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Order metrics and order maps of octahedron packings

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HIGHLIGHTS

- We propose the concept of the maximally dense random packing (MDRP).
- A local cubatic order metric is proposed to measure the local order degree.
- We obtain the order map of octahedron packings.
- The thresholds of order metrics are determined by Monte Carlo simulations.

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ABSTRACT

We apply the ideal octahedron model and the relaxation algorithm in generating octahedron packings. The cubatic order parameter $[P_4]_1$, bond-orientational order metric Q_6, and local cubatic order parameter P_{4local} of the packings are calculated and their correlations with the packing density are investigated in the order maps. The border curve of packing density separates the geometrically feasible and infeasible regions in the order maps. Observing the transition phenomenon on the border curve, we propose the concept of the maximally dense random packing (MDRP) as the densest packing in the random state in which the particle positions and orientations are randomly distributed and there is no nontrivial spatial correlations among particles. The MDRP characterizes the onset of nontrivial spatial correlations among particles. A special packing with a density about 0.7 is found in the order maps and considered to be the MDRP of octahedra. The P_{4local} is proposed as a new order parameter for octahedron packings, which measures the average order degree in the neighborhoods of particles. The $[P_4]_1$, Q_6 and P_{4local} evaluate the order degree of orientation, bond orientation and local structures, respectively and are applied simultaneously to measure the order degree of the octahedron packings. Their thresholds in the random state are determined by Monte Carlo simulations.

1. Introduction

The packing of octahedra has become one of the focuses of particle packing, and has been researched by simulations [1–8] and experiments [8,9] in the last few years. As one of Platonic solids, the densest packing of octahedra is the optimal lattice packing [1,2], known as the Minkowski lattice with a density of 18/19 [10,11]. Henzie et al. [8] showed that Ag octahedra could self-assemble into their conjectured densest packings and tended to form an exotic superstructure with complex helical motifs by inducing depletion attraction through excess polymer in solution. Jiao and Torquato [3] generated the maximally random jammed (MRJ) packing of octahedra with a density of 0.697 ± 0.005. They also found that the MRJ packing is isostatic and has hyperuniform quasi-long-range correlations. Smith et al. [4,5] studied the athermal jamming

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threshold state of soft frictionless octahedra whose density is about 0.686 ± 0.001. Their results suggested that the average number of face–face contact is a suitable order parameter to determine the jamming state of faceted particle systems [4]. The random loose packing (RLP) and the random close packing (RCP) of octahedral particles were obtained by Baker and Kudrolli via experiments [9] with the packing densities of 0.52 and 0.64, respectively. Considering that octahedron and cube both have octahedral symmetry and are extremes in the class of octahedral symmetry grains, the evolution of the packings of octahedral symmetry particles was studied [5,6]. Meanwhile, the packing properties of superballs, of which the shapes interpolate between cubes and octahedra via spheres, were also researched [12–14].

A number of methods have been employed to measure the order degree in particle packings. Some are the functions of the radial distance, for instance, the orientational correlation function [3,15,16], face–face correlation function [7,15,16] and radial distribution function [7,15,16]. These methods reflect some microscopic properties of a packing structure, but they cannot well distinguish between order and disorder or measure the order degree quantitatively [17]. Other methods tend to give a macroscopic parameter, such as the nematic order parameter [18–20], the cubatic order parameter [21] and the bond-orientational order metric [22–24]. These parameters are often applied to reflect the order degree of orientation or bond orientation in packing structures. Nevertheless, none of these parameters can evaluate all the order forms alone. Generally, several methods should be employed simultaneously to evaluate the overall order degree of a packing structure. Besides the bond-orientational and orientational order forms, the local order structures have been studied as well [5,8,17]. The clusters which are local order structures are the main order forms in quasi-random packings [17,25] and are different from the order of bond orientation or orientation. The size and topological structure of a cluster are closely connected to the packing configuration and packing density [25–28]. As for the packing of octahedra, no effective method has been used to evaluate the local order.

With respect to the random packing of octahedra, some special states with different packing densities have been proposed, such as the random close packing [9,29,30], random loose packing [9], jamming threshold [4,5] and maximally random jammed [3,29,31] states. All these states are often known as the "random packings". The main difficulty in the descriptions of these special random packing states is how to define "random" or evaluate the order degree clearly. In general, several order metrics may need to be used simultaneously to evaluate the overall order degree of a packing and a packing structure is more random with smaller order metric values. However, the order metric values should not be zero even in the random state because order structures may occur under a small probability as a random fluctuation, which is also a property of random. A packing is in the random state when the particle positions and orientations are randomly distributed and there is no nontrivial spatial correlations among particles. Therefore, an order metric of the random state should not be a constant value, but is in a certain range although it is quite small. In this work, we use the cubatic order parameter, bond-orientational order metric, and local cubatic order parameter to evaluate the random degree of octahedra packings, and their thresholds in the random state are determined via Monte Carlo (MC) simulations [26,32–34]. A packing will be random if all its order metrics applied are in the corresponding threshold intervals.

In this work, we propose a new special state of particle packings termed as the maximally dense random packing (MDRP). We define a packing as a MDRP if it satisfies the two conditions as follows. Firstly, the packing must be random, i.e. all the order metric values are in the corresponding threshold intervals of the random state. Secondly, the packing density is maximum which means that the packing is the densest packing on the premise of the random state. The concept of the MDRP is obviously not the same as the RCP since the random condition should be satisfied for the MDRP while order level is not evaluated in the RCP. Meanwhile, the MDRP also has differences with the MRJ packing. Firstly, jamming is not a necessary condition of the MDRP, i.e. a MDRP can be unjammed, while a MRJ packing must be jammed. Secondly, A MDRP must be random enough, while a MRJ packing may have remarkable local ordered structures to achieve jamming, such as the MRJ packings of cubes and tetrahedra. The most advantage of the MDRP is that the packing configuration is in the same order level of the random state for any shaped particle. Therefore, the MDRP is an appropriate state to be used in the density comparison of the random packings of variously shaped particles. We note that the particle packing here is a configuration of non-overlapping hard particles confined to a volume of fixed size with periodic boundary condition. The packing is a geometric one with no considerations about mechanical or thermodynamic stability.

In summary, the purpose of this work is to compute a number of order metrics of octahedron packings and investigate the order maps as well as the special states on the maps. We use the ideal polyhedron model and the relaxation algorithm [15,17,34–40] to generate a large number of packing configurations of octahedra. The cubatic order parameter and bond-orientational order metric are applied to evaluate the orientational and bond-orientational order of octahedron packings, respectively. Then, we propose a new order parameter which measures the average orientational order in the neighborhoods of particles and is demonstrated to well estimate the order degree of local structures in octahedron packings. These three order metrics are used simultaneously to measure the overall order degree of the packing structures of octahedra. Their thresholds in the random state are determined by MC simulations. The order maps of packing density vs. order metrics are depicted, and the MDRP of octahedra is selected and its packing structure is analyzed and compared with the MRJ packing.

2. Model and algorithm

The ideal octahedral model, which has sharp corners and is mathematically accurate, is used in this work to simulate the packing of octahedra. The edge length of the octahedron noted as L is set to be 10.00 in this work. The model is a hard particle model without any deformation. Fig. 1(a) shows an ideal octahedron.