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Voronoi diagram as an analysis tool for spatial properties for ceramics

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While research in ceramics has focused on physical experiments, the need for computational aids is increasing more and more. Among several computer simulation tools for the design and analysis of various aspects of ceramics, the Voronoi diagram is introduced in this paper. The Voronoi diagram is a powerful tool in computational geometry which provides all spatial information among geometric objects in a system with an efficient data structure. In this paper, we present the properties of Voronoi diagrams and introduce various applications appropriate for research in ceramics.

Key words: Voronoi diagrams, spatial analysis, computational geometry.

Introduction

Until recently, major approaches in material science research, including ceramics, have been based mainly on experiments using physical instruments. While this trend is, and will continue to be, the main-stream of research in ceramics, computer simulation has started a new paradigm in material science research.

Suppose that we have a powder consisting of several particles. In many cases, the spatial distribution of particles in various conditions is one of the major research interests in ceramics. The shapes of grains are also important factors to be considered in the design and manufacturing of ceramics [2, 7].

Even though there are several methods to analyze the spatial characteristics of the particles or grains, physical experiments usually use scanning electron microscopy to take photographs of the material surface. The pictures are then visually analyzed to identify and describe new phenomena. However, physical experiments followed by visual inspections are frequently costly and time consuming. Besides, this approach can be rather imprecise.

Computer simulation, on the other hand, can replace physical experiments if the environment of the experiment can be appropriately modeled. Simulation is usually less expensive and can produce results faster. If the model is constructed correctly, the results can be very close to the real experiment. Besides, the results are usually produced quantitatively.

Among various simulation techniques in material science, in this paper we will introduce the Voronoi diagram to analyze the spatial characteristics of a material so that the analysis can be easily reflected in the material design and manufacture.

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Voronoi diagram

Suppose that a finite number of distinct points, which we call *generators*, are given in a space. If we allocate all locations in this space with the closest member of the generators, the result is a partition of the space into a set of regions. Such a partition is called the Voronoi diagram of given point set, and each region is called a Voronoi region [1, 9].

Figure 1 illustrates an example of a Voronoi diagram for six point-generators. As shown in the figure, a location Q in a region corresponding to generator P_1 is always closer to P_1 than P_i, i = 2, 3, 4, 5, and 6. In this example, a Voronoi region, VR1, is a polygon consisting of all such locations in the plane. The distance is the ordinary Euclidean distance, in other words, $d(q_1$,

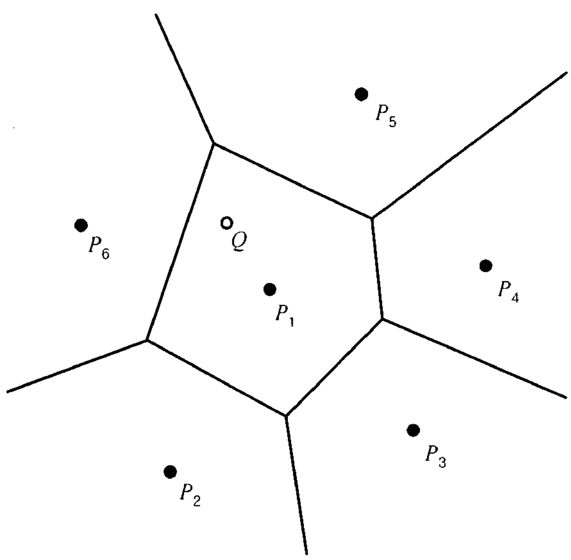

Fig. 1. Voronoi diagram of a point set in a plane.

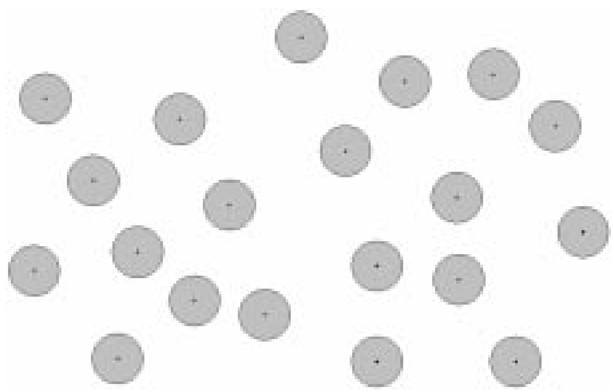

Fig. 2. Particles distributed on a plane.

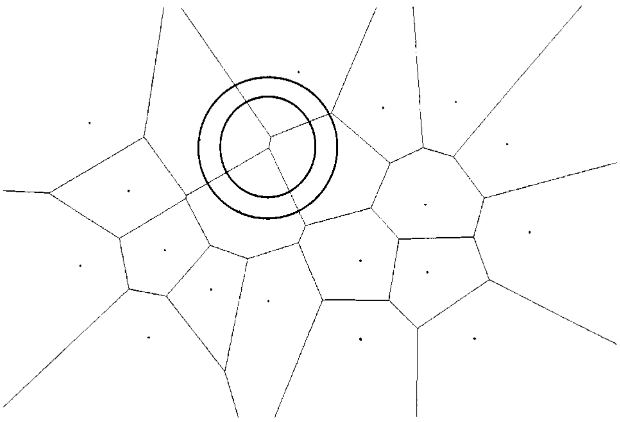

Fig. 3. Point set Voronoi diagram. The larger circle is the largest empty circle of point set and the smaller circle corresponds to the largest open space among particles.

$q_2)=\sqrt{(x_1-x_2)^2+(y_1-y_2)^2}$ where $q_1=(x_1, y_1)$ and $q_2=(x_2, y_2)$. Note that a Voronoi region is always a bounded convex polygon except at the exterior generators.

In Fig. 3, the larger circle is the largest empty circle computed from the point set Voronoi diagram and the smaller circle corresponds to the largest open space existing among the particles with the prescribed spatial distribution. Note that the largest open space can be easily found from the largest empty circle by subtracting the radius of the particle. Once the Voronoi diagram is given, the time to find the largest circle is linear with respect to the number of particles since the Voronoi diagram is usually stored in an efficient data structure such as a Winged-Edge data structure. Therefore, the integral and global properties, such as the distribution of open spaces in a given material, can also be easily computed by the fast computation of the distribution of empty space among the particles.

If a Voronoi diagram is given, it is also possible to compute other important geometric properties without much difficulty. For example, the time to compute the average number of boundaries between grains is also linear with respect to the number of particles. Similarly, the grain with the maximum or minimum number of grain boundaries can also be easily located.

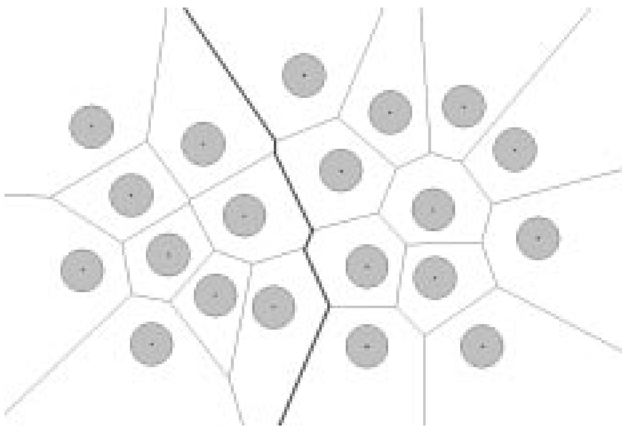

Fig. 4. The largest channel.

Suppose that we want to find one or more paths through which another particle can pass freely without touching given particles. Such paths can be easily identified once the Voronoi diagram is given and stored in Winged-Edge data structure. Among these paths, one with the minimum or maximum travel distance can be computed without much computational effort. Figure 4 is an example of such a diagram showing a path through which the largest particle can pass freely between two sites in the powder distribution.

Suppose that a material is polycrystalline, meaning that it consists of many individual crystals that are randomly distributed and oriented. If a picture of the material surface is taken by an electron microscope, it is then possible to estimate where and when the crystallization of each grain started on the surface. This type of problem is called the generator recognition problem in computational geometry [9]. Assuming that the grain boundaries are potential Voronoi edges, the locations of generator points can be computed. Therefore, if the crystallization process is assumed as a point set Voronoi diagram, the seed points at which the crystallization started can be found. The distribution of these seed points can be very useful information.

Computation of a Voronoi diagram

There have been several reports of research to compute the Voronoi diagram of a point set. They can be categorized as the following approaches: incremental, divide-and-conquer, plane sweep, lift-up, and flip. Among these approaches, the lift-up approach is significant due to its capability to incorporate the error-free computation of the diagram using exact computation [4, 9].

It has been found that a Voronoi diagram can be computed in $O(n \log n)$ time where n is a number of points [10]. Note that we use a symbol $O(g(n))$ to indicate the time complexity of our algorithm to give an upper bound of the time taken by the algorithm for a given number of input data [3]. For example, a Voronoi diagram of 10,000 points can be computed and stored in Winged-Edge data structure in less than 2 or 3 seconds with a Pentium III with 128 MB main memory [8].

Conclusions

In this paper, we have introduced the possibility of the Voronoi diagram to analyze the spatial properties of a set of particles. Especially, when the particles can be modeled by circles with identical radii, the problem can be precisely approached by the Voronoi diagram. The Voronoi diagram of point set can be computed very rapidly by any of several algorithms. For future work, it is necessary to find appropriate problems that can be solved using Voronoi diagrams.

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