Physics Letters A 378 (2014) 835–838

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Excluded volumes of clusters in tetrahedral particle packing

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ARTICLE INFO

Article history:
Received 30 October 2013
Received in revised form 21 December 2013
Accepted 14 January 2014
Available online 21 January 2014
Communicated by A.R. Bishop

Keywords:
Excluded volume
Cluster
Packing
Tetrahedra

ABSTRACT

We investigate the excluded volumes of clusters in tetrahedral particle packing using an ideal tetrahedron model and Monte Carlo simulation. Both the influences of the size and topology of clusters on the excluded volume are studied. We find that the excluded volumes of the dimer composed of two tetrahedra and the wagon wheel composed of five tetrahedra are relatively lower than other cluster forms. For large clusters, the excluded volume decreases when the topology of a cluster approaches the wagon-wheel geometry. The results give an explanation to the cluster distribution which demonstrates that the dimer and wagon wheel are the dominative cluster forms in the packing structure of tetrahedra.
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1. Introduction

As an example of the 18th problem proposed by Hilbert in 1900 about the densest packing of a given shape [1], the packing of regular tetrahedra has achieved significant advances in the last few years, and becomes a prosperous research area in particle packing, granular material and discrete geometry. Chen et al. [2] presented the densest packing of regular tetrahedra so far with a crystalline structure of dimers which has a density about 0.8563. For the disordered packing of tetrahedra, macroscopic and microscopic properties have been well studied via simulations [3–10] and experiments [11–13]. However, the theoretical packing density limit is still unknown, and further investigations should be carried out to explore the dense packing structure of tetrahedra.

It has been well observed that tetrahedra assemble into some special cluster forms in various packings both from simulations and experiments. Common cluster forms are the dimer (bipyramid), wagon wheel (pentagonal dipyramid), nonamer, icosahedron and tetrahelix [3]. Our recent investigation [10] showed that the relative amount of particles in clusters increases linearly with the growth of the packing density, and the relation is irrelevant to the packing generation method. We termed the hierarchical random packing of clusters as a "quasi-random packing" [10]. We also found that the dimer and wagon wheel are the two dominative cluster forms in the packing structure of tetrahedra [14]. For instance, in a quasicrystal packing structure of tetrahedra [3], the volume fractions of dimers and wagon wheels are about 23.58% and 13.58%, respectively, which are significantly larger than other cluster forms. However, the reason for the phenomenon is still out of reach. In this work, we try to explain the phenomenon via the concept of excluded volume.

The concept of excluded volume was introduced by Werner Kuhn in 1934. In granular and polymer systems, the excluded volume refers to the volume that is inaccessible to other particles as a result of the presence of the first one [15,16]. It was believed that the excluded volume is closely related to packing density, although their relationship is not quite clear yet. Philipse [15] proposed a random contact model and demonstrated that the random packing density has an inverse relation with the excluded volume for long spherocylinders. Gravish et al. [17] and Meng et al. [16] tried to explain the variation of packing density by the excluded volumes of non-convex U particles and curved spherocylinders, respectively. Recently, Baule et al. [18] presented a theoretical framework for packing density prediction based on the concept of the Voronoi excluded volume. Many works have been done to calculate the excluded volume of a single particle, however, the excluded volumes of clusters are rarely referred to in previous works.

The excluded volume of a complex shape particle is usually difficult to calculate [19]. Recently, Torquato and Jiao [20] derived an explicit formula for the excluded volume of a convex hyperparticle of arbitrary shape. As for a tetrahedron and derivative clusters, only the tetrahedron and dimer are convex bodies, and all other cluster forms are non-convex. However, it is rather difficult to give an explicit formula for the excluded volumes of non-convex clusters. Fortunately, the Monte Carlo simulation [16,17,21] provides an optional means to estimate the excluded volume.

The purpose of this work is to compute and analyse the excluded volumes of clusters in tetrahedral particle packings, which are important to the understanding of the packing density and

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http://dx.doi.org/10.1016/j.physleta.2014.01.023

packing structure. We will compare the excluded volumes in different cluster sizes as well as in the same cluster size but different cluster types to investigate the effects of the size and topology on the excluded volume. We also compare the excluded volumes of clusters with face–face joints to those of clusters with other face–face contacts. Thereafter, we try to explain the distribution of cluster types in tetrahedral particle packings using their excluded volumes. Finally, we explore how the excluded volume is related to the packing density.

2. Model and method

All the clusters in tetrahedron packings can be treated as a variety of topological structures of tetrahedra. The particle model used in this work is the ideal tetrahedral model with sharp corners, and its roundness ratio [7] $\gamma = 0$. Clusters defined here are composed of tetrahedra with continuous face–face joints. A face–face joint can be regarded as a strict face–face contact, which satisfies that the two faces are parallel, contacted and coplanar [10]. The size of a regular tetrahedron is measured by its side length. In the three dimensional Euclidean space, the vertex coordinates can be obtained by using a coefficient matrix which describes the relationship between the vertexes and the centroid of the tetrahedron in a local coordinate system. Other geometric properties of the tetrahedron can be easily expressed in terms of the vertex coordinates.

A contact detection algorithm is applied to detect whether two tetrahedra are contacted with each other. In our simulations, we consider two tetrahedra to be contacted if their minimum distance is less than 2.0×10^{-6} (the side length of the tetrahedron is within the spectrum from 1 to 5). First we detect whether their circumscribed spheres are overlapped. If they are not overlapped, the two tetrahedra are surely separated. Then whether the vertexes of a tetrahedron are inside or on the face of the other one is checked. When such vertex exists, the two tetrahedra are overlapped. Afterwards, we detect if one of the edges of a tetrahedron has an intersection point with one of the faces of another tetrahedron. If such edge exists, the two tetrahedra are overlapped. Otherwise, they are separated.

The ideal tetrahedron model is employed to construct cluster models. Each cluster consists of a number of tetrahedra with continuous face–face joints. A tetrahedron has four faces, and each of them can respectively generate a new tetrahedron which has a common face with the original one. Therefore, the cluster model can be built by generating tetrahedra in a certain topological order on a tetrahedron. Meanwhile, by detecting whether two tetrahedra belonging to different clusters are contacted, we can judge if the two clusters are overlapped accordingly.

Twenty typical cluster types in tetrahedron packings are shown in Fig. 1. We note that only clusters with face–face joints, which are very common in simulation and experimental results [10], are considered in this work, except the last one (2-a) with a face–face contact. The cluster type is unique if the cluster consists of less than four tetrahedra, namely the 1-tetrahedron, 2-dimer and 3-trimer for the cluster size of 1, 2 and 3, respectively. The three types of the clusters consist of four tetrahedra, namely the 4-cluster, are termed as 4-a, 4-b and 4-c shown in Fig. 1. There are seven topological structures for 5-cluster, while only six typical types of 6-cluster are considered in this work. These cluster types are also illustrated in Fig. 1. Additionally, a different type of 2-cluster (2-a) is analysed as well to compare the excluded volume of face–face joint clusters with that of other face–face contact clusters.

For a particle with a convex or non-convex shape, the excluded volume can be calculated by the generalised expression as follows

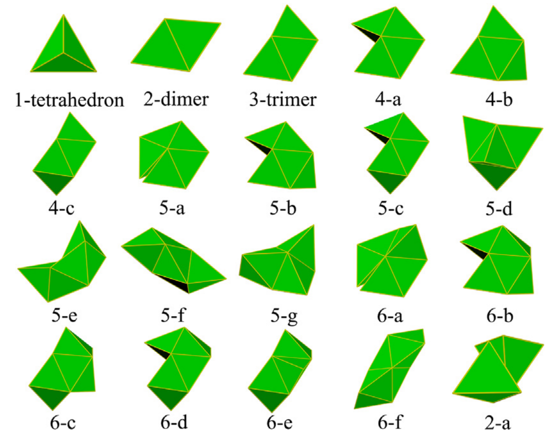

Fig. 1. Typical cluster types in tetrahedron packings with face–face joints. The last one (2-a) is a different two-particle cluster with a face–face contact.

$$V_{ex} = \int_{\boldsymbol{\Omega}} p(\boldsymbol{r}, \boldsymbol{\omega}) \Theta\big(s(\boldsymbol{r}, \boldsymbol{\omega})\big)\, d\boldsymbol{r}\, d\boldsymbol{\omega} \tag{1}$$

where $\boldsymbol{\Omega}$ is the whole three dimensional Euclidean space, $p(\boldsymbol{r}, \boldsymbol{\omega})$ is the positional and orientational probability density function, $\Theta(x)$ is the unit step function, and $s(\boldsymbol{r}, \boldsymbol{\omega})$ is the minimum distance between the central particle and the particle with the centroid position $\boldsymbol{r}$ and orientation $\boldsymbol{\omega}$. If the two particles are overlapped, the minimum distance is determined as -1. For the particles in a random packing, the probability density is uniform, that is $p(\boldsymbol{r}, \boldsymbol{\omega}) = 1$. We thus obtain the following formula

$$V_{ex} = \int_{\boldsymbol{\Omega}} \Theta\big(s(\boldsymbol{r}, \boldsymbol{\omega})\big)\, d\boldsymbol{r}\, d\boldsymbol{\omega} \tag{2}$$

In this work, excluded volumes are mostly obtained through the Monte Carlo simulation [16,17,21]. In a Monte Carlo procedure, a cubic box with a side length L is applied as a sampling space. Then we put one particle at the centre of the box with an arbitrary orientation. Another identical particle is generated in the sampling space with an arbitrary position and orientation, and whether it is contacted with the central one is detected. The procedure is carried out iteratively and N_c particles are detected to be contacted with the central one. Finally, the excluded volume of the particle can be estimated as

$$V_{ex} = \lim_{N \to \infty} \frac{N_c}{N} V_s \tag{3}$$

where $V_s = L^3$ is the volume of the sampling space, N is the total number of tested particles. In fact, Eq. (3) is an equivalent expression of Eq. (2) using a computer simulation scheme. We also introduce the concept of the relative excluded volume which is defined as

$$V_{rex} = \frac{V_{ex}}{V} \tag{4}$$

where V is the volume of the particle. Therefore, the relative excluded volume V_{rex} is dimensionless, and is a constant for a given shaped particle. For example, the V_{rex} is 8 for a sphere.

After a number of attempts, we find that the influence of the dimension of the sampling space on the excluded volume can be eliminated when $L \geqslant 50$ while the side length of the tetrahedron is within the spectrum from 1 to 5. The effect of the number of tests N on the excluded volume is also explored. The excluded volume changes little when N reaches 10^9. The excluded volume of each cluster is computed four times and averaged to reduce errors. With $L = 50$ and $N = 10^9$, the relative error of the excluded

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