Modeling of the material structure using Voronoi diagrams and tessellation methods

Larysa Burtseva[1,a], Frank Werner[2,b], Benjamin Valdez Salas[1,c], Alexey Pestryakov[3,d], Rainier Romero[4,e], Vitalii Petranovskii[5,f]

[1]Autonomous University of Baja California, Mexicali 21280, Mexico

[2]Otto-von-Guericke University, Magdeburg 39106, Germany

[3]Tomsk Polytechnic University, Tomsk 634050, Russia

[4]Polytechnic University of Baja California, Mexicali 21376, Mexico

[5]Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autonoma de Mexico, Ensenada 22800, Mexico; On the sabbatical leave at: Departamento de Investigación en Zeolitas de la Universidad Autónoma de Puebla, Puebla 72570, Mexico.

[a]burtseva@uabc.edu.mx, [b]frank.werner@ovgu.de, [c]benval@uabc.edu.mx, [d]pestryakov@yandex.ru, [e]rromerop@uabc.edu.mx, [f]vitalii@cnyn.unam.mx

January 7, 2015

Abstract: Tessellation methods are a relatively new approach for modeling the structure of a material. In this paper, such structures are interpreted as sphere packing models, where molecules and atoms represent spheres of equal or different size. Based on the review of the literature, it is shown that the tessellation approach is a powerful method for modeling and simulating such structures with desirable metric and topological properties. Two basic tessellation methods are considered more in detail: the Delaunay tessellation and the Voronoi diagram in Laguerre geometry, as well as some of their generalizations. The principal concepts of both tessellation methods are briefly explained for a better understanding of the application details. It is noted that packing models created by tessellation methods are not based on the use of the gravity camp effect, which is a difference to numerical and mathematic programming modeling approaches. Therefore, tessellation methods permit the development of structures without taking into account the gravitation, what is important for modeling the structure on the microscopic and nano levels, where the influence of the gravitation is studied insufficiently. A review of the related literature is given, focusing on the details of the tessellation method and the particle size distribution.

Keywords: Voronoi diagram, Delaunay tessellation, Laguerre geometry, Voronoi statistics, material structure, packing.

MSC: 11H31; 05B45

1. Introduction

In recent years, the literature on computational geometry and computer graphics shows an increasing interest for the tessellation approach based on Voronoi diagrams to model different structures. These diagrams were defined and generalized by G. F. Voronoi in 1908, meanwhile they are traced back to earlier works by Descartes and Dirichlet. In the simplest form, a Voronoi diagram can be defined as follows: Given some number of points in the plane, their Voronoi diagram divides the plane according to the nearest-neighbor rule: Each point is associated with the region of the plane closest to it. A detailed up-to-date survey was given by Aurenhammer [1]. The author noted three main reasons for such an interest of the researchers for this subject: 1) Voronoi diagrams naturally arise in various situations using a visual perception guided by intuition. 2) Interesting and surprising mathematical properties related to geometrical structures led several authors to believe that the Voronoi diagram is one of the most fundamental constructions defined by a discrete set of points. 3) These diagrams have proved to be a powerful tool in solving seemingly unrelated computational problems. In addition, he indicated three useful respects when the application of Voronoi diagrams is efficient and practical: 1) as a structure per se that describes explicitly natural processes, 2) as an auxiliary structure for investigating and calculating related mathematical objects, 3) as a data structure for algorithmic problems that are inherently geometric ones.

One can meet Voronoi diagrams in a large number of fields in science and technology, even in art. They have found numerous practical and theoretical applications in astronomy, epidemiology, geophysics, meteorology as well as in computer graphics. An impressive application of the tessellation approach in architecture was shown in the paper [2] .

The tessellation methods based on Voronoi diagrams are widely used for modeling material structures, representing an interconnected net of cells packed into a given space as a cluster of spherical particles or crystals. These methods are also useful to obtain various statistics of the corresponding models [3-5]. The interest of the authors of this paper falls into the use of these methods for modeling structures containing mono- and multi-sized spheres, which represent the atoms and molecules of a material in this case. The special interest of the authors for the tessellation approach can be explained by the reason that it does not use the gravitational field effect to model dense packings, in contrast to numerical modeling and mathematical programming methods, which are strictly based on the gravitation [6].

This paper reviews the tessellation methods based on Voronoi diagrams applied to sphere packing models. A short description of the concepts used is given in Section 2. In Sections 3 and 4, various generalized tessellation methods employed for mono- and multi-disperse packings, respectively, are reviewed. Some concluding remarks finish the paper.

2. Tessellation methods based on a Voronoi diagram

The Voronoi-Delaunay tessellation as well as the Voronoi diagrams in Laguerre geometry also referred to as radical or power tessellation, are two basic tessellation methods found in the literature related to material structure modeling.

2.1 Voronoi-Delaunay tessellation

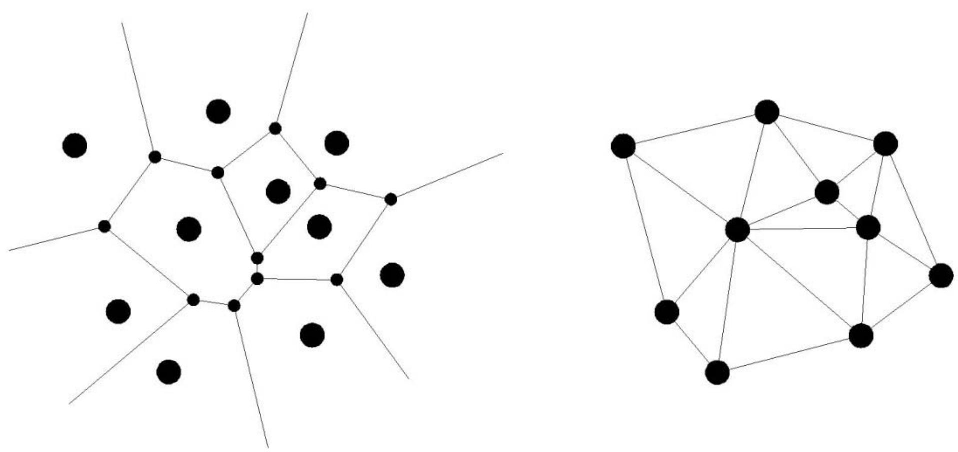
A generic definition of Voronoi diagrams was given first by Aurenhammer [1]. Let S denote a set of n points in the plane called sites. For two distinct sites $p, q \in S$, the dominance of p over q is defined as the subset of the plane being at least as close to p as to q:

$\mathrm{dom}(p, q) = \{x \in \boldsymbol{R}^2 | \delta(x, p) \le \delta(x, q)\}.$

Here δ denotes the Euclidean distance function and dom(p, q) is a closed half-plane bounded by the perpendicular bisector of p and q, which separates all points of the plane closer to p from those closer to q. The region of a site $p \in S$ is the portion of the plane lying in all of the dominances of p over the remaining sites in S:

$\mathrm{reg}(p) = \cap_{q \in S\text{-}\{p\}} \mathrm{dom}\ (p,q).$

The boundary of a region consists of at most n – 1 edges and vertices. Each point on an edge is equidistant from exactly two sites, and each vertex is equidistant from at least three sites. As a consequence, the regions of a plane form a polygonal partition called the *Voronoi diagram* or *Dirichlet tessellation*, $V(S)$, of the finite point-set S. A region reg(p) cannot be empty, and $V(S)$ contains exactly n regions, some of them are necessarily unbounded. An example of a Voronoi diagram for nine sites is given in Figure 1 (a).



a) b)

Fig. 1. Voronoi diagram (a) and Delaunay tessellation (b) for seven sites.

Voronoi was the first who considered the dual of this structure, where any two-point sites, whose regions have a boundary in common, are connected. Later, in 1934, his successor Boris Delaunay concluded that two-point sites are connected if and only if they lie on a *circle*, whose interior contains no points of S. Posteriorly, the dual of Voronoi diagrams got the name of *Delaunay tessellation* or *Delaunay triangulation* (Figure 1 b). The Voronoi polyhedron is directly related to the connectivity of particles, like the thermal conductivity or interparticle forces, while the Delaunay cell is related to the connectivity of pores in a packing, e.g., permeability [7]. The reader can find a more detailed mathematical description in [8].

A generalization of this approach leads us to a Delaunay empty sphere moving inside the Voronoi region so that it touches at least three objects at any time moment (Figure 2).

A Voronoi-Delaunay tessellation is widely used for modeling structures, which permit an interpretation as dense packings of mono-sized spheres. Such packings are characterized by a direct contact of spheres, defined numerically by the coordination number, whose limit for the mono-disperse case is known to be 12.

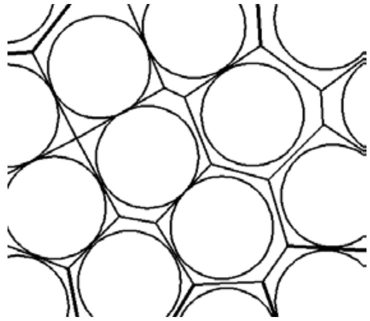


Fig. 2. A representation of the Voronoi-Delaunay tessellation in the plane

2.2 The Voronoi diagram in Laguerre geometry

For multi-disperse sphere structures, the Voronoi-Delaunay tessellation is not an appropriate method because then the regions can cut spheres or the adjacent spheres are not necessarily in contact. Sugihara (2002) noted that in generalized Voronoi diagrams some good properties have disappeared, particularly, the edges are complicated curves in the generalized Voronoi diagrams while they are portions of straight lines in the ordinary one. One possible alternative is the *Voronoi diagram in Laguerre geometry*, also referred to as the radical or power tessellation, which is an extension of the concept of the Voronoi diagram in the ordinary Euclidean geometry for n points to the one in the Laguerre geometry for n circles of different radii in the plane, where the distance between a circle and a point is defined by the length of the tangent line.

The possible mutual positions of a radical (power) line, also called locus, were illustrated in Imai at al. [9] (Figure 3). The locus of the points being equidistant from two circles c_i and c_j is a straight line, called the radical axis of c_i and c_j, which is perpendicular to the line connecting the two centers of c_i and c_j (Figure 3 a, b, c). If two circles intersect, their radical axis is the line connecting the two points of intersection. If three circles c_i, c_j and c_k intersect, and the centers are not on a line, then the three radical axes among c_i, c_j and c_k meet at a point, which is called the radical center of c_i, c_j and c_k (Figure 3 d).

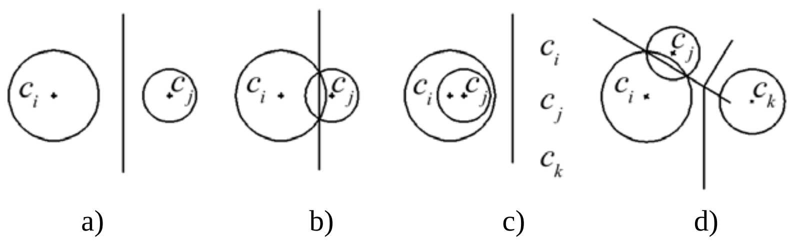


Fig. 3. Radical or power lines of two a) separated, b) overlapped, and c) included circles, and d) three circles.

Let $G = \{c_1, c_2, \ldots, c_n\}$ be a set of n circles in the plane $\mathbf{R}^2$, and let P_i and r_i be the center and the radius of the circle c_i, $i = 1,\ldots, n$. For the point P and the circle c_i, the Laguerre distance from P to c_i is defined as follows:

$$d_L(P, c_i) = d(P, P_i)^2 - r_i^2,$$

where $d(P, P_i)$ denotes the Euclidean distance between P and P_i. Let P be outside c_i, and l be the line that passes through P and the tangent to c_i. The Laguerre distance $d_L(P, c_i)$ is the square of the distance between P and the point of contact of l with c_i. If the generating circles are mutually disjoint, a point on an edge of the diagram has tangent line segments with equal lengths to the associated two generating circles. Figure 4 shows the geometrical representation of the Laguerre distance [10]. The Laguerre distance is not a kind of a distance in a mathematical sense; it represents a 'degree of farness' only.

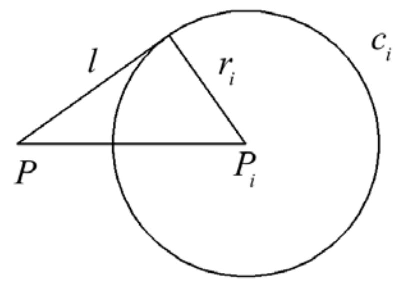


Fig. 4. The geometrical representation of the Laguerre distance *l*.

The *Laguerre Voronoi region* for c_i is defined as follows:

$R(G; c_i) = \{P \in \mathbf{R}^2 \mid d_L(P, c_i) < d_L(P, c_j), j \neq i\}$.

A corner of a Voronoi region is called a Voronoi point, and a boundary edge of the Voronoi region is called a *Voronoi edge*. Each point on an edge is equidistant from exactly two sites, and each vertex is equidistant from at least three sites. As a consequence, the regions are edge-to-edge and vertex-to-vertex, that is to say, they form a partition of the plane into the regions $R(G; c_1)$, $R(G; c_2)$,…, $R(G; c_n)$. This partition is called the *Laguerre-Voronoi diagram* for G, and the elements of G are called the *generating circles* or *generators*. A Voronoi edge is perpendicular to the great circle passing through the centers of the two generating circles. A

For a more detailed description of Laguerre-Voronoi diagrams, the reader can consult the works of Imai et al., [9], Aurenhammer [1] and Sugihara [10].

Similar to the Delaunay tessellation, the radical one divides the whole packing space into a set of non-overlapping convex polyhedra, and each polyhedron contains exactly one particle. The plane used in the radical tessellation to separate two close particles is the assembly of the points with equal tangential distance to the two spheres, different from the bisecting plane. The touching spheres have a common face; larger spheres tend to have larger cells than smaller ones.

The Laguerre-Voronoi diagram is the dual to a regular triangulation and vice versa as well as the Delaunay cell is the topological dual to the Voronoi polyhedron. The vertices of the regular triangulation are the spheres (germs) of the corresponding power diagram, the edges correspond to faces and the vertices of the power diagram are the orthogonal centers of the triangulation. The weight is similar to the distance, and it enables some control of the size of grains. The larger the weight is, the bigger is the grain.

If the radii of all spheres in the set are equal (or all weights are equal), the Voronoi-Delaunay tessellation is obtained.

3 Modeling structures containing mono-sized spheres

Since the seminal works of Bernal [11] and Finney [12] a tridimensional generalization of the ordinary Delaunay-Voronoi tessellation method was used for the study of liquids [3] and the modeling of structures containing mono-sized spheres. The main idea is to construct a system of space-filling convex cells, where each cell contains exactly one sphere. In this case, the Voronoi diagram, or region, is a polyhedron defined as the portion of space, or the set of all points surrounding that sphere and being closer to that sphere than to any other one [13]. The interstices within a packing form a continuous network of interconnecting pores or voids. Two Delaunay cells are considered to be adjacent if they have one face in common. The connectivity between pores is restricted by the void area in the face of two adjacent Delaunay cells. For illustrations, see, e. g., [5, 13, 14].

In 1998, Mac Laughin has demonstrated that the smallest Voronoi cell is the regular dodecahedron circumscribing the sphere [13]. For mono-sized spheres, the ratio of the sphere volume to the cell volume is 0.754697, which is very close to Kepler's limit 0.74048, given for the face-centered cubic close packing and the hexagonal close packing in a volume filled by identical spheres. It is considered as the best upper bound on the largest possible coefficient of the occupation of space and a convenient method to model a dense structure of particles. Then, the geometry of the packing can be described by the geometrical characteristics of the cells. The tessellation techniques are able to predict the metric and topological properties of such a structure and its statistical analysis.

The Delaunay-Voronoi tessellation is may be a more complex method for modeling dense structures compared with numerical and mathematical programming methods. Nevertheless, the two last ones are strictly based on the use of the gravitational field effect, meanwhile the influence of the gravitation on the packing structures on molecular and nano levels are less studied.

The structures of the lattices generated by randomly packed spheres were extensively studied over a long time period because of its importance as a predictive model in many processes involving granular materials, nevertheless they may be applied to study a wide range of structures. The research was centered principally on measuring the packing properties and the acquisition of void distribution models. Utilizing a tessellation approach, the authors also discussed a convenient polyhedron shape. The tetrahedral tessellation, where the vertices of each tetrahedron are the centers of four neighboring spheres, is a useful method for modeling structures containing equivalent spheres. Other available methods mentioned in the related literature are square, triangular and hexagonal tessellations, which are composed of area-filling squares, triangles and hexagons, respectively [4]. The variants of a Delaunay-Voronoi tessellation describing the models for different structures, which were found in the literature, are reviewed below.

In the works of, McGeary [15], Mason [3], Chan and Ng [4], Zou and Yu [16] and Van Antwerpen [17], a random packing of equivalent spheres is described in terms of a tetrahedral tessellation. The selection of a tetrahedron as the basic unit in these studies was based on the known observation that the average coordination number of a random packing of equal spheres is about six, with three on the top and three on the bottom. Such tetrahedra are related to Voronoi polyhedra. Each face on the Voronoi polyhedron contributes one edge to the network of the tetrahedron.

McGeary [15] described a ball-bearing model in terms of tetrahedral subunits in random close packed lattices of uniform spheres. Zou and Yu [16] and Van Antwerpen [17] analyzed the voids associated with tetrahedral structures. Each tetrahedral structure contained a central pore and four outer constrictions. Although the four connections associated with each pore varied in their sizes, nevertheless the pores joined by a common constriction were similar in their size.

Studying the drainage of a liquid from porous materials, Mason [3] highlighted two principal concepts concerning the material: there is a network of *interconnections* within the material, comprised of *pores* defined as small regions of that network. Some materials, for example, foams can be very highly interconnected. The capillary properties of such pores define the capillary pressures and in isolation from the network, they determine whether the liquid can fill or drain an individual pore. In a random sphere packing the most convenient pore is a tetrahedral subunit formed by joining the centers of neighboring not necessarily touching spheres together. A method of generating these tetrahedra was given. Some capillary properties of the assembly are derived using an approximation for the draining and filling curvatures of the pore spaces.

Chan and Ng [4] applied a tetrahedral tessellation to a computer-generated, random packing of nearly equal spheres confined in pore chambers. The objective was to identify the tetrahedral pores and then to determine the geometrical characteristics of the pore space. The tessellation procedure began with a seed tetrahedron. Then, in a crystal growth-like manner, tetrahedra are added one at a time to the seed until a cluster of non-overlapping, space-filling tetrahedra was formed. Each tetrahedron had a pore chamber and four constrictions, one on each of its four triangular faces. A simulating algorithm was proposed. A statistical analysis allowed the determination of various correlations among the pores and constrictions.

Nolan and Kavanagh [5] applied the Voronoi-Delaunay tessellation technique that was able to predict accurately the transport properties of the porous medium for an ordinary diffusion. The authors compared the distribution of the pore polyhedra in a random close packing of equal-sized spheres obtained using a computer simulation with experimental data obtained by previous workers. The analysis of the results suggested that the structure of a random close packing is characterized by irregular octahedral and planar configurations rather than tetrahedral as previously thought.

In the paper by Yang et al. [18], the topological and metric properties of Voronoi polyhedra for uniform fine spherical particles were analyzed and facilitated by the Voronoi tessellation. They were quantified as a function of the particle size and the packing density. The authors have shown that the average sphericity coefficient of the Voronoi polyhedra varied with the packing density. Moreover, with decreasing the particle size or the packing density, the average face number of the Voronoi polyhedra decreased, and the distributions of the face number and the edge number became broader and more asymmetric; (ii) the average perimeter and the area of the polyhedra increased, and the distributions of the surface area and the volume of the polyhedron become more flat and can be described by the log-normal distribution.

The Voronoi-Delaunay approach for the analysis of the free volume, considering packing of balls confined in a cylinder, was described in [14], where a generalized Voronoi diagram was used as the underlying data structure. Two problems were considered: i) an efficient construction of the confined Voronoi diagram inside a cylindrical boundary, and ii) an analysis of the Voronoi network to study the distribution of the empty spaces (voids) in the system. An algorithm was proposed to calculate the Voronoi network for 3D systems. Explicit formulas to compute the coordinates of the Voronoi vertex were provided. The algorithm was implemented and tested in a 3D system for packings with disordered structure, representing a bed of spherical particles in cylinders of different radii. The models were obtained by using the Monte Carlo relaxation method.

In the works of Khirevich et al. [19] and Khirevich et al. [20], the Voronoi-Delaunay tessellation was used for the analysis of the mass transport properties and the morphology of different packing structures.

4 Modeling complex structures using tessellation methods

Commonly, the properties of multi-component structures are studied and modeled with methods appropriate for random (close) packings of multi-sized spheres, when the spheres of different radii are considered as atoms and molecules of a material. The density, the radial distribution function, the contact coordination number, as well as the correlations between different characteristics are useful parameters describing any packing. The related literature of the recent years shows a growing interest of the researchers to use the tessellation methods in this area, therefore Voronoi statistics, such as the number of cell faces and the edges per face, the surface area and the volume per polyhedron, appear as typical characteristics of a structure.

In this section, we give a brief review of the works applying tessellation techniques to model and study structures, which contain multi-sized components, focusing mainly on the tessellation method used for a specific particle size distribution, which is considered as the more significant factor when the resulting structure is analyzed. For illustrations, see, e. g., Fan et al. [21], Lochmann et al., [22], Redenbach [23], Wu et al. [24], Yi et al., [25].

In the paper by Fan et al. [21], the Poisson-Voronoi diagram was considered using the Laguerre-Voronoi approach. The Poisson-Voronoi diagram is a kind of a Voronoi diagram with the set of points generated through a homogeneous Poisson point process. A Poisson-Voronoi diagram is composed of an array of convex, space-filling and non-overlapping polyhedrons, which represent the grains of the polycrystalline material. The polyhedra of the Poisson-Voronoi diagram possess the properties that four edges share a vertex and three faces share an edge, which are also observed in real material. Fan et al. [21] proposed a model based on a random closed packing of spheres, called the RCP-LV diagram, which is probably better than the Poisson-Voronoi diagram in the simulation of the microstructure of real polycrystalline materials because it is based on real material characteristics instead of inadequate ones used in the Poisson-Voronoi diagram: the average number of faces per polyhedron, the range of the coefficient of variation of the grain volumes, and the polyhedron volumes obeyed a lognormal distribution instead of a gamma distribution.

The work of Yang et al. [7] presented a numerical study of the pore structure of fine particles. Pores and their connectivity are then analyzed in terms of a Delaunay tessellation. The geometries of the pores are represented by the size and shape of Delaunay cells and quantified as a function of the packing density or the particle size. It was shown that the cell size decreased and the cell shape became more spherical with increasing packing density. A general correlation existed between the size and shape of the cells: the larger the cell size relative to the particle size is, the more spherical is the cell shape. The size distribution of the Delaunay cells was described by the lognormal distribution. A formula for the probability function was given.

An application of tessellation-based methods, which includes the analysis of correlations between the cell face and coordination numbers was proposed in the paper by Lochmann et al., [22]. An analysis of the geometrical organization of disordered packings of spheres with different statistical methods was performed. Four different structures were considered: mono-sized, binary, power-law and Gaussian size distributions. The comparison of basic geometrical characteristics such as the packing fraction, the two-point probability function, the pair correlation function and the coordination number has shown that these characteristics can have quite different forms, which are closely related to the radius distribution. The description was refined by means of tessellation-related characteristics, which enable a quantitative description of the different local arrangements by means of the number of cell faces and edges per face. A depth analysis of the coordination number, which is the fundamental topological parameter, is given for different radii distributions. In this paper, the tessellation employed was the radical one (or the Laguerre-Voronoi one).

In the paper by Redenbach [23], Laguerre tessellations generated by random sphere packings were employed as models for the microstructure of cellular or polycrystalline materials, using lognormal or gamma distributions of the volumes, because these distributions were often suggested for the size distributions of grains (cells) in granular (cellular) materials. The Laguerre cells on the volume fraction in the sphere packing and the coefficient of variation of the volume distribution were studied in detail. The authors studied the dependence of the geometric characteristics of the Laguerre cells on the volume fraction in a sphere packing and the coefficient of variation of the volume distribution. The moments of certain cell characteristics were described by polynomials, which allows one to fit tessellation models to real materials, such as open polymer and aluminum foams, without further simulations. The author considered relatively dense packings with 66.7%, where the cell volumes, as well as the sphere volumes, were approximately lognormally distributed. The topology parameters, the number of facets per cell and the number of edges per facet and their tessellation characteristics were analyzed. The procedure was illustrated by the examples of open polymer and aluminium foams.

The Laguerre-Voronoi tessellation based on a random close packing of spheres was performed by Wu et al., [24]. The authors considered this method as a successful one for modeling and characterizing two-phase composites. First, it was generated with two groups of spheres and each group has its own volume distribution, basically lognormal, by using a modified rearrangement algorithm. Then a Laguerre-Voronoi diagram was performed basing on the sphere packing to generate the grains of the two phases, thus the model of a two-phase composite was obtained. Various geometrical and topological characterizations were conducted, yielding useful information about this kind of composite. Three groups of representative parameters were selected to characterize the particle shape, the local and the overall geometrical distributing patterns: 1) the form factor; 2) the nearest neighbor distance, and 3) the second-order intensity function and the pair distribution function. Three aspects were selected as general descriptions of the composite models: 1) the volume fraction of constituent phases; 2) the mean and standard deviation of the grain volume; 3) the grain volume distribution. Several topological parameters were computed. The authors concluded that the model and the characterization based on a random close packing of spheres using a Laguerre-Voronoi diagram are effective for analyzing the composite microstructure.

In the paper by Yi et al. [25], the packing structures for ternary mixtures were analyzed by the radical tessellation. The metric and topological properties of each polyhedron were studied as a function of the volume fractions of constituent components. The studied properties included the number of edges, the area and the perimeter per radical polyhedron face, and the number of faces, the surface area and the volume per radical polyhedron. The properties of each component of a mixture were shown to be strongly dependent on the volume fractions. The authors concluded that the radical tessellation can be successfully used to model different properties of multi-sized packings and the development of a predictive method to describe the effect of the particle size distribution on the structural properties of the packing of particles. The authors noted that the structural results based on the Voronoi or radical tessellation are increasingly used in the literature and gave some examples of these results.

The Laguerre-Voronoi diagrams were used in the paper [26] for performing a numerical approach to study the effects of a grain size distribution and the stress heterogeneity on the yield stress of polycrystals. The numerical scheme was used for the generation of polycrystalline microstructures. It combines the Lubachevsky-Stillinger algorithm for a dense packing of spheres [27] with power diagrams. It has been shown that the combination of a dense-sphere packing and Laguerre-Voronoi diagrams provides a convenient way to produce microstructures with a prescribed grain size distribution.

5 Conclusions

In many cases the three-dimensional structural model of a matter can be interpreted as spheres packed in the available space, therefore the methods of sphere packings should be used to model and study such structures. The tessellation approach based on Voronoi diagrams is a powerful method to creare mono-sized sphere packings as well as multi-sized ones. The tessellation techniques are able to predict the metric and topological properties of a structure and its statistical analysis.

The basic tessellations are the Voronoi-Dalaunay and the Laguerre-Voronoi ones, for the modeling and analysis of mono-sized and multi-sized sphere packings, respectively, meanwhile researchers adapt these principal approaches to the peculiarities of the problem. The tessellation methods permit the development of structures without taking into account the gravitation, what is important for modeling the structure on the microscopic and nano levels, where the influence of the gravitation is studied insufficiently. The possibilities of the tessellation methods are still unexhausted. Aurenhammer [1] and Yao [8] pointed out several kinds of a generalized Voronoi diagram and their potential applications, which has certain features and can be crucial in prospective researches.

Acknowledgements

This work was supported by the Department of Postgraduate and Research of the UABC, Project No. 111/739.

References

[1] F. Aurenhammer. Voronoi diagrams--a survey of a fundamental geometric data structure. ACM Comput. Surv. 23 (1991) 345-405.
[2] H. Pottmann, C. Jiang, M. Höbinger, J. Wang, P. Bompas & J. Wallner. Cell packing structures. Computer-Aided Design (2014 In press).
[3] G. Mason. A model of the pore space in a random packing of equal spheres. Journal of Colloid and Interface Science 35 (1971) 279-287.
[4] S. K. Chan & K. M. Ng. Geometrical characteristics of the pore space in a random packing of equal spheres. Powder Technology 54 (1988) 147-155.
[5] G. T. Nolan & P. E. Kavanagh. Octahedral configurations in random close packing. Powder Technology 83 (1995) 253-258.
[6] L. Burtseva, A. Pestryakov & V. Petranovskii. Monosized sphere packing approach in the nanoporous structure modeling. Strategic Technology (IFOST), 2012 7th International Forum on, 18-21 Sept. 2012. 1-6.
[7] R. Y. Yang, R. P. Zou, A. B. Yu & S. K. Choi. Pore structure of the packing of fine particles. Journal of Colloid and Interface Science 299 (2006) 719-725.
[8] F. F. Yao. Computational Geometry Handbook of Theoretical Computer Science: Algorithms and complexity. Elsevier Science Publishers. (1990) 343-380l.
[9] H. Imai, M. Iri & K. Murota. Voronoi Diagram in the Laguerre Geometry and Its Applications. SIAM Journal on Computing 14 (1985) 93-105.
[10] K. Sugihara. Laguerre Voronoi diagram on the sphere. Journal for Geometry and Graphics 6 (2002) 69-81.
[11] J. D. Bernal. A Geometrical approach to the structure of liquids. Nature 183 (1959) 141-147.
[12] J. L. Finney. Materials Science and Engineering 23 (1976) 199-205.
[13] C. Marchal. Study of the Kepler’s conjecture: the problem of the closest packing. Math. Z. 267 (2011) 737-765.
[14] V. A. Luchnikov, M. L. Gavrilova, N. N. Medvedev & V. P. Voloshin. The Voronoi–Delaunay approach for the free volume analysis of a packing of balls in a cylindrical container. Future Generation Computer Systems 18 (2002) 673-679.
[15] R. K. Mcgeary. Mechanical packing of spherical particles. Journal of the American Ceramic Society 44 (1961) 513-522.
[16] R. P. Zou & A. B. Yu. The packing of spheres in a cylindrical container: the thickness effect. Chemical Engineering Science 50 (1995) 1504-1507.
[17] W. Van Antwerpen, C. G. Du Toit & P. G. Rousseau. A review of correlations to model the packing structure and effective thermal conductivity in packed beds of mono-sized spherical particles. Nuclear Engineering and Design 240 (2010) 1803-1818.
[18] R. Y. Yang, R. P. Zou & A. B. Yu. Voronoi tessellation of the packing of fine uniform spheres. Physical Review E 65 (2002) 041302/1-8.

[19] S. Khirevich, A. Höltzel, A. Daneyko, A. Seidel-Morgenstern & U. Tallarek. Structure–transport correlation for the diffusive tortuosity of bulk, monodisperse, random sphere packings. Journal of Chromatography A 1218 (2011) 6489-6497.

[20] S. Khirevich, A. Höltzel, A. Seidel-Morgenstern & U. Tallarek. Geometrical and topological measures for hydrodynamic dispersion in confined sphere packings at low column-to-particle diameter ratios. Journal of Chromatography A 1262 (2012) 77-91.

[21] Z. Fan, Y. Wu, X. Zhao & Y. Lu. Simulation of polycrystalline structure with Voronoi diagram in Laguerre geometry based on random closed packing of spheres. Computational Materials Science 29 (2004) 301-308.

[22] K. Lochmann, L. Oger & D. Stoyan. Statistical analysis of random sphere packings with variable radius distribution. Solid State Sciences 8 (2006) 1397-1413.

[23] C. Redenbach. Microstructure models for cellular materials. Computational Materials Science 44 (2009) 1397-1407.

[24] Y. Wu, W. Zhou, B. Wang & F. Yang. Modeling and characterization of two-phase composites by Voronoi diagram in the Laguerre geometry based on random close packing of spheres. Computational Materials Science 47 (2010) 951-961.

[25] L. Y. Yi, K. J. Dong, R. P. Zou & A. B. Yu. Radical tessellation of the packing of ternary mixtures of spheres. Powder Technology 224 (2012) 129-137.

[26] F. Lavergne, R. Brenner & K. Sab. Effects of grain size distribution and stress heterogeneity on yield stress of polycrystals: A numerical approach. Computational Materials Science 77 (2013) 387-398.

[27] B. Lubachevsky & F. Stillinger. Geometric properties of random disk packings. J Stat Phys 60 (1990) 561-583.