and annihilation. This is confirmed by detailed analyses of the contact-network autocorrelation functions to be presented elsewhere [15]. These functions are qualitatively similar to those previously presented for two dimensions [5].

We have thus been able to establish, as predicted by the microscopic model [3], that above a threshold of vibration, the compactivity (which we measure operationally by the inverse of the packing fraction) rises in response to an applied vibration, whereas below this, it *falls*. In addition, and more crucially, by monitoring the dynamic correlation functions mentioned above, we have been able to consolidate the link between a rise in packing fraction and a predominance of collective motions, and vice versa. This confirms our earlier conjecture [3] that the mechanism of collective relaxation is an efficient way of minimizing voids, which is also a result that has been obtained theoretically [11]. In future work [15], we aim to show that the competition between single-particle and collective relaxation mechanisms contributes significantly to the surface properties of a sandpile.

In conclusion, we have devised a novel simulation method which enables us, with its ability to probe cooperative dynamics, to focus on different microscopic relaxation mechanisms at the particulate level. We have verified earlier theoretical predictions [3], and have obtained a consistent picture of the relaxational dynamics in this rich and fascinating system.

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