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Maximally dense random packings of spherocylinders

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ABSTRACT

A spherocylinder, a convex 3D object consisting of a cylinder with two hemispherical ends, can possess a wide range of aspect ratios and is one of the most studied non-spherical particle shapes. Previous investigations on disordered spherocylinder packings yielded inconsistent packing characteristics, especially the packing density φ, indicating that density alone is not sufficient to uniquely characterize a packing. In this paper, we delineate in the density–order–metric diagram (i.e. order map) the border curve that separates geometrically feasible and infeasible packings of congruent spherocylinders via the geometric-structure approach, i.e., by generating and analyzing a large number of packing configurations with a diversity of densities and degrees of order generated via a relaxation algorithm. We find that the border curve possesses a sharp transition as the packing density increases, i.e., the initial increase of φ is not associated with any notable increase of the degree of order, while beyond a threshold φ value, the increase of density is strongly positively correlated with the increase of order. This allows us to propose the concept of maximally dense random packing (MDRP) state for spherocylinders, which corresponds to the transition point in the boarder curve and characterizes the on-set of nontrivial spatial correlations among the particles. It can also be considered as the maximally dense packing arrangement of spherocylinders without nontrivial spatial correlations. The degree of order of a spherocylinder packing is quantified via the nematic order parameter (S) and the local order metric (S_{Local}), which respectively characterize the level of global orientational order and local order in particle clusters. The latter metric S_{Local}, which measures the average order in the neighborhoods of particles with the second Legendre polynomial, is a new order metric for spherocylinder systems. We find that the packing density of the MDRPs initially increases with the increase of the aspect ratio w from 0, and reaches the maximal value of 0.725 when $w = 0.5$, then drops with further increase of w. The MDRP at $w = 0.5$ is verified to be jammed via a Monte Carlo jamming-testing algorithm and thus, should also represent the maximally random jammed (MRJ) packing state as well.

1. Introduction

Elongated particles are ubiquitous in nature and industry. The aspect ratio, defined as the ratio of the length to the diameter of the largest cross section of a particle, is a common shape parameter for spherocylinders, cylinders, cones, ellipsoids, super-ellipsoids and curved spherocylinders. Spherocylinders, 3D convex objects consisting of a cylinder with two hemispherical ends, have smooth surfaces and can be easily represented via a rigorous mathematical model or by a sphere assembly model. In molecular systems, e.g. liquid crystals, hard parallel spherocylinders are usually used as the fundamental models to study the ordering phenomena. Much attention has been paid on the phase transition in such systems and the elongation effect of the spherocylinders on the mechanically stable phases has been well studied [1,2]. Particle packing is a long studied problem in discrete geometry, which has been a fascination for mathematicians for centuries [3]. Dense particle packings have also been employed as models for a variety of condensed matter systems in equilibrium and non-equilibrium, such as low-temperature states of matters, heterogeneous materials, colloids and granular media [4–6]. Packing problems also arise in a variety of industrial applications, including powder milling and mixing in consumer goods industry and dense multiphase granular flow in oil industrial. It is well known that the initial packing configuration and particle characteristics can significantly affect the discharge dynamics in a hopper flow and segregation behaviors during transportation of powders.

In the last three decades, the packing of spherocylinders has been investigated mainly via numerical simulations. For the ordered packing of spherocylinders, the maximum packing density ($\phi_{\max}$) at a specific aspect ratio can be given by [7]

$$\phi_{max} = \left(\frac{\pi}{\sqrt{27}} + \frac{\pi}{\sqrt{12}}w\right) \Big/ \left(\sqrt{\frac{2}{3}} + w\right). \quad (1)$$

The aspect ratio w of a spherocylinder is here defined as the ratio of the length to the diameter of the cylinder part. In particular, when

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the aspect ratio tends to infinity, the maximum packing density of spherocylinders reaches the packing density of the densest packing of identical disks in two-dimension, which is $\pi/\sqrt{12}\approx 0.9069$. Generally, the maximum packing density of spherocylinders is lower than that of cylinders with the same length and diameter, because of the hemispherical ends.

For the disordered packing of spherocylinders, most studies showed that the optimal shape which gives the highest packing density is the one with $w = 0.5$ [8–12]. Deviation from the optimal aspect ratios will decrease the packing density. However, the reported values of disordered packing densities for spherocylinders in literature are not consistent with each other, which range from 0.64 to 0.722 [8–18]. This strongly suggests that the packing density alone is not sufficient to uniquely characterize a disordered packing [19]. Here, we employ the "geometric-structure" approach, which emphasizes the analysis of individual packing configurations, regardless of their possibilities of occurrence in an ensemble nor the specific protocols used to generate the packings [4]. Disordered packings with the same density can possess a variety of degrees of order and distinct local particle arrangements/ clusters and structural properties. Such local particle clusters should be identified and statistically quantified via proper local order metrics in order to characterize the associated packings. In the comparison of packing properties among particles with various shapes, the same packing state should be used and the same order degree should be ensured. The prevalent packing states in disordered packings are the random close packing (RCP) [20,21] and the maximally random jammed (MRJ) [19,22,23] states. The RCP state does not explicitly consider the degree of order in packings but rather uses an entropic measure to determine the most disordered state. Consequently, one can always increase the packing density by increasing the order level in a "random packing" [19]. The MRJ state represents the most random state in jammed packings, the determination of which sensitively depends on the specific order metrics employed [24]. Therefore, there may be significant differences in the degree of order in MRJ packings of particles with various shapes when quantified using different order metrics. For example, the MRJ packing of tetrahedra was found to have considerable local ordered structures, and thus, could also be considered as the quasi-random packing which is a disordered packing of clusters with significant local order [25,26].

In this paper, we delineate in the density–order–metric plane (i.e. order map) the border curve that separates geometrically feasible and infeasible packings via comprehensive numerical studies. We find that the border curve possesses a sharp transition as the packing density φ increases, i.e., the initial increase of φ is not associated with any notable increase of the degree of order, while beyond a threshold φ value, the increase of density is strongly positively correlated with the increase of order. This allows us to propose the concept of maximally dense random packing (MDRP) state for spherocylinders, which corresponds to the transition point in the boarder curve and characterizes the on-set of nontrivial spatial correlations among the particles. It can also be considered as the maximally dense packing without nontrivial spatial correlations. Since the initial increase of φ from zero is not associated with any notable increase of order in the packing, there is a spectrum of packing states with varying density but similar and very low degrees of order, as quantified via specific order metrics described below, that are statistically indistinguishable from those associated with a state in which the particle positions and orientations are Poisson distributed. We therefore consider these packing states "fully random", since they possess order metrics that are significantly smaller than all of the other geometrically feasible packings. The MDRP is then the one possessing the largest φ among all those "random" packings.

We note that such "random" packings are not characterized by a unique lowest value of order metric, but rather a range of statistically indistinguishable low values. The metrics should not always be zero because ordered structures may occur under a small probability even in the fully random state compatible with the non-overlapping conditions, which is also a property of randomness. Here, we use thresholds of the order metrics to distinguish the "fully random" states to packings with notable order. Such threshold values are determined from a statistical method based on the results of Monte Carlo (MC) simulations. The MDRP state distinguishes itself from the RCP state since the definition of the former explicitly takes into account the degree of order. Therefore, the MDRP is a comparable state among random packings of particles with various shapes. MDRP also differs from the MRJ, since jamming is not a necessary condition for the MDRP, which only considers geometrically feasible packings. For example, a MDRP can be unjammed, and a MRJ packing may have remarkable structures of local orders, such as the MRJ packings of cubes and tetrahedra.

To determine the degree of order in spherocylinder packings, several methods have been employed. The nematic order parameter S is a commonly used parameter for global orientational order [11,27]. Nevertheless, it does not reflect the local order of clusters which are crucial constituents for quasi-random packings [26]. The pair radial distribution function [9,11] and orientational pair radial distribution function [12] have also been employed to identify the local orders in the packings, but they are neither straightforward nor quantified. Cluster analysis has received intensive attentions in the last few years [28–30]. This technique defines local ordered structures as clusters and quantifies the local order via the number of such clusters. In this work, we define the cluster of spherocylinders as an assembly of parallel and contacting particles. We also propose a new order metric S_{Local} to quantify the local order. Thresholds of the order metrics representing the fully random state are determined from a statistical method based on MC simulations. Subsequently, the relation between the packing density and order metrics, i.e. the order maps, can be depicted and investigated, and the MDRPs can be determined from the order maps.

The goal of this work is to provide a general approach to systematically investigate the entire spectrum of geometrically feasible packings of spherocylinders. Specifically, we focus on all geometrically feasible packing configurations, including both ordered and disordered packings that are respectively associated with the equilibrium and non-equilibrium states of spherocylinder systems, instead of the equilibrium phase behavior of the system. We use the analytical model for the particle shape and the relaxation algorithm to generate a diversity of packing configurations of spherocylinders. We find that the nematic and local orders in clusters are the main source of ordered structures in geometric spherocylinder packings. The nematic order parameter and the novel local order metric, which is distinguished from those usually used in equilibrium systems, are separately introduced to evaluate the levels of the global and local orders in a geometric spherocylinder packing configuration. The order maps of packing density vs. order metrics are depicted at different aspect ratios, and the MDRPs are determined from the order maps, which is a well defined packing state for different particle shapes. The optimal shape and the variation of packing properties as a function of aspect ratio are also studied. Moreover, the MDRP at $w = 0.5$ is verified to be jammed using a MC algorithm [31]. Finally, we note that although in this work, we focus on idealized particle shape (i.e., identical spherocylinders) and interaction (i.e., frictionless hard-particle), we believe that our results have practical implications to real granular systems. For example, the variety of statistic packing configurations can be readily used as initial input configurations for subsequent granular dynamics simulations using LIGGGHTS or MFIX software tools. In addition, the local organizing principles and cluster statistics derived based on the identical spherocylinders are generic, and can be immediately applied to real granular systems with similar particle characteristics.

2. Model and algorithm

The sphero-polyhedron model [32], which describes a particle as a set of points with the distance to an inner polyhedron no larger than a given value R, is employed in this work. The sphero-polyhedron