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Modeling structures of open cell foams

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ABSTRACT

This work proposes an original geometrical model based on randomly packed spheres using Laguerre-Voronoi tessellations to simulate geometrical and topological characteristics in the microstructure of open cell foams. The model can be used to analyze the effect of coefficient of variation on the pores distribution in real foams. The distribution of foam-cell volumes in foam structures generated in this work is dependent on the log-normal distribution of sphere volumes in corresponding randomly packed spheres. The statistical data of modeled foam structures, including distribution of the cell volume, face and edge number is very close to the characteristics of real materials. The results also show that a higher coefficient of variation in the sphere diameter would decrease the average number of faces per cell. The average number of faces varies from 13.56 to 14.43 for different coefficients of variation of sphere diameter, while the average number of faces in the Poisson-Voronoi tessellation structures is approximately 15.5. Furthermore, the porosity of foam structures, ε, decreases with the ratio of strut diameter to the average diameter of randomly packed spheres, $d_s/E(d)$, while the specific surface area of foams, S_V, increases with $d_s/E(d)$.

1. Introduction

Open cell foams: ceramic, metal, or polymer, have been used in a wide range of industrial areas since they typically possess high specific surface area, high porosity, and efficient thermal insulation [1,2]. In biomedical applications, open cell foams can be viewed as the scaffolds in implantations to reconstruct bones of human body [3,4]. For chemical engineering applications, open cell foams serve as filters, heat exchangers, and catalyst supports due to their strong corrosion resistance and good high temperature resistance [5–7]. Open cell metallic foams are utilized to construct media for heat energy storage since they usually have an enclosed porous structure [8–11].

A number of papers present different models to build open cell foam structures. In general, three approaches exist to model the foam structures. The first method uses the Kelvin cell to obtain the structure. The Kelvin cell, i.e. so-called tetrakaidecahedron in some publications, has fourteen faces (eight hexagonal and six quadrilateral) and twenty-four vertices as shown in Fig. 1. Lord Kelvin studied the bubbles packing pattern in foams. Lord Kelvin (1887) stated that the Kelvin cell was the best shape with minimal surface area for packing equal-sized objects together to fill space. This method entails modeling an idealized periodic cell structure as shown in Fig. 2. The Kelvin cell was viewed as an optimal reconstruction model of real foam structures for a long period. However, Kelvin's model shows some unusual mechanical behaviors that have not been verified by researchers in real materials [12]. The random disorder in real materials might be responsible for those unusual mechanical behaviors [13]. At present some researchers have already claimed that the Kelvin cell cannot obtain certain mechanical properties of real foams due to its lack of randomness, which is an important feature in real foams, and Kelvin's model is anisotropic, which is clearly not the structure of real foams [12,13].

In order to obtain the structure with so-called random disorder, many studies used different methods to consider the randomness of real foam, which are defined as the second approach modeling the foam structures in this work. Habisreuther et al. [14] obtained a randomization of the Kelvin structure by changing the positions of vertices of the ordered Kelvin multi-cells structure using vectors with stochastic directions and stochastic values.

Many other researchers generated the random models by Voronoi tessellation, Laguerre-Voronoi tessellation or Poisson-Voronoi tessellation. With this model, random seed points first are set in space and then a cell is generated by defining the space that is closer to its seed point than to any other points. The randomness of this structure is strongly influenced by the spatial distribution of the seed points. However, the number of struts per vertex of the

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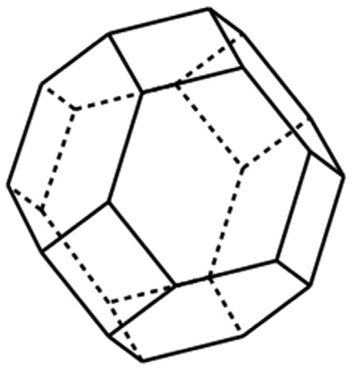


Fig. 1. Structure of Kelvin cell.

structures generated by Voronoi tessellations is higher than that of real foam structures, and the structural parameters of foam structures obtained by Poisson-Voronoi tessellation is different from real foams [14,15]. Wejrzanowski et al. [15] proposed a three-dimensional model for open cell foams using Laguerre-Voronoi tessellation. They also compared the porosity and surface area with the experimental data. The structures developed by Wejrzanowski et al. are closer to real foams than that of the other two tessellations. Skibinski et al. [16] reported the validation of the modeling method (Laguerre-Voronoi tessellation) developed in the literature [15] by comparing the pressure drop obtained for modeled structures with the pressure drop of commercial foams and calculated the permeability of open cell foams. The results also state a relationship between pore size distribution and permeability.

The third method uses digitized images or tomographic images of the foams to reassemble the structures of real foams. X-ray micro-tomography (μCT) and magnetic resonance imaging (MRI) are very powerful tools that can obtain the architecture and microstructures of materials in a non-destructive and non-invasive way. This approach also is called 3D reconstruction technology, which reconstructs a three-dimensional model using two-dimensional image slices such as μCT and MRI stacks [17,18]. However, three-dimensional models obtained this way are unable to represent all investigated foam structures. Such models are very unique for each individual foam sample. Moreover, because the reconstruction process is high-cost, complicated and time-consuming, this technology is not always feasible.

To determine foam properties and investigate the effects of geometrical parameters on foam properties, a general statistical foam model is necessary. In this work, a general model is developed which possesses a random spatial structure and is isotropic, but still has a roughly uniform cell size. A non-periodic arrangement of seed points with a pre-selected size distribution is obtained with LAMMPS (an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator). Random foam structures then are generated using Laguerre-Voronoi tessellations. This model could provide the effects of geometrical parameters on the topological properties of foams. To evaluate the generated model in this work, a series of parameters are discussed, such as the average number of faces per foam cell, porosity, and specific surface area, etc.

2. Methods and modeling

The model (referred to as the LV foam model) generated in this work is a kind of Laguerre-Voronoi tessellation based on the randomly closed packing of spheres. Voronoi tessellation and Laguerre-Voronoi tessellation are the tools that usually are used to obtain the polycrystalline structures of certain materials or to division spaces in many fields.

2.1. Laguerre-Voronoi tessellation

Laguerre-Voronoi tessellation (LVT) is a kind of weighted Voronoi tessellation [19]. For any point p_i in set S, a weight r_i is provided to get a weight set $r = \{r_1, r_2, \ldots, r_n\}$, and the distance between p_i and any point q is given by:

$$d_L(p_i, q) = \{[d_V(p_i, q)]^2 - r_i^2\}^{1/2} \tag{1}$$

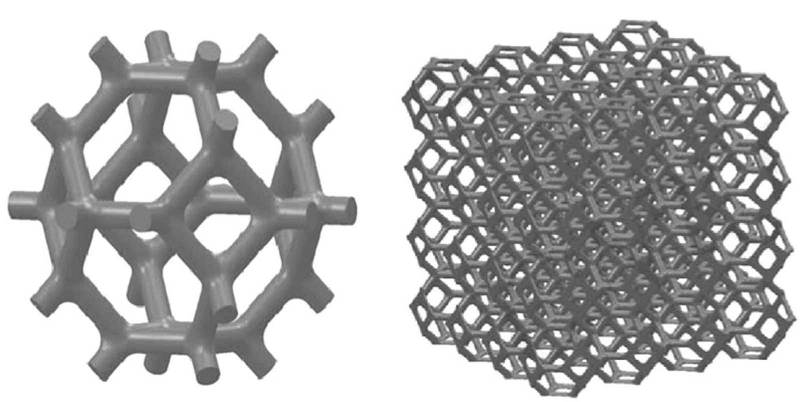
A cell corresponding to point p_i is defined as:

$$\upsilon_L(p_i) = \{p | p \in R^3, d_L(p, p_i) < d_L(p, p_j), i \neq j\} \tag{2}$$

and the set of all cells, $V_L(S, r) = \{\upsilon_l(p_1, p_2, \ldots, p_n)\}$, is referred to as an LV diagram as shown in Fig. 3. Here $\upsilon_l(p_i)$ is the dominant region of p_i with a weight of r_i. From Fig. 3(c), an LV diagram consists of convex polyhedrons without overlaps interconnected in a topological manner.

2.2. Randomly packed spheres

Randomly packed spheres have been extensively studied by both experiments and computer algorithms [20–22]. Among the research methods, computer simulations used to generate randomly packed spheres can be divided into two categories: collective rearrangement algorithms and sequential generation



(a) (b)

Fig. 2. (a) Single Kelvin cell, and (b) Kelvin multi-cells model.