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DEM Simulation of Experimental Dense Granular Packing

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Abstract. In this study we present numerical analysis performed on the experimental results of sphere packings of mono-sized hard sphere whose packing fraction spans across a wide range of $0.59 < \Phi < 0.72$. Using X-ray Computed Tomography (XCT), we have full access to the 3D structure of the granular packings. Numerical analysis performed on the data provides the first experimental proofs of how densification affects local order parameters. Furthermore by combining Discrete Element Method (DEM) and the experimental results from XCT, we investigate how the inter-granular forces change with the onset of crystallization.

Keywords: Sphere packing; Granular materials; Order parameters; Force Chains

PACS: 45.70.Cc; 45.70.-n; 45.70.Qj

INTRODUCTION

The hard spheres packing model has gained considerable attentions in the field of condensed matter physics due to its outstanding ability in reproducing the essential structural properties of liquids¹, crystals, glasses, colloidal suspensions², granular media and even in optimization problems such as those in information theories³. Numerous experimental studies have shown that mechanically stable packings of mono-sized spheres can be generated at different densities from $\sim 0.55\%$ ⁴⁻⁶ called the Random Loose Packing (RLP) bound to $\sim 0.64\%$ ⁷ known as the Random Close Packing (RCP) limit. Numerical simulations, on the other hand, have been able to produce packings of spheres from the RLP limit of ~ 0.55 ⁸ to the maximum density of 0.74 ⁸ which corresponds to HCP or FCC configurations. Previous structural analyses revealed that massive structural reorganization occurs in the packing when RCP limit is passed⁸. In a series of novel experiments we produce sphere packings whose densities range from ~ 0.59 to ~ 0.72 ⁹. In this paper we present a numerical study of these packings investigating the evolution of their geometrical and mechanical properties. We show the emergence of local and global orders as the system undergoes structural transitions.

I. Sample Information

Fourteen dense packings of spherical acrylic beads have been prepared using a shaker allowing for both

vertical and horizontal vibrations. Three packing geometries of rectangular cube, triangular prism and cylindrical used in this study provide a wide range of boundary conditions for our packings. XCT is used to digitally access the internal 3D structure of each sample with a spatial resolution of 4.78 microns. Bead centers, diameters as well as the packing density are readily calculable from the CT images^{10,11}. Table I summarizes basic statistics of the packings derived from the CT data. A number of limitations come with the XCT technique; chief amongst them is the limited spatial resolution (voxel size). Additionally during the binarization process, where the tomograms are thresholded, small amount of uncertainties on the bead centers and diameters are introduced. The thresholding (segmentation process) of the tomograms causes an overestimation of grains radii, which in turn affects the detection of true grain-grain contacts¹². In order to overcome the limitations imposed by XCT, the resulting data of the XCT namely position and radius of each grain is fed into a Discrete Element Method (DEM) code. We use LIGHHHTS, an open-source DEM code widely used in granular community¹³. The particles are then let to relax under the gravity according to the Hertz-Mindlin contact law. Grains interact via a repulsive force proportional to the amount of overlaps between them and their Young's modulus.

An important advantage of combining the experimental data from XCT with the DEM simulations is the ability to access inter-granular forces as well as precise definition of grain contacts which

otherwise could not be available directly from the raw CT data¹⁴.

Figure 1 shows a 2D slice through the tomogram of a cylindrical packing. Our packing protocol produces dense packings where both random and crystal phases coexist.

As a result the packing density is not uniform within each sample and there are regions of high and low densities. Second column of Table 1 reports the mean density of the whole packing for each sample. In order to investigate the geometrical properties, each sample was divided into non-overlapping cubic sub-volumes each containing about 4000 grains. In the following sections, we discuss methods to characterize such packings in terms of their geometrical and mechanical signatures.

Figure 1. A 2D slice through the tomogram of sample 5.

TABLE 1. Summary of the experimental samples used in this study. The first column is the type of container of the grains. The second column is the number of grains used in analysis of the data. This is less than the number of grains in the experiments since to remove boundary effects 3 layers of grains has been fixed while relaxing the spheres. The third column is the packing fraction of the whole system as explained in the text. The forth column is the diameter of the grains used. The last column is the polydispersity caused by the thresholding methods.

Container	N	Φ	D	P
1 Cylinder	26498	0.59	1.62	$2.6 \cdot 10^{-3} \%$
2 Cylinder	25797	0.61	1.62	$1.96 \cdot 10^{-3} \%$
3 Cylinder	27555	0.60	1.62	$1.96 \cdot 10^{-3} \%$
4 Cylinder	27665	0.61	1.62	$1.89 \cdot 10^{-3} \%$
5 Cylinder	31005	0.64	1.62	$4.3 \cdot 10^{-3} \%$
6 Cylinder	175452	0.69	1.00	$4.6 \cdot 10^{-3} \%$
7 Cylinder	111201	0.63	1.00	$8.81 \cdot 10^{-3} \%$
8 Triangular prism	58596	0.71	1.00	$5.51 \cdot 10^{-3} \%$
9 Triangular prism	58675	0.70	1.00	$5.3 \cdot 10^{-3} \%$
10 Triangular prism	53246	0.64	1.00	$5.83 \cdot 10^{-3} \%$
11 Rectangular cube	52098	0.60	1.00	$17 \cdot 10^{-3} \%$
12 Rectangular cube	21143	0.72	1.62	$3.52 \cdot 10^{-3} \%$
13 Rectangular cube	21007	0.70	1.62	$3.7 \cdot 10^{-3} \%$
14 Rectangular cube	22430	0.70	1.62	$3.55 \cdot 10^{-3} \%$

II. Geometrical Characterization

To characterize the rich and diverse local structures of our packings, we use two of the common local order parameters, (q_l, w_l) , that are routinely used to analyze the local structural motifs in granular systems¹⁵:

$$q_l = \left(\frac{4\pi}{(2l+1)} \sum_{m=-l}^{m=l} |q_{lm}(i)|^2 \right)^{1/2}$$

where $q_{lm}(i) = N_{nn}(i)^{-1} \sum_{j=1}^{N_{nn}(i)} Y_{lm}(r_{ij})$ and Y_{lm} are the spherical harmonics and r_{ij} are the vectors connecting the centers of spheres i and j and:

$$w_l = \sum_{\substack{m_1, m_2, m_3 \\ m_1+m_2+m_3 \neq 0}} \begin{bmatrix} l & l & l \\ m_1 & m_2 & m_3 \end{bmatrix} \times q_{lm_1}(i) q_{lm_2}(i) q_{lm_3}(i)$$

Here we have chosen $N_{nn}(i)$ to be the first twelve neighbors of each sphere. The bracket is the Wigner 3j symbol. These two quantities show the emergence of local and global order in the system. From w_l a new and extremely sensitive measure of the structural order parameter w_6^{hh} can be derived as $\hat{W}_6(w_6^{hh}) = 1/2$ ¹⁵. $\hat{W}_6$ is the cumulative distribution function¹⁵:

$$\hat{W}_6(x) = \int_{-\infty}^x n(w_6) dw_6$$

Figure 2 and 3 show the behavior of q_6 and w_6^{hh} as a function of the packing fraction. Comparison of

Figure2. Order Parameter q_6 .

figures 2 and 3 shows that the advantage of w_6^{hh} over q_6 clearly showing structural transition at RCP and the onset of crystallization at $\Phi=0.68$. It is noteworthy that w_6^{hh} shows three distinct regions: *i.* pre-RCP, $\Phi < 0.64$ *ii.* the coexistence phase $0.64 < \Phi < 0.68$ and *iii.* the start of FCC or HCP domination $\Phi > 0.68$. Note that q_6 results are more scattered due to the difference in the values

of q_6 for *fcc* and *hcp* order ($q_6^{fcc} \approx 0.57$ and $q_6^{hcp} \approx 0.48$). Such difference is far less pronounced for w_6^{hh} ($w_6^{fcc} \approx -1.31 \times 10^{-2}$ and $w_6^{hcp} \approx -1.25 \times 10^{-2}$)¹⁵.

Figure 3. Order Parameter w_6^{hh} .

Figure 4 shows the presence of both types of these orders for a sub-volume of sample 6 which has a packing fraction above the RCP limit.

Figure 4. Probability Distribution Function and Cumulative Sum of Parameter q_6 .

III. Mechanical Characterization

One of the most investigated parameters in the literature of sphere packing is the average number of neighbors for each grain or coordination number. It is important to note that the difference between the mechanical coordination number Z which includes the contacts with non-zero force and geometrical coordination number z which can also include 'trivial' contacts with zero force¹⁶ also known as near contact⁸. Even in the case of numerical simulations with perfectly mono-sized spheres, due to the round off errors in calculating the overlap between two neighboring particles that may not be quite in contact (giving rise to a zero force) but close enough to be considered as contributing to the geometrical coordination number¹⁶.

The Modified Radial Distribution Function (MRDF) introduced by Makse et al¹⁷ can distinguish between the real touching grains leading to mechanical coordination number and those which are close enough

to be considered neighbors. The MRDF is formulated as follows:

$$g_z(r) = \frac{1}{N} \frac{R^2}{r^2} \sum_i \sum_{j \neq i}^N \theta\left(\frac{r_{ij}}{r-R}\right) \theta\left(\frac{r+R}{r_{ij}}\right)$$

where R is the radius of particles, N is the number of particles, r_{ij} is the distance of two particle's centers and θ is the Heaviside step function. Figure 5 shows $g_z(r)$ as a function of $\Delta(r)$ which is defined as $\Delta(r) = \frac{r-R}{2R}$ for three sub-volumes of sample 7 with different packing fraction. The value of $g_z(r)$ in the limit of $\Delta(r) \rightarrow 0$ corresponds to the mechanical coordination number Z and the maximum value of $g_z(r)$ can be taken as the geometrical coordination number

Figure 5. MRDF for three sub-volumes.

The slight polydispersity in our sphere packings has an immediate effect on $g_z(r)$ function as shown in figure 6 therefore making it impractical to use the limit of $\Delta(r) \rightarrow 0$.

Figure 6. Effect of polydispersity on MRDF. The blue line shows that in case of polydispersed spheres MRDF expands in an interval around $\Delta(r)=0$ so it is not possible to tell at which value of $\Delta(r)$ $g_z(r)$ corresponds to mechanical coordination number.

In order to find the mechanical coordination number, we resort to the DEM simulations through which detailed inter-granular forces are calculated. Simply by counting the number of contacts with none-zero force we are able to obtain the mechanical coordination number. We carry out such calculations for all the sub-volumes within each of the fourteen samples. Figure 7

and 8 show the mechanical coordination number as a function of packing fraction. Sub-volumes belonging to each sample are shown with different symbols. Our results show a plateau between packing fractions 0.64 and 0.68 where the number of mechanical coordination number remains more or less constant.

Figure 7. Mechanical coordination number for samples 1, 6, 7, and 11

Figure 8. Mechanical coordination number for other samples.

This region known as the “coexistence region” contains a mixture of ordered and disordered phases. This result is remarkable; as such plateau has only been suggested previously through simulations in perfectly mono-sized spheres⁹. Beyond the packing fraction of 0.68 the ordered phase dominates and crystalline regions begin to span across the system.

Figure 9 shows the geometrical coordination number versus the packing fraction. Our results of the geometrical coordination number are in good agreement with previous experimental observation.¹⁰ However we show a greater data resolution over a large range of packing fractions from pre-RCP to FCC.

Figure 9. Geometrical Coordination Number as a Function of Packing Fraction

IV. Conclusions and Outlook

In summary we have shown, through a novel set of experiments, that sphere packings with partially ordered regions can be produced. By combining experiments with XCT imaging and DEM simulations, we were able to calculate a wide range of geometrical and mechanical properties in our packings. We showed the emergence and evolution of local and global order parameters for disorder, partially ordered and HCP as well as FCC phases as the packing becomes denser. Furthermore we have shown, for the first time, the existence of a plateau in the mechanical coordination number for packing densities of $0.64 < \Phi < 0.68$ where local orders emerge and gradually dominate the system with increasing packing density. The nature of such plateau and its connection with the topology of force network will be investigated in our future work.

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