Vertical ordering of rods under vertical vibration

M. Ramaioli,[1,2,*] L. Pournin,[1] and Th. M. Liebling[1]

[1]*Mathematics Institute, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

[2]*Nestlé PTC Orbe, CH-1350 Orbe, Switzerland*

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Granular media composed of elongated particles rearrange and order vertically upon vertical vibration. We perform pseudo-two-dimensional discrete element model simulations and show that this phenomenon also takes place with no help from vertical walls. We quantitatively analyze the sizes of voids forming during vibrations and consider a void-filling mechanism to explain the observed vertical ordering. Void filling can explain why short rods are less prone to align vertically than long ones. We cannot, however, explain, invoking just void filling, the existence of an optimum acceleration to promote vertical ordering and its dependence on particle length. We finally introduce an interpretation of the phenomenon, by considering the energetic barriers that particles have to overcome to exit a horizontal or a vertical lattice. By comparing these energetic thresholds with the peak mean particle fluctuant kinetic energy, we identify three different regimes. In the intermediate regime a vertical lattice is stable, while a horizontal is not. This interpretation succeeds in reconciling both dependencies on vibration acceleration and on particle length.

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I. INTRODUCTION

Over the last half decade, the research for understanding the complex collective behavior of granular media has progressively been shifting its focus from spherical to the more relevant nonspherical particles. Real-world grains are indeed far from being spherical and particle geometry is commonly thought to strongly influence the behavior of dense granular media. Getting better insight into the behavior of monodisperse anisotropic media subject to vibration is a key step towards explaining compaction mechanisms [1] in real granular media. Moreover, such insight is also needed to interpret the segregation of mixtures of anisotropic particles just as understanding the behavior of vibrated monodisperse spheres has been a key to interpret sphere size segregation over the last decade [2,3].

Stokely *et al.* [4] studied grain orientation and voids in two-dimensional piles of prolate grains. A density dependent isotropic-nematic transition was reported by Galanis *et al.* [5] in a horizontal pseudo-two-dimensional box vibrated vertically, showing the important role of walls. The importance of particle shape in such a configuration was studied too [6]. Ribière *et al.* [7] showed the importance of convection and Abreu *et al.* [8] used Monte Carlo methods to simulate compaction of spherocylinders and shape segregation from spheres. Experiments by Villaruel *et al.* [9], Blair *et al.* [10], and Lumay *et al.* [11] showed that rods can orient vertically when vibrated vertically in a cylindrical container. Blair invoked first void-filling to interpret qualitatively this phenomenon. Volfson *et al.* [12] studied the dynamics of a set of bouncing rods and the spontaneous development of a horizontal velocity.

The modeling archetype for elongated grains is the spherocylindrical rod: a cylinder with a hemisphere at each end. It is fully characterized by two geometric parameters: its total length L and the diameter D, identical for the cylinder and the hemispheres. Williams [13] simulated random packings of spheres and spherocylinders by mechanical contraction. Pournin *et al.* [14] proposed a DEM capable of handling spherocylinders, used to reproduce experiments by Villaruel *et al.* and later extended DEM to three-dimensional particles with more complex shapes [15]. The vertical ordering of spherocylinders in a cylindrical container was explained by the reaction torque occurring when a rod touches the curved sidewall with both tips in a nonhorizontal position [14].

In a previous paper [16] the authors linked rod vertical alignment with the shape segregation of rods from spheres. It was shown experimentally that vertical ordering takes place also in a vertically vibrated, pseudo-two-dimensional, flat container as shown in Fig. 1. Vertical alignment was reached regardless of initial orientation. Those observations suggested an intrinsic tendency of rods to evolve toward a vertical arrangement, even in the absence of curved walls. DEM simulations were found to agree with experiments.

In this paper we study the influence of particle geometry and vibration acceleration on rod vertical ordering, simulating the rearrangement of particles of different lengths in a box with lateral periodic boundaries. We consider void filling as a possible mechanism explaining vertical ordering and show the limits of such interpretation. We finally introduce the notions of mean particle fluctuant kinetic energy and potential energy barriers and use them to explain the effect of

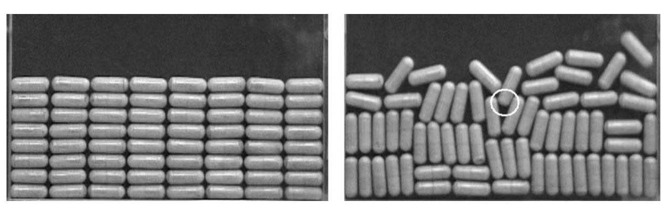

FIG. 1. Experiments from Ref. [16]. Initial configuration on the left. Rod configuration after 1650 s vibration on the right.

*marco.ramaioli@epfl.ch

TABLE I. Ordering simulations of particles of different elongations.

	Particle L (mm)	Acceleration (g)
Sim. 4	23.0	1,1.2,1.5,2,3,4,6
Sim. 5	17.5	3
Sim. 6	16.0	1.5,3,4
Sim. 7	14.4	3
Sim. 8	12.9	3
Sim. 9	12.2	3
Sim. 10	11.9	3
Sim. 11	11.5	2,3,4,6

particle geometry and vibration acceleration on rod vertical ordering.

II. DEM SIMULATION SETUP

We use molecular dynamics DEM to simulate the rearrangement of 256 particles of different lengths in a flat pseudo-two-dimensional container vibrated vertically. Details about the DEM used in the present study can be found in Refs. [14,15].

Simulation conditions can be found in Table I. All simulations start from a horizontal lattice and use particles whose diameter is D=0.0081 m. The box is 0.009 m thick and has lateral periodic walls. Simulation 4 uses the same particle geometry used in Ref. [16] and a periodic box whose width (0.768 m) is four times the width of the real box considered there. The behavior of particles of different lengths is investigated through simulations 4 to 10, using periodic walls allowing to host initially 256 particles ordered in 8 horizontal layers. The lateral periodicity is therefore reduced proportionally to the reduction in particle length. In addition to varying particle length, we also modulated the vibration amplitude as to achieve different peak accelerations as summarized in Table I. Vibration frequency is kept constant at 12.5 Hz.

We varied the lateral periodicity using the longest particles, observing some effect on the ordering kinetics, but no effect on the steady-state ordering. The smallest periodicity tested (64 particles) showed strong fluctuations of the mean angle around the steady state value, due to the strong sensitivity to local lattice defects that are created by the vibrations. A population of 256 particles (and the corresponding periodicity), turned out to be a good compromise to observe steady state ordering in a reasonable computational time.

III. RESULTS

Figure 2 shows the rearrangement occurred in simulation 4 after 1200 s: rods have rearranged away from the initial horizontal order, toward a predominantly vertical lattice. Our box does not have vertical sidewalls that can promote vertical ordering when inclined rods touch them as observed macroscopically in Ref. [16] or microscopically with the depletion-induced torque [17] in colloids. Observing vertical

FIG. 2. Simulations 4: Rearrangement after 1200 s of vibrations. Initially the particles were ordered horizontally. Lateral walls are periodic.

ordering in such a periodic setup confirms that this phenomenon takes place also in the absence of help from the walls. During rearrangement all the particles translate horizontally, similarly to what observed in experiments [12].

To quantify the rod rearrangement, Fig. 3 shows the time evolution induced by 3 g vibrations of the mean angle with the horizontal plane of the bottom-most two layers of the medium. The longest particles of simulation 4, order vertically as observed in Fig. 2, till reaching a fairly vertical steady state. To appreciate the degree of robustness of the results we report three repetitions of simulation 4, obtained varying the initial arrangement. These three different initial states are obtained by perturbing the initial horizontal lattice with a very short inclined vibration. The ordering dynamics follows reasonably well the three regimes proposed by the adsorption-desorption model [18]: the mean angle of the bottom-most two layers varies initially as $1/t$, then as $1/\ln(t)$, finally it follows an exponential decay. Figure 3 also shows that the shortest rods (simulation 11) do not achieve ordering but an angle only slightly above the random angle of 45°, while the intermediate rods of simulation 8 achieve a very good ordering. It can also be observed that the shorter the particles, the more readily the initial horizontal lattice is broken up. This suggests that under same vibrations very long rods might stay trapped in a horizontal lattice.

A more detailed insight into the effect of particle length on steady state vertical ordering can be gained from Fig. 4. Here we consider the effect of particle length on the ordering achieved after 1400 s of vibration at 3 g. On the left axis we plot the mean angle with the horizontal plane of the bottom-most two layers of the medium, which shows a maximum for 12.9 mm rod length (simulation 8). On the right axis we

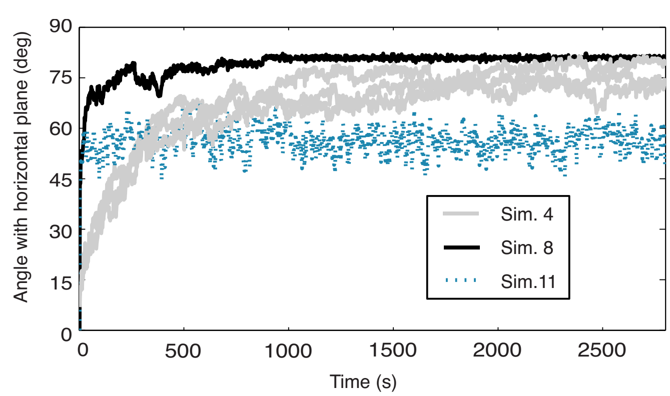

FIG. 3. (Color online) Simulations 4, 8, and 11: Influence of particle length on vertical ordering induced by 3 g acceleration. Plot against time of the mean angle with the horizontal plane of the bottom-most two layers of the medium.

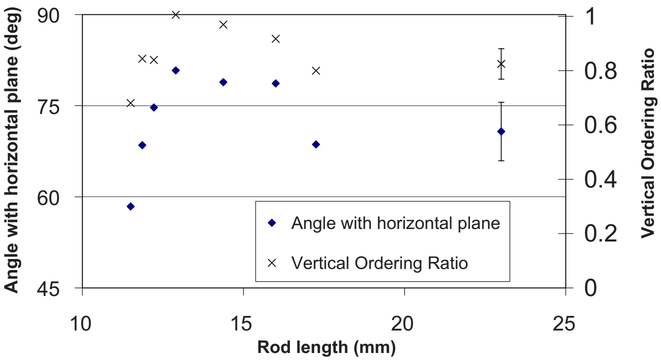

FIG. 4. (Color online) Effect of rod length on the vertical ordering achieved after 1400 s vibration at 3 g: Mean angle with the horizontal plane of the bottom-most two layers of the medium (left axis) and vertical ordering ratio (right axis).

consider the vertical ordering ratio defined as the ratio between the mean angle of the bottom-most two layers of the medium and the maximum angle achievable within each layer. Indeed 12.9 mm rods used in simulation 8 reach the maximum angle they can achieve, considering the lateral periodicity of the box.

Figure 5 shows the effect of varying acceleration on the vertical ordering ratio of the shortest particles used in simulation 11 (triangles), intermediate used in simulation 6 (squares), and longest particles used in simulation 4 (circles). The shortest particles, which do not order vertically at 3 g as described previously, do so at 2 g acceleration. At 3, 4, and 6 g acceleration, they reach an angle approaching the random angle of 45°, while below 1.5 g they stay rather horizontal. The intermediate (simulation 6) particles stay in the initial horizontal lattice at 1.5 g, while they order vertically at 3 g. They do not achieve a complete ordering at 4 g, similarly to what is observed with shorter particles in simulation 8 at 3 g. The longest particles (simulation 4) stay horizontal at 2 g, they order vertically at 3 g, as discussed above, and even better at 4 g. At 6 g the initial horizontal lattice is broken very quickly but the medium stays in a random configuration. We observe therefore the existence of an optimum

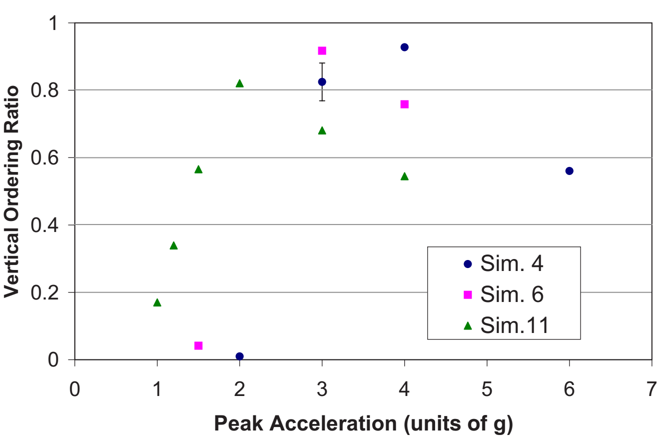

FIG. 5. (Color online) Influence of the acceleration on the vertical ordering ratio achieved after 1400 s of short (simulation 11), intermediate (simulation 6) and long rods (simulation 4).

acceleration to promote vertical ordering. This acceleration is around 4 g for the longest particles used in simulation 4, closer to 3 g for the intermediate particles used in simulation 6 and to 2 g for the shortest particles used in simulation 10.

IV. IS VERTICAL ORDERING LINKED TO VOID SIZES?

How can the rods' intrinsic tendency to form a vertical lattice and the behavior of particles of different lengths be explained? When a granular medium is vibrated, gravity drives particles from upper layers to fill voids that may appear in the lower layers. We showed that spherocylinders orient vertically, regardless of boundary or initial conditions. During the rearrangement through vibrations, a frequent emergence of holes of the size of the particle diameter can be observed. An example of such a hole is highlighted with a white circle in Fig. 1. Such holes can host only particles that are rather vertical. The void-filling mechanism, usually explaining size segregation of spheres [19], may therefore also be at the origin of the vertical ordering of spherocylinders, as already conjectured by Blair *et al.* [10].

To test this interpretation, we analyzed the size distribution of the holes within the medium using the intersect length distribution (ILD) approach. We considered several thousand lateral snapshots of the medium configuration at different moments in time during simulation 4 and filled the holes between the particles with horizontal segments, whose length was taken as a measure of the void size. The symmetry breaking introduced by the vertical orientation of the vibration conditioned our choice of considering horizontal segments.

We focused on two classes of holes: short holes, whose length falls in-between the diameter and the length of the rods and elongated holes, whose length is greater than rod length. Short holes cannot host a horizontal particle: they clearly drive the particles in the medium to orient vertically, if particle neighbors allow this rearrangement. Elongated holes can host a particle at a generic orientation. If a horizontal particle lands in such a hole, its orientation is not modified. If several vertically aligned particles fall into an elongated hole, their orientation is not modified either. However, a long hole can induce a particle of generic orientation falling into it to orient horizontally, thus acting as a horizontal wall, if particle neighbors do not prevent this.

We define λ_s and λ_l as the total length of respectively the short and long voids and λ_t the total void length. For instance, the probability of a void to belong to the class λ_s is

$$P_s = \frac{\lambda_s}{\lambda_t}. \tag{1}$$

Similarly, indicating the medium porosity as ε, we can express the porosity due to small holes as

$$\varepsilon_s = \varepsilon P_s. \tag{2}$$

To judge on the validity of the void-filling interpretation, it is important to look at the void distribution in the portion of the vibration cycle when the medium is bouncing and the par-

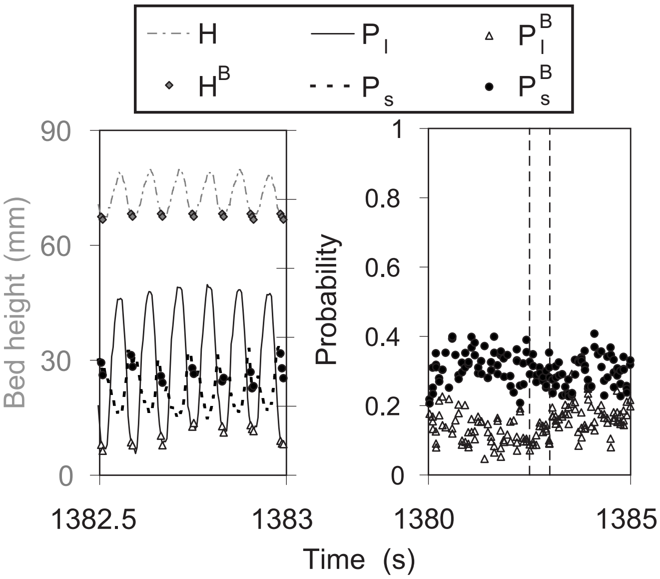

FIG. 6. Simulation 4: Left: detail of the time evolution of the medium height (H, top curve, left axis), and of the probability P_s, P_l of occurrence of short and long voids (bottom curves, central axis). Dots on each curve (H^B, P_s^B, P_l^B) identify the rebounds. Right: P_s^B, P_l^B along several vibration cycles. The dashed area corresponds to the time window magnified on the left side of the figure.

ticles are forced to fill the available holes below their previous positions. The top-left curve in Fig. 6 shows the time evolution of the height of the medium H (left vertical axis) along few vibration cycles, the bottom-left curves that of the probability P_s, P_l of the short and long void classes (right vertical axis). We carefully analyzed the height of the medium to identify instants within the vibration cycles where the medium bounces. These were characterized by a double condition: the medium height is below the threshold of 70 mm (about three particle lengths) and it is decreasing. The diamondlike gray points on the top-left curve of Fig. 6 highlight the value of the medium height when the medium bounces H^B. At those rebounds, the probabilities of the two void classes P_s^B, P_l^B are indicated, respectively, with black circles and white triangles in the bottom-left quadrant. One can see that short holes (of length in between the rod diameter and length) are more probable than long holes. The right side of Fig. 6 shows the probability of the void classes at rebounds P_s^B, P_l^B over a longer time-span and confirm this characteristic pattern: on average about 33% of the void volume within the medium belongs to short holes that promote vertical ordering. This supports void filling as an interpretation for vertical ordering. A lower percentage of the void volume, about 15%, belongs to holes longer than particle length. The gap between the two probabilities is even bigger at an earlier stage, before reordering.

To appreciate the influence of particle length, Fig. 7 compares the porosity at bouncing due to short holes for simulations 4, 8, 10, 11. Shorter particles (simulation 11) show a lower porosity due to short voids, which promote vertical ordering. This observation is in agreement with the lower tendency of short particles to align vertically, shown in Fig. 3. It thus supports the void-filling interpretation, suggesting

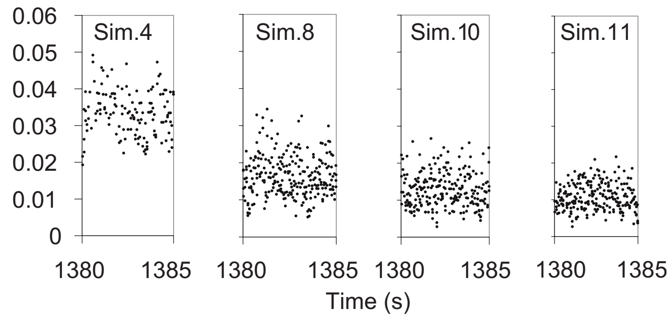

FIG. 7. Influence of particle length on the porosity ε_s^B inducing rods to verticalize. From left to right: simulations 4, 8, 10, 11. The porosity due to long holes ε_l^B is similar for these four simulations and is omitted.

that a minimum availability of small voids is needed for vertical ordering to occur. ε_l^B is similar for these four simulations and is omitted.

In Sec. III we discussed the effect of acceleration on ordering (Fig. 5). An optimum acceleration exists to promote vertical ordering, higher for the longest particles (simulation 4) than for the shortest particles (simulation 11). Applying the same ILD approach to these simulations, we obtain the void distributions shown in Fig. 8. For all accelerations, ε_s^B is higher for long particles (simulation 4) than for short particles (simulation 11) as already observed for an acceleration of 3 g. The height of the medium as well as the porosity contributed by the long and short voids also increase monotonically with acceleration. As already commented, Fig. 5 shows that significant vertical ordering occurs in simulation 11 at 2 g, while a random arrangement is obtained for higher accelerations. Therefore, the monotonic dependence of ε_s^B on

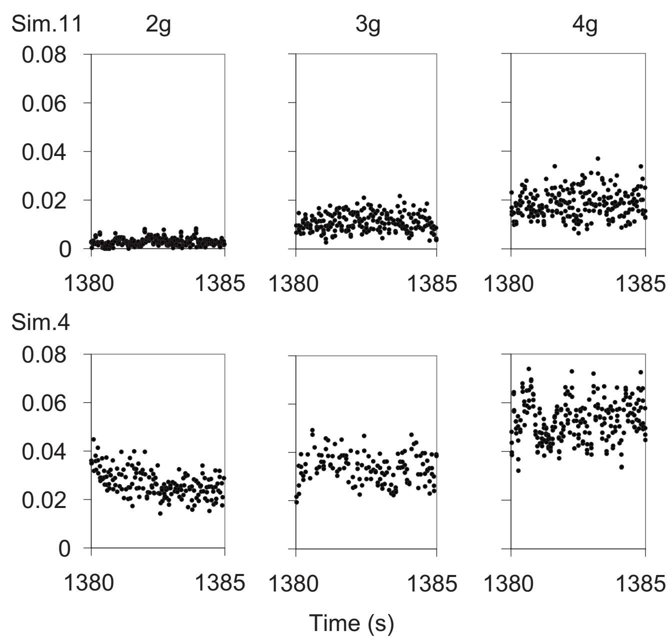

FIG. 8. Effect of acceleration on the porosity ε_s^B inducing rods to verticalize. Acceleration changes from 2 to 3 to 4 times gravity moving from left to right. Simulations 11 with short particles are at top; simulations 4 with long particles are at bottom.

acceleration does not, by itself, allow a clear and thorough interpretation of the dependence of vertical ordering on acceleration reported in Fig. 5. This led us to an alternate explanation to vertical ordering, which we describe next.

V. POTENTIAL ENERGY BARRIERS

Holes are needed to allow any reordering in the medium. Their sizes can influence the reordering, but cannot clearly explain its dependence on acceleration. The evolution of a horizontal or vertical lattice is affected on one side by the rate of creation of the lattice, which is conditioned by the appearance of holes, but also by the rate of its break up. A lattice can be broken up because particles are either expelled from it or rotating into a different orientation. Such a particle has to overcome different energetic barriers. A rod of mass m jumping out of a horizontal resp. vertical lattice has to overcome an energetic barrier of

$$U_H = mgD, \quad \text{respectively,} \quad U_V = mgL. \tag{3}$$

A rod rotating from a horizontal into a vertical position has to overcome an energetic barrier of

$$U_R = mg(L/2 - D/2). \tag{4}$$

For the range of particle lengths and the diameter considered in this study, the following inequalities hold:

$$U_R < U_H < U_V. \tag{5}$$

Shaking a horizontal lattice of rods with a low energy input is insufficient to break the horizontal lattice. Increasing the energy input allows the medium to reach the rotational threshold. In this intermediate range of accelerations, the rods have enough energy to break away from a horizontal lattice through rotation, but not to jump out of a vertical lattice. If energy input is close to the energy barrier that a rod needs to overcome to jump out of a vertical lattice, the latter becomes unstable too and the medium tends to orient at a random angle.

These energetic barriers must be compared with an appropriate measure of the energy available to the vibrated rods. The motion of each particle can be separated into a bulk motion due to sinusoidal vibration and a fluctuation due to collisions. Only the fluctuant part can generate a relative motion of a particle with respect to their neighbors. We therefore define the mean fluctuant kinetic energy of the rods as

$$\widetilde{E_K} = \frac{m}{N} \frac{\sum_{i=1}^{N} (v_i - \bar{v})^2}{2}. \tag{6}$$

We will not venture here into the still open question of defining a granular temperature, but simply call this quantity an energy. This quantity is found to follow periodic variations insensitive to any rearrangement of the rods. We normalize the mean fluctuant kinetic energy of the rods by the rotational and vertical potential energy barriers. Of particular interest are the peaks of these ratios, which give an insight into the ability of the system to break an existing arrangement.

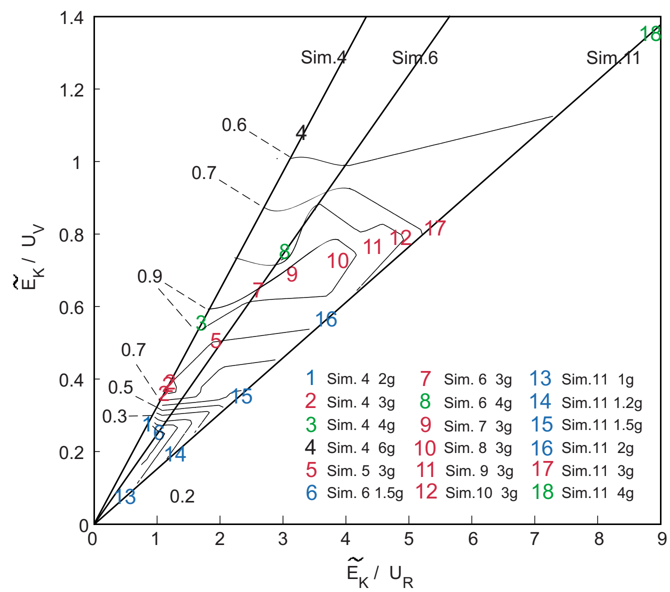

FIG. 9. (Color online) Phase diagram summarizing the peak values of fluctuant kinetic energy normalized by the rotational potential barrier on x axis and by the vertical potential barrier on y axis. Simulations with same rod geometry and increasing acceleration describe a ray moving away from the origin. Contours represent an interpolation of the VOR: zero corresponds to a horizontal orientation, one to the most vertical orientation that rods can achieve. Colors help grouping simulations based on their acceleration: blue identify acceleration lower than 2 g, red 3 g acceleration, green 4 g and black 6 g.

In Fig. 9 we use the peaks of these two ratios to interpret all the results in the form of a phase diagram. A point corresponds to one simulation with given particle elongation and acceleration. Simulations with same rod geometry and increasing acceleration describe a ray moving away from the origin. Contours represent an interpolation of the vertical ordering ratio (VOR): zero corresponds to a horizontal orientation, one to the most vertical orientation that rods can achieve. At low energy input, when not enough energy is available to overcome the rotational barrier ($E_K/U_R < 1$), the initial horizontal lattice is stable and no rearrangement occurs. At intermediate energy input, when rotation is enabled, rearrangement occur leading to a vertical lattice. When an excess of energy is available and rods can overcome the energy barrier to jump out of a vertical lattice ($E_K/U_V > 1$), the system breaks the initial lattice, but evolves toward a random orientation. The transitions between the three regimes are smooth and steady state orientation with intermediate angles are reached across transitions.

VI. CONCLUSION

Vertical ordering of a vertically vibrated medium of rods initially in a horizontal lattice seems intrinsic to particle anisotropy, occurs regardless of initial conditions, and also with no help from side walls. While short particles break away rapidly from the initial lattice but evolve toward a random orientation, longer ones have more difficulties leaving the initial horizontal lattice and they evolve toward a vertical lattice. Too mild a vibration can prevent breakage of the horizontal arrangement, whereas a too vigorous one can prevent the vertical ordering, leading to a random orientation. Thus an optimal acceleration promoting vertical ordering exists, which increases with rod length. We can explain through void filling why long rods tend to orient vertically as opposed to short rods, by assuming that a minimum availability of short voids is needed. However, invoking just void filling, no clear explanation of the dependence on vibration intensity can be found. We therefore consider the energetic barriers that particles need to overcome to exit a horizontal or a vertical lattice. Comparing the maximum available fluctuant kinetic energy with these energetic thresholds, we can identify three regimes. At low energy input, the initial horizontal lattice is stable. At intermediate energy the particles cannot escape from a vertical lattice, which is thus stable. At too high energy input, even the vertical lattice becomes unstable. The notion of low and high energy input depends on rod length, thus reconciling both the effects of the particle length and vibration acceleration on vertical ordering.

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