Powder Technology 338 (2018) 67–78

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Uniform and decoupled shape effects on the maximally dense random packings of hard superellipsoids

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ARTICLE INFO

Article history:
Received 11 December 2017
Received in revised form 27 February 2018
Accepted 20 June 2018
Available online 25 June 2018

Keywords:
Superellipsoid
Order parameters
Shape effects
Maximally dense random packing

ABSTRACT

The superellipsoid model is a rich geometric model and is convenient to study the particle shape effects on random packings. The particle shape significantly influences the macroscopic and microscopic structure properties of random packings. In this work, we find uniform and decoupled shape effects on the maximally dense random packings (MDRPs) of hard superellipsoids. Slightly changing the surface shape or elongating (compressing) the particles may influence the random packing density significantly. The influences of surface shape parameter p and aspect ratio w on the random packing densities are decoupled. For the aspect ratio effects, all the packing density curves show “M” type with various p. Meanwhile, the aspect ratio effects are applicable to all the symmetric particles with three equal main cross sections when $w = 1.0$. For the surface shape effects, the packing density curve is also in “M” type with various w. The maximum of the random packing density is obtained at $p \approx 0.7, 2.0$ and $w \approx 0.7, 1.5$. Moreover, we obtain the MDRPs of hard superellipsoids via the inverse Monte Carlo packing method with a wide range of the surface shape parameter. The normalized local cubatic order parameter and a new normalized local bond-orientational order parameter are used to evaluate the order degrees of orientations and bond-orientations in random packings, respectively. The local analyses of the MDRPs of superellipsoids are carried out via the Voronoi tessellation. Two linear relationships between the mean and standard deviation of the reduced Voronoi cell volumes are obtained. Our findings should lead to a better understanding of random packings and are helpful in guiding the granular material design.

1. Introduction

Since Bernal [1] and Scott's [2] studies on the monodisperse sphere packings, the random particle packings have been applied in many fields such as the structures of liquids, glasses, heterogeneous materials and granular media [3–8]. The random packings of spherical and non-spherical particles are widely studied in decades and the particle shape significantly influences the macroscopic (microscopic) structure properties of random packings. The packing density of the Random Close Packing (RCP) of spheres is about 0.64 [1], which is close to that of the Maximally Random Jammed (MRJ) packing of spheres [9]. Previous studies demonstrate that introducing asphericity to the particle shape will change the structure properties and increase the random packing density above that of spheres. The asphericity of a particle can be increased via elongating (compressing), i.e. changing the aspect ratio, such as the spherocylinders [10–19] and ellipsoids [13, 20–27]. Meanwhile, changing the surface shape can also increase the asphericity, for example, the superballs [28]. These two shape factors are independent and fundamental in particle morphology. Therefore, systemically investigating the aspect ratio and surface shape effects on the random packings is important and meaningful.

The superellipsoid model [29] is a rich geometric model and is convenient to study the particle shape effects. It is believed that 80% of shapes of solids can be represented by superellipsoids [30, 31]. Superellipsoids are used to model symmetric particle geometries with a range of aspect ratios and edges ranging from rounded to spiky in shape [32], such as spheres, ellipsoids, superballs, and cylinder-like, cuboid-like, octahedron-like particles. The densest packing of different shaped superellipsoids has been studied by a number of researchers. For example, the densest packing of spheres is the Face-Centered Cubic (FCC) packing or Hexagonal Close Packing (HCP), which was proved by Hales in 2005 [33]. The densest known ellipsoid packings are the SM2 crystal [34] and the SQ-TR crystal [35] for different aspect ratios. The densest known superball packings are the Bravais lattices with different lattice vectors when the surface shape parameter varies [36]. Moreover, the phase behaviors of superballs were well studied by Batten et al. [37] and Ni et al. [38] The phase behaviors of spheroids [39–41] and biaxial ellipsoid [42] have also been systemically investigated.

As for the random packings of different shaped superellipsoids, the aspect ratio effects on the random packing density were not always uniform. The random packings of spheroids were studied by many

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https://doi.org/10.1016/j.powtec.2018.06.033

researchers [13, 20–27] and all their results demonstrated that the packing density reaches the maximum value when the aspect ratio is about 0.7 or 1.5 and the packing density of sphere is a local minimum, which means that slightly elongating or compressing the spheres via ellipsoids will improve the random packing density. Similarly, changing the surface shape away from spheres via superballs will also improve the random packing density, as shown by Jiao et al. in ref. [28]. Furthermore, Delaney et al. [24] and Zhao et al. [27] studied the aspect ratio effects on the random packings of superellipsoids which are elongated or compressed superballs. The random packing density curves are in "M" type when the superball is close to a sphere with the surface shape parameter $p = 5/7, 5/6, 1.0$ and 1.5. Here the shape parameter $p = m/2 = 1/\zeta$, where m is the shape parameter defined in ref. [24] and ζ is the blockiness defined in ref. [27]. However, when the superball is much closer to a cube with $p = 2.0$ and 2.5, the packing density curves are not in "M" type and the maximum value is obtained at the aspect ratio $w = 1.0$ [24, 27]. This is because their packings must be mechanically stable or jammed. The randomness must be compromised and ordered structures dominate to keep the packing structure mechanically stable or jammed when the particle shape is close to an ideal cube. In other words, the final superellipsoid packings in their work are not always on the same random degree and the aspect ratio effects are not uniform as a result of mechanical stability or jamming. Additionally, the maximal surface shape parameter p of superballs already studied is 3.0 [24, 27, 28], which is far from that of the ideal cube. The evolution of the random packings of superballs varying from sphere to cube and the maximal value on the packing density curve are still not well described. Meanwhile, the surface shape effects on the random packings of superellipsoids with different aspect ratios have not been well studied.

In order to compare the packing densities of different shaped particles in a same random state, we introduced the concept of the Maximally Dense Random Packing (MDRP) [19, 43, 44]. The MDRP is defined as the densest packing in the random state in which the particle positions and orientations are randomly distributed as quantified by specified order metrics. The packing density of the MDRP corresponds to a sharp transition in the order map, which characterizes the onset of nontrivial spatial correlations among the particles [43]. The MDRP is regarded as a glass state of hard particle systems with an artificial constraint and is always random. For particles which are good glass formers, the packing density of the MDRP is close to that of the RCP or MRJ packing, such as the MDRPs of octahedra [43] and spherocylinders [19]. However, for bad glass formers which are easy to crystalize, the MDRP is more random with lower packing density, such as the MDRPs of cuboids [44]. Two approaches have been utilized to obtain the MDRP. One is the enumeration method [19, 43], in which the MDRP is chosen as the maximally dense one among varieties of random packings already generated by common random packing algorithms. However, for bad glass formers, the enumeration method may fail to obtain the MDRP because the packing structures are easy to crystalize with common random packing algorithms. The other method is the inverse Monte Carlo packing method [44] in which the MDRP is directly generated via an artificial constraint. The artificial constraint is carried out via the order parameters and is used to prevent the presence of seed crystals or nuclei around which crystal structures form creating a solid.

In this work, we obtain the MDRPs of hard superellipsoids via the inverse Monte Carlo packing method [44] in which the formation of the local ordered structures is suppressed rigorously. The normalized local cubatic order parameter [44] and a new introduced normalized local bond-orientational order parameter are used to evaluate the local order degrees of orientations and bond-orientations, respectively. The influences of surface shape parameter p and aspect ratio w on the random packing densities are systematically investigated. As for the aspect ratio effects, all the packing density curves show "M" type with the minimal value at $w = 1.0$ and two maximal values at $w \approx 0.7, 1.5$. Meanwhile, the packing density curves also show "M" type for surface shape effects. The maximal packing density is obtained at $p \approx 0.7, 2.0$ and the minimal packing density is obtained at $p = 1.0$. Therefore, the surface shape and aspect ratio effects for superellipsoid packings are decoupled. The local analyses of the MDRPs of superellipsoids are carried out via the Voronoi tessellation [45]. Two linear relationships between the mean and standard deviation of the reduced Voronoi cell volume are obtained when the surface shape parameter $p \le 1.5$, or $p \ge 2.0$. Our findings should lead to a better understanding of random packings.

The rest of the paper is organized as follows: in Section 2, we introduce the superellipsoid model and the overlap detection algorithm we use. Then we give the definitions of the order parameters and describe the inverse Monte Carlo packing method which is applied to generate the MDRPs. Finally, the simulation results of the MDRPs of superellipsoids are discussed in Section 3, and concluding remarks are provided in Section 4.

2. Methodology

In this part, we firstly introduce the superellipsoid model [29] and the Perram and Wertheim (PW) potential [46] used to detect overlaps between superellipsoids. Then the order parameters are proposed to evaluate the orientational and bond-orientational order degrees of superellipsoid packings, including the normalized local cubatic order parameter [44] and a new normalized local bond-orientational order parameter. Finally, we describe the inverse Monte Carlo packing method which is used to generate the MDRPs of superellipsoids.

2.1. The superellipsoid model

The superellipsoid model [29] is a rich geometric model and is convenient to study the particle shape effects. It is believed that 80% of shapes of solids can be represented by superellipsoids [30, 31]. Superellipsoids are used to model symmetric particle geometries with a range of aspect ratios and edges ranging from rounded to spiky in shape [32]. The surface function of a superellipsoid in the local Cartesian coordinates is defined as [29].

$$\left[\left(\left|\frac{x}{a}\right|\right)^{2p_0} + \left(\left|\frac{y}{b}\right|\right)^{2p_0}\right]^{\frac{p_1}{p_0}} + \left(\left|\frac{z}{c}\right|\right)^{2p_1} = 1.0 \qquad (1)$$

where a, b and c are the semi-major axis lengths in the direction of x, y, and z axes, respectively, and p_0, p_1 are the surface shape parameters determining the sharpness of particle edges. The superellipsoids degenerate to ellipsoids when $p_0 = p_1 = 1.0$, and are superballs if $p_0 = p_1$, $a = b = c$. Moreover, the surface will be an ideal octahedron with $p_0 = p_1 = 0.5$, $a = b = c$ and a cube with $p_0 = p_1 = +\infty$, $a = b = c$. In this work, we focus on the random packings of superellipsoids which are elongated or compressed superballs with $a = b$ and the surface shape parameter $p = p_0 = p_1$. The aspect ratio w, which is defined as $w = c/a$, is used to describe the aspect ratio effects. Then the surface function in Eq. (1) degenerates to

$$\left(\left|\frac{x}{a}\right|\right)^{2p} + \left(\left|\frac{y}{a}\right|\right)^{2p} + \left(\left|\frac{z}{wa}\right|\right)^{2p} = 1.0 \qquad (2)$$

Fig. 1 shows some typical superellipsoid examples used in this work with different p and w. The surface shape parameter p ranges from 0.7 to 5.0 with the aspect ratio w varies from 0.5 to 2.0. Meanwhile, the packings of octahedra and cuboids, two extremities of superballs with p equal to 0.5 and infinity, respectively, are also studied via the ideal polyhedral model [43]. The shapes of superellipsoids are close to octahedra when p is smaller than 1.0 and are close to cuboids when p is larger than 1.0. Meanwhile, the superellipsoids are compressed if w is smaller than 1.0 and are elongated if w is larger than 1.0, as seen in Fig. 1.

The overlap detection algorithm we use is based on the Perram and Wertheim (PW) potential introduced in ref. [46]. The generalization of