Micromechanical Simulation and Analysis of One-Dimensional Vibratory Sphere Packing

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We present a numerical method capable of reproducing the densification process from the so-called random loose to dense packing of uniform spheres under vertical vibration. The effects of vibration amplitude and frequency are quantified, and the random close packing is shown to be achieved only if both parameters are properly controlled. Two densification mechanisms are identified: pushing filling by which the contact between spheres is maintained and jumping filling by which the contact between particles is periodically broken. In general, pushing filling occurs when the vibration intensity is low and jumping filling becomes dominant when the vibration intensity is high.

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Particle packing is an important subject in scientific research and industrial application [1,2]. Previous studies of uniform spheres have identified two reproducible states in terms of the packing fraction C [3,4]: random loose packing (RLP, $C \leq 0.60$) and random close packing (RCP, $C = 0.64$). The RCP has been extensively studied in the past decades because of its relation to the so-called maximally random jammed state that is related to phase transition [see [5–8] for example]. Much work has also been conducted on investigating the transition from the RLP to RCP. Experimentally, it has been confirmed that the RCP can be realized by one-dimensional (1D) compaction [4,9] or vibration [3,10–12]. However, the mechanics governing the transition is difficult to study because of the lack of information about the force network and structural rearrangement. In principle, this difficulty can be overcome by computer simulation. Many simulation algorithms have been developed aiming to reproduce the RCP under vibration or other conditions [see [13–17] for example].

The formation of a packing is a dynamic process which involves various interparticle forces. Therefore, a successful simulation method must take into account all dynamic factors related to both geometry and force. As noted by Liu *et al.* [16], most of the previous methods involve different assumptions and criteria for packing growth and stability and ignore the forces, hence failing to produce results fully comparable to those measured, particularly when forces rather than the gravity are dominant. This remark applies to the densification under vibration that is governed by external mechanical forces. Indeed, deficiency can be observed in the previous studies [13–15]. For example, the packing generated by Tory and Jodrey [13] gives a packing fraction comparable to the RCP but a much lower mean coordination number. Tapping or vibration even loosens the RLP according to the algorithm of Mehta and Barker [14]. The model of Philippe and Bideau [15] overcomes this problem but may have limited application because it has not taken into account the friction and other interparticle forces. Dynamic simulation based on the so-called discrete element method (DEM) can overcome this deficiency. The validity and advantage of this simulation technique have been clearly demonstrated by various investigators [16,18–24]. In recent years, understanding the role of different interparticle forces and their spatial and statistical distributions in a packing emerges to be an important area in granular research [see [25–28], for example]. The use of such dynamic simulation is therefore even more attractive.

Here we extend the method used in our previous work [19] to study the transition from the RCP to RCP under 1D vibration. We will first show that the densification process can be reproduced with the method employed, and then analyze the densification mechanisms in relation to structure and interparticle forces.

We simulated the packing of 2000 particles with a set of parameters same as those used for glass beads [19]. Different material properties will affect their associated forces and hence results [20,23]. This is also the case for packing under vibration, although this is not concerned in this Letter. All simulations started from the random generation of spheres with no overlap in a rectangular container of a length $12d$ (= sphere diameter) with periodic boundary conditions imposed in the horizontal directions.

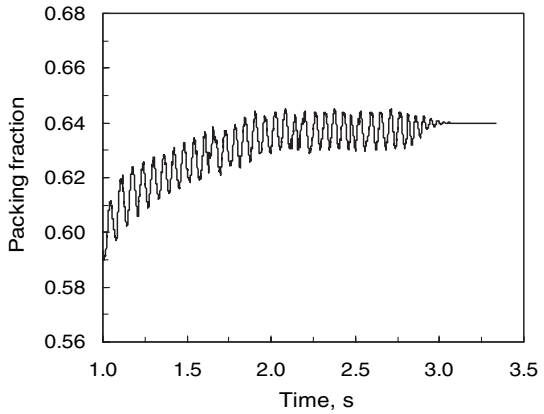

FIG. 1. Evolution of the packing fraction when $A = 0.1d$ and $\omega = 100$ rad/s.

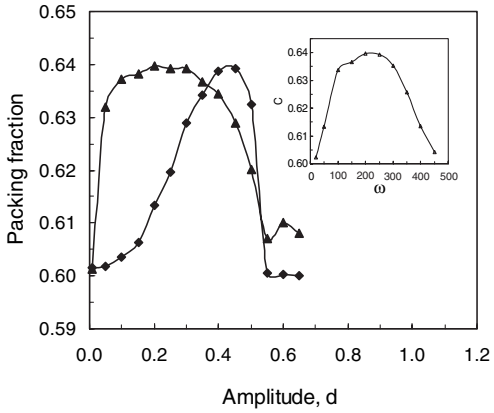

FIG. 2. Effect of amplitude A on packing fraction C for different vibration frequency ω: ◆, $\omega = 50$ rad/s; ▲, $\omega = 200$ rad/s. The inset shows the effect of ω on C when $A = 0.2d$.

The spheres were allowed to fall down under gravity. After 1 s when all particles were settled to form a packing of $C = 0.588$, the container base, which has the same properties as particles, was vibrated in the vertical direction according to: $Z(t) = A\sin[\omega(t - t_0)]$, where Z is the vertical displacement at time t, A and ω, are, respectively, vibration amplitude and frequency, and t_0 (= 1 s in this work) is the starting time of vibration. The values of A and ω used in this work are 0.01–$0.65d$ and 20–500 rad/s, respectively. We calculated the packing fraction for a section of bed at the height from $1/4Z_{\max}$ to $3/4Z_{\max}$ ($Z_{\max}$ = the maximum height of the packed bed). We also used a larger number of spheres (up to 10 000) in some simulations and obtained almost identical results, indicating the wall effect has been satisfactorily eliminated in this work.

Figure 1 shows the evolution of packing fraction C during vibration when $A = 0.1d$ and $\omega = 100$ rad/s. Three regions can be identified. The first region is from 1 to about 2 s, where C increases with time. The fluctuation observed corresponds to the vibration which compresses and relaxes the packing periodically. In the second region, packing fraction simply fluctuates around a constant value. The third region started at $t = 2.8$ s when vibration stopped, and particles gradually settled down to form a stable packing. The three regions were observed for all the simulations conducted, although the packing fraction of the final packing varies with operational conditions. For this particular case, $C = 0.64$. Note that the present densification process is more related to that in a conventional vibratory experiment [10,11], which differs from the one that induces a deexcitation period in order to obtain the RCP [12,15]. Rosato and Yacoub [21] also used DEM to study particle packing under vibration. However, their work differs from ours considerably. This can be reflected from the simulation conditions. For example, they only used 600 spheres and conducted two simulations. The packing fraction obtained varied from 0.53 to 0.60 in their work. They hence did not obtain the RCP and discuss the densification mechanisms.

Different ω and A may result in different final state and packing fraction. Figure 2 shows their effects. For a given ω or A, C increases with A (or ω) to a maximum and then decreases. The maximum packing fraction corresponds to the RCP. When ω is high, high C can be obtained in a wide range of amplitude. On the contrary, vibration at a low frequency requires relatively a large and narrow range of amplitude to produce high packing fraction. Although not fully valid [21], the concept of vibration intensity $\Gamma = A\omega^2$ is often used to examine the combined effect of A and ω [12,15]. Increasing Γ can increase the external energy or force that can be used to transform a packing from a loose to dense state. Γ must be high enough to break down the interparticle locking or bridges among particles initially formed. However, a too large Γ may excite the packing too much, and the final packing state is produced under the condition similar to pouring particles to form a packing. In that case, packing fraction is low, varying with the deposition rate [20,29]. Such packing behavior may correspond to different convective regimes under vibration [30,31].

To test if the densest packing corresponds to the RCP at a microscopic level, we compared the simulated and measured structural data. The so-called measured data were from Finney's packing for uniform spheres [4], as used elsewhere [32]. Figure 3(a) shows the frequency distribution of coordination numbers. The results were obtained using a cutoff distance $1.05d$. That is, a contact between two particles is counted if their center distance is less than $1.05d$. It can be seen that the distribution shifts to the right, corresponding to the densification from the loose to dense packing. Notably, the simulated and mea-

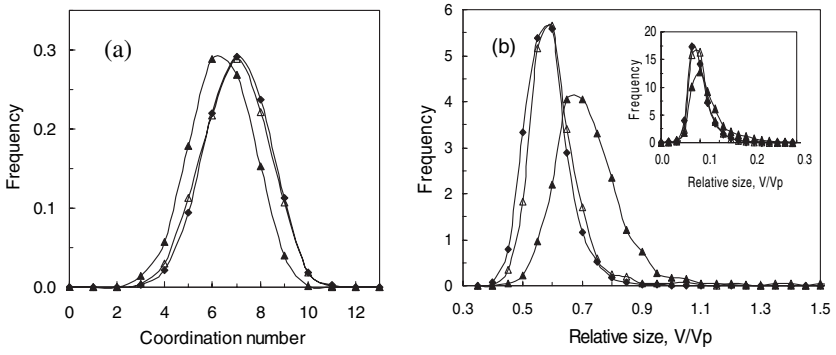

FIG. 3. Frequency density distribution of coordination numbers (a), Voronoi and Delaunay (inset) subunits (b) for different packing: ▲, loose packing; ◆, dense packing; and △, Finney's packing [4]. V and V_p are, respectively, the void volume of a subunit and the volume of a particle. The RCP was produced when $A = 0.2d$, and $\omega = 200$ rad/s.

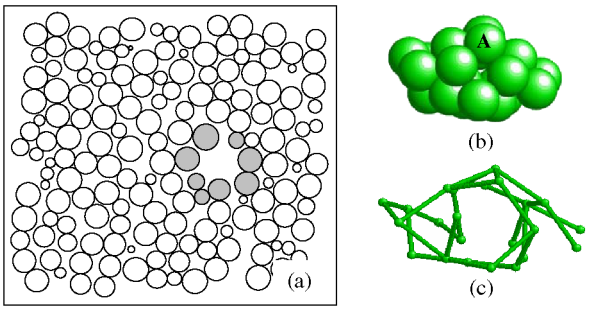

FIG. 4 (color online). Existence of a macropore formed by 23 spheres: (a) identified from the simulated RLP by the greyed particles from two-dimensional slice scanning, (b) three-dimensional visualization, and (c) the connection among the 23 spheres.

sured distributions for the dense packing are quite comparable, particularly considering the experimental error and the fact that Finney's packing was obtained under conditions more similar to 1D (radial) compaction rather than vibration [4,9]. This agreement clearly indicates that, different from the previous simulations [13], the RCP can be reproduced without the loss of realistic structural information such as coordination number.

The good agreement between the measured and simulated structures for the RCP can be further verified from the results of Voronoi and Delaunay subunits, as shown in Fig. 3(b). Different from the coordination number which varies with the critical distance, Voronoi-Delaunay tessellation generates a unique configuration of a packing, so that the resultant comparison is more definite. We also examined the packing structures corresponding to the RCP, obtained with different A and ω. The results indicated that the structure is very comparable, not sensitive to the way to reach the densest state.

The above facts confirm that the RCP is indeed a critical state of particle packing and it can be achieved in different ways. Gotoh and Finney [33] discussed this packing state based on a statistical geometrical argument. We believe that the RCP is the densest state uniform spheres can achieve when packed under the effect of one 1D dominant force. Its packing fraction can be sightly higher than 0.64, as implied by Fig. 1 (Region 2), which corresponds to an unrelaxed state during vibration. Higher packing fractions are achievable when 3D vibration is used, which will be discussed in detail separately. This consideration may apply to other packing systems, e.g., amorphous solids or glasses involving different types of forces and packing conditions which may, however, function similarly.

According to Bernal [34], micropores should be small and cannot accommodate a particle, and macropores may be large enough to accommodate a particle. Figure 3(b) clearly indicates that there are macropores in the RLP. Scanning the packing slice by slice indeed shows the existence of macropores. Figure 4 shows one example, where the macropore consists of 23 spheres in three dimensions. The densification under vibration must be linked to the elimination of these macropores. The governing mechanisms can be elucidated by tracing the motion of the particles during the transition from the RLP to RCP.

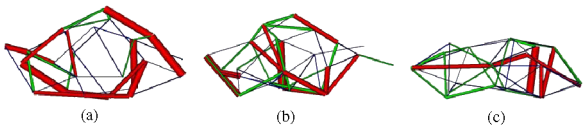

FIG. 5 (color online). Evolution of the force structure when $A = 0.05d$ and $\omega = 180$ rad/s for the macropore in Fig. 4: (a) $t = 1.016$ s, (b) $t = 1.037$ s, and (c) $t = 1.062$ s.

Two different mechanisms were identified from such analysis: pushing filling (PF), in which contacts between spheres are maintained, and jumping filling (JF), in which contacts between particles may be broken during in a densification process. Figure 5 shows the evolution of the normal contact force structure corresponding to the PF mechanism for the macropore identified. The force structure is represented by sticks which link the centers of two contact particles, and whose thickness is proportional to the magnitude. It can be seen from Fig. 5 that the original contacts among the particles are maintained in their rearrangement to produce a dense structure and more contacts in response to the change in forces. Our results indicate that the PF mechanism dominates when the bed is vibrated with relatively low Γ. Figure 6 shows the force evolution when the JF mechanism is effective. It is clear that the original force network for the macropore is broken for some particles during vibration. This occurs when Γ is relatively high. Interestingly, while the final packing structure is almost the same, the force structure differs [Fig. 5(c) versus Fig. 6(c)], indicating that the force structure is more closely related to the history of formation.

The two mechanisms can also be identified from the variation of coordination number of a particle. We took particle "A" shown in Fig. 4(b) as an example. Figure 7 shows the variation of the contact for this particle under different vibration conditions (here the critical distance is d to link to contact forces). Clearly the fluctuation of coordination number when the PF mechanism is dominant is not as large as that when the JF mechanism is effective. To a large degree, the coordination number increases steadily to its maximum when the PF mechanism is dominant. On the contrary, when the JF mechanism is dominant, the coordination number fluctuates significantly because of the broken and established connections with surrounding

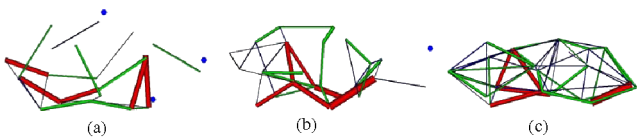

FIG. 6 (color online). Evolution of the force structure when $A = 0.45d$ and $\omega = 90$ rad/s for the macropore in Fig. 4: (a) $t = 1.016$ s, (b) $t = 1.048$ s, and (c) $t = 1.072$ s.

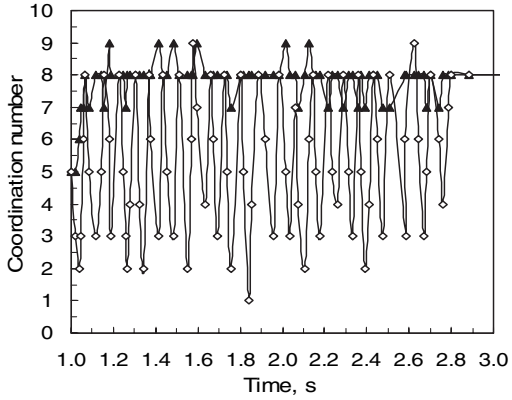

FIG. 7. Variation of the coordination number of particle "A" in Fig. 4, obtained when: ▲, $A = 0.05d$, $\omega = 180$ rad/s; and ◇, $A = 0.45d$ and $\omega = 90$ rad/s.

particles. Instability and hence uncertainty are involved in the formation of a stable packing. Consequently, the RCP and high C can be obtained within a relatively narrow range of A for a given ω (Fig. 2).

In summary, we have shown that the transition from the RLP to RCP under vertical vibration can be satisfactorily reproduced by the DEM. For a given material, the degree of densification is significantly affected by vibration frequency and amplitude. The RCP can only be obtained when vibration frequency and amplitude are properly controlled. We identified two mechanisms governing the densification: pushing filling and jumping filling. In general, pushing filling or jumping filling becomes dominant when vibration intensity is low or high. The two mechanisms may be comparable to those identified by other investigators [14,30,35] who used different techniques and experimental conditions. For example, Pouliquen *et al.* [35] analyzed the trajectory of a single particle and used the concept of caging to explain the random motion of particles in a densification process. The DEM-based studies as shown in this Letter can help clarify this matter because the analysis is based on not only the trajectories but also the transient contact and force network of particles. The slow relaxation and compaction of particles under vibration is related to various most basic problems of granular matter [31]. Granular dynamics simulation offers a convenient way to probe the underlying physics complementing physical experiments that may experience a difficulty in generating detailed results at particle and microstructural scales.

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[1] R. M. German, *Particle Packing Characteristics* (Metal Powder Industries Federation, Princeton, NJ, 1989).
[2] *Disorder and Granular Media*, edited by D. Bideau and A. Hansen, Random Materials and Processes Series (Elsevier Science Publishers B.V., North-Holland, 1993).
[3] G. D. Scott, Nature (London) **188**, 908 (1960).
[4] J. L. Finney, Proc. R. Soc. A **319**, 479 (1970); for experimental details, see: J. D. Bernal and J. L. Finney, Nature (London) **214**, 265 (1967).
[5] J. D. Bernal, Proc. R. Soc. A **280**, 299 (1964).
[6] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, Rev. Mod. Phys. **68**, 1259 (1996).
[7] S. Torquato, T. M. Truskett, and P. G. Debenedetti, Phys. Rev. Lett. **84**, 2064 (2000).
[8] C. S. O'Hern *et al.*, Phys. Rev. E **68**, 011306 (2003).
[9] K. Kawakita and K.-H. Lüdde, Powder Technol. **4**, 61 (1971).
[10] J. E. Ayer and F. E. Soppet, J. Am. Ceram. Soc. **48**, 180 (1965).
[11] G. D. Scott and D. M. Kilgour, Br. J. Appl. Phys. **2**, 863 (1969).
[12] J. B. Knight *et al.*, Phys. Rev. E **51**, 3957 (1995).
[13] W. S. Jodrey and E. M. Tory, Powder Technol. **30**, 111 (1981).
[14] A. Mehta and G. C. Barker, Phys. Rev. Lett. **67**, 394 (1991).
[15] P. Philippe and D. Bideau, Phys. Rev. E **63**, 051304 (2001).
[16] L. F. Liu, Z. P. Zhang, and A. B. Yu, Physica (Amsterdam) **268A**, 433 (1999).
[17] *Granular Matter: An Interdisciplinary Approach*, edited by A. Mehta (Springer-Verlag, Berlin, 1994).
[18] K. Z. Y. Yen and T. K. Chake, J. Appl. Phys. **71**, 3164 (1992).
[19] R. Y. Yang, R. P. Zou, and A. B. Yu, Phys. Rev. E **62**, 3900 (2000).
[20] Z. P. Zhang *et al.*, Powder Technol. **116**, 23 (2001).
[21] A. D. Rosato and D. Yacoub, Powder Technol. **109**, 255 (2000).
[22] L. E. Silbert *et al.*, Phys. Rev. E **65**, 031304 (2002).
[23] R. Y. Yang, R. P. Zou, and A. B. Yu, J. Appl. Phys. **94**, 3025 (2003).
[24] O. Skrinjar and P. L. Larsson, Comput. Mater. Sci. **31**, 131 (2004).
[25] C.-H. Liu *et al.*, Science **269**, 513 (1995).
[26] F. Radjai *et al.*, Phys. Rev. Lett. **77**, 274 (1996).
[27] R. Blumenfeld, Phys. Rev. Lett. **93**, 108301 (2004).
[28] C. Goldenberg and I. Goldhirsch, Nature (London) **435**, 188 (2005).
[29] J. C. Macrae and W. A. Gray, Br. J. Appl. Phys. **12**, 164 (1961).
[30] P. Philippe and D. Bideau, Phys. Rev. Lett. **91**, 104302 (2003).
[31] P. Richard *et al.*, Nat. Mater. **4**, 121 (2005).
[32] G. J. Cheng, A. B. Yu, and P. ZuIli, Chem. Eng. Sci. **54**, 4199 (1999).
[33] K. Gotoh and J. L. Finney, Nature (London) **252**, 202 (1974).
[34] J. Bernal, Nature (London) **183**, 141 (1959).
[35] O. Pouliquen, M. Belzons, and M. Nicolas, Phys. Rev. Lett. **91**, 014301 (2003).