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Crystal structure extraction in materials using Euclidean Voronoi diagram and angular distributions among atoms

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In the evaluation of material properties, the structural configuration of atoms constituting the material is of importance. Presented in this paper is a mathematical and computational methodology to efficiently classify a given atomic structure of an arbitrary material into groups of atoms defining *BCC*, *FCC*, and *HCP* crystal structures. The approach is based on the angular distributions among neighboring atoms efficiently identified by a computational geometry technique called a Voronoi diagram. Usually a Voronoi diagram consists of Voronoi regions for each atom where a Voronoi region consists of points in space which is closer to an associated atom than the others. Due to the computational efficiency of a Voronoi diagram, the proposed approach becomes more powerful as the number of atoms is increased.

Key words: Crystal Structure, Voronoi Diagram, Geometric Algorithm, Angle distribution.

Introduction

The evaluation of physical properties in materials from a microscopic viewpoint has been an aim of material science for several decades. The technique to understand and control microscopic systems is important because it provides a way to control material properties. As technologies are developed, the similar evaluation and design of materials on even an atomic scale have become more important. Since the understanding of atomic structure inherently contains geometric aspects in addition to the physics among atoms, it is important to make observations on the spatial properties among atoms which constitute materials [1, 2].

Materials consist of atoms. When atoms are contiguous in 3-dimensional space with a regular structure, the aggregate of atoms is called a grain. As the size of a grain under investigation becomes smaller such as on a nano scale and as more atoms are considered simultaneously, the need for computer simulation is inevitable to evaluate material properties. Even though there have been a strong desire to understand the spatial structure among atoms in a simulation, there have been not sufficient computational tools to meet such a requirement [1, 2].

Presented in this paper is a mathematical and computational theory for extracting grains of different crystal structures of Body-Centered Cubic (*BCC*), Face-Centered Cubic (*FCC*), and Hexagonal Closed-Packed (*HCP*) from a set of atoms constituting a material. To devise such a computational tool, we provide a few geometric observations on the fundamental three crystal structures so that a computational algorithm can be built on them. Based on the geometric observations, a very well-known computational geometrical tool called the Voronoi diagram is introduced so that a geometrical observation can be easily applied. It is noteworthy that a group of Russian scientists lead by Medvedev has been working on a similar problem with a slightly different perspective [3-8]. As early as 1987, Medvedev developed a theory to extract local geometric structures among nearly atoms using Voronoi diagram [9].

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Voronoi Diagram

Suppose that a finite number of distinct geometric entities, which we call *generators*, are given in a space. If we allocate all locations in this space with the closest member among the generators, the partition of the space into a number of regions results. Such a partition is a tessellation of the space and called the Voronoi diagram of given generators where each region is called a Voronoi region [14].

Mathematically speaking, a Voronoi diagram in 3D can be defined as follows. Suppose that $G=g_1, ..., g_n\} \subset R^3$, where $1 < n < \infty$, are a set of generators. Then, $VR(g_i)=\{x \mid d(x, g_i) \leq d(x, g_j)$ for $i \neq j\}$ is called a *Voronoi region* for g_i where $d(p_1, p_2)$ is a distance between p_1 and p_2, and the set given by $VD=\{VR(g_1), ..., VR(g_n)\}$ is called a *Voronoi diagram* for the set G. Even though there can be different definitions of distances depending on applications, the *Euclidean distance* is

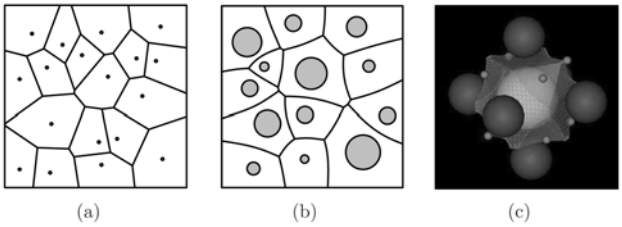

Fig. 1. (a) Point, (b) Circle, and (c) Sphere set Voronoi diagram.

usually employed in most problems as in this paper. In other words, $d(p_1, p_2)=\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}$ where $p_1=(x_1, y_1, z_1)$ and $p_2=(x_2, y_2, z_2)$.

Shown in Fig. 1 are three examples of such Voronoi diagrams in 2 and 3D. Fig. 1(a) shows an example of a Voronoi diagram for points in a plane. Hence, any location in a polygon is closer to the generator point, shown as a black dot, in the polygon than any other point in the space. Shown in Fig. 1(b) is a similar diagram but with circles instead of points as generators. Hence, any location in a curved Voronoi region is closer to the circle in the region than to any other circles in the plane. On the other hand, Fig. 1(c) illustrates a similar Voronoi diagram of spheres in 3D. Hence, the curved polyhedron illustrates the Voronoi region for a sphere at the center of the structure.

While the computational technique for an ordinary Voronoi diagram of points in 2 and 3D has been known quite well and efficient programs are available, the Voronoi diagrams for circles and spheres were not possible to compute until very recently. According to [10-12], Voronoi diagram of thousands of circles can be now computed in a few seconds while one for one thousand spheres can be computed in the order of ten's of seconds with a low-end personal computer.

Given a Voronoi diagram such as Fig. 1(a), let's define an edge between two point generators which share a Voronoi edge. If we apply this operation for all such pairs, we can get another tessellation called a *Delaunay triangulation* as shown in Fig. 2. Hence, the

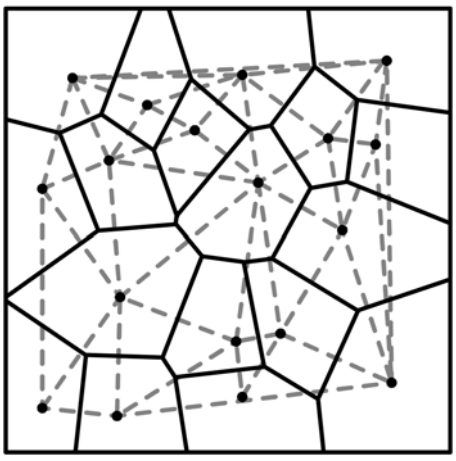

Fig. 2. Delaunay triangulation.

Voronoi diagram and Delaunay triangulation are said to be dual to each other. Note that the dual transformation can be done in a linear time with respect to the number of Voronoi [13].

Once either a Voronoi diagram or a Delaunay triangulation is given in an efficient data structure, it is quite easy to traverse immediate neighbors for a given generator. For example, if a particular generator is given, its immediate neighboring generators can be located in the linear time of the number of neighbors. In a planar case of Delaunay triangulation, for example, a triangle next to a particular triangle can be found in a constant time. In 3D, a similar observation holds and a neighboring tetrahedron for a particular tetrahedron can be located in a constant time. Therefore, a neighbor search for a given 3D atomic structure can be very efficiently done once its Voronoi diagram is computed [12, 15, 17, 18].

While the computation of an ordinary point set Voronoi diagram can be done by a library such as CGAL, its counterpart for spheres with different radii has become possible only very recently [21]. In CGAL, for example, the topology of an ordinary Voronoi diagram is represented by a Delaunay triangulation which is the dual of the Voronoi diagram.

Geometric Observations in Fundamental Crystal Structures

It is known that there are three fundamental crystal structure types in most materials: Body-Centered Cubic (*BCC*), Face-Centered Cubic (*FCC*), and Hexagonal Closed-Packed (*HCP*). From a geometrical viewpoint, *BCC* has a cubic unit cell with atoms located at all 8 corners of the cell and a single atom at the center of the cube. Each of the eight corner atoms can be considered to play the role of the center atom when neighboring cubes are considered altogether. Similarly, *FCC* has also a cubic unit cell with atoms located at each of the 8 corners and the 6 centers of all faces of the cube. *HCP*, on the other hand, assigns 17 atoms at the appropriate places around a hexagonal cylinder: 12 atoms at the corners of the hexagonal cylinder, an atom for each of top and bottom hexagonal faces of the cylinder, and 3 atoms inside the cylinder.

Based on these configurations of atoms, we have made a few geometric observations so that they can be used for the assessment of material properties. Shown in Fig. 3(a) is a model of the *BCC* structure consisting of identical atoms and Fig. 3(b) illustrates the Voronoi region of the center atom among the 9 given atoms. It should be remembered that such a *BCC* structure repeats itself in the crystal. Since the center atom is located at the center of the unit cell, the eight neighboring atoms are located in the space at an identical distance. In addition, the angles formed at the center atom with respect to the two immediate

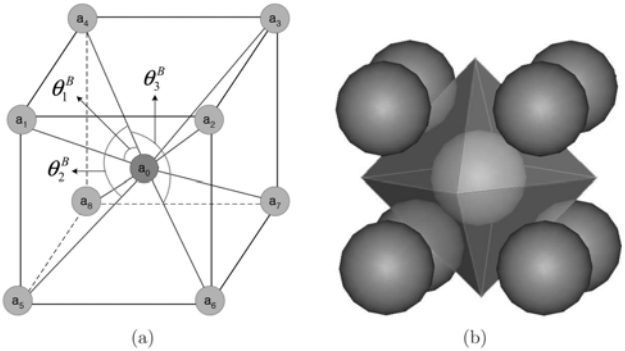

Fig. 3. (a) a geometric model of *BCC*-structure and (b) the Voronoi region for the center atom with respect to only eight neighboring atoms in the *BCC*-structure.

neighbors are also identical.

From the model, we can define three different kinds of angles among the atoms in the system: θ_1^B, θ_2^B, and θ_3^B. θ_1^B is defined at the center atom with respect to two immediate neighboring atoms at the vertices of the cube. For example, an example of angle type θ_1^B is the angle $\angle a_1a_0a_4$ since the atoms a_1 and a_4 are immediate neighbors from each other. Similarly, $\angle a_1a_0a_5$ and $\angle a_1a_0a_2$ are also instances of θ_1^B. θ_2^B is defined at the center atom with two non-immediate neighboring and non-diagonal atoms at the vertices. For example, the angles $\angle a_1a_0a_6$ and $\angle a_1a_0a_5$ are the examples of θ_2^B. Lastly, θ_3^B is defined at the center atom with respect to diagonal atoms at the vertices. For example, the angles $\angle a_1a_0a_7$ and $\angle a_2a_0a_8$ are examples of θ_3^B. Shown in Fig. 3(b) is a Voronoi region of the center atom with respect to only eight neighboring atoms.

Based on the above-described *BCC*-model, we can draw a simple yet important lemma regarding the angles in the model as follows. Part 1 discusses the distribution of different angles in the system and Part 2 discusses the values of different angles.

Lemma 1 Suppose that a *BCC* unit cell is given. Then, the following holds.

1. There are 28 distinct angles, in total, defined at the center atom with respect to the vertex atoms.
2. There are 12 cases of θ_1^B angles, 12 cases of θ_2^B angles, and 4 cases of θ_3^B angles defined at the center atom.
3. $\theta_1^B \approx 70.5288^o$, $\theta_2^B \approx 109.4712^o$, and $\theta_3^B = 180.0000^o$.

Proof: (Part 1 and 2) Since there are 8 vertex atoms, there can be $\binom{8}{2}=28$ distinct angles defined at the center atom in a *BCC* unit cell. For a vertex atom a_1, there can be three θ_1^B with vertex atoms a_2, a_4 and a_5. Since there are eight vertex atoms, there can be 3*8=24 combinations of angles where each angle is doubly counted. Hence, there are 12 cases of θ_1^B angles in a *BCC* unit cell. A similar argument holds for θ_2^B. Since there is only one diagonal atom for a given vertex atom, there are only 4 cases of θ_3^B angles in a *BCC* unit cell.

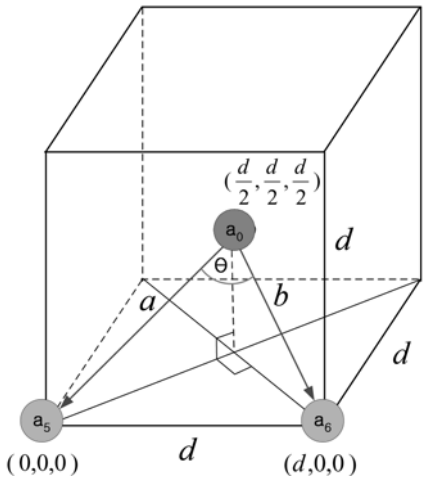

Fig. 4. θ_1^B angle in *BCC*.

(Part 3) Assuming that the constituting atoms are equally sized, we can find the value of angle θ_1^B as follows. Let c_i be the center of atom a_i. Suppose that the centers c_5, c_6, c_0 of atoms a_5, a_6, a_0 be located at the origin, (d, 0, 0), and (d/2, d/2, d/2) in the coordinate system, respectively.

Let $\vec{a}=c_5-c_0$ and $\vec{b}=c_6-c_0$. Then, $\vec{a}=\left(\frac{-d}{2},\frac{-d}{2},\frac{-d}{2}\right)$ and $\vec{b}=\left(\frac{d}{2},\frac{-d}{2},\frac{-d}{2}\right)$. Hence, the inner product $\vec{a}\cdot\vec{b}=\frac{-d^2}{4}+\frac{d^2}{4}+\frac{d^2}{4}=\frac{d^2}{4}$. Note $\|a\|=\sqrt{\left(\frac{-d}{2}\right)^2+\left(\frac{-d}{2}\right)^2+\left(\frac{-d}{2}\right)^2}=\sqrt{\frac{3d^2}{4}}$ and $\|b\|=\sqrt{\left(\frac{d}{2}\right)^2+\left(\frac{-d}{2}\right)^2+\left(\frac{-d}{2}\right)^2}=\sqrt{\frac{3d^2}{4}}$. Therefore, $\theta_1^B \approx 70.5288^o$ can be obtained since $\theta=\cos^{-1}\left(\frac{a\cdot b}{\|a\|\|b\|}\right)=\cos^{-1}\left(\frac{d^2/4}{\sqrt{\frac{3d^2}{4}\frac{3d^2}{4}}}\right)=\cos^{-1}\left(\frac{1}{3}\right)$. Since $\theta_2^B=\pi-\theta_1^B$, it turns out that $\theta_2^B \approx 109.4712^o$. θ_3^B is obviously 180^o. □

Closer investigation of *FCC* and *HCP* structures provides similar observations, and we summarize them here without the details of the derivation.

Lemma 2 Suppose that a *FCC* unit cell is given. Then, the following holds.

1. There are 66 distinct angles, in total, defined at the center atom with respect to the vertex atoms.
2. There are 24 cases of θ_1^F angles, 12 cases of θ_2^F angles, 24 cases of θ_3^F angles, and 6 cases of θ_4^F angles defined at the center atom.
3. $\theta_1^F = 60^o$, $\theta_2^F = 90^o$, $\theta_3^F = 120^o$, and $\theta_4^F = 180^o$.

Lemma 3 Suppose that a *HCC* unit cell is given. Then, the following holds.

1. There are 66 distinct angles, in total, defined at the

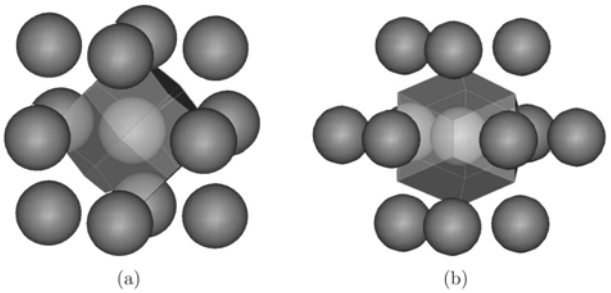

Fig. 5. Voronoi regions for a center atom: (a) *FCC*-Model and (b) *HCP*-Model.

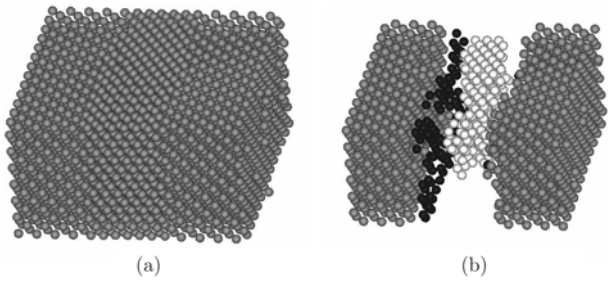

Fig. 6. (a) Al-Co 5458 atoms-Gray: NONE and (b) *BCC*, *FCC*, and *HCP* atoms after extraction-Black: *BCC*, Gray: *FCC*, and White: *HCP*.

center atom with respect to the vertex atoms.

2. There are 24 cases of θ_1^H angles, 12 cases of θ_2^H angles, 3 cases of θ_3^H angles, 18 cases of θ_4^H angles, 6 cases of θ_5^H angles, and 3 cases of θ_6^H angles defined at the center atom.

3. $\theta_1^H = 60^o$, $\theta_2^H = 90^o$, $\theta_3^H \approx 109.4712^o$, $\theta_4^H = 120^o$, $\theta_5^H \approx 146.4426^o$, and $\theta_6^H = 180^o$.

Crystal Structure Extraction

The above-discussed three lemmas can be efficiently used to extract the boundaries of crystal structures for a given set of atoms. The most critical part of the process is to locate the neighboring atoms for a given atom, we take advantage of an Euclidean Voronoi diagram of atoms constituting the material. Since the neighbors can be easily located once a Voronoi diagram is available, the calculation of angles and distances among neighbors can be done easily.

Let $A=\{a_1, ..., a_n\}$ be a material substrate consisting of atoms a_i. Then, let $VD(A)$ be the Euclidean Voronoi diagram of the atoms. Given $VD(A)$, we apply Lemmas 1 through 3 for each atom and check if the atom satisfies one of the lemmas. By collecting the set of atoms satisfying each lemma, we can isolate a grain with a single crystal structure.

Figure 6 shows an example of such an experiment. In Fig. 6(a), there are 5,458 atoms generated by molecular dynamics software XMD 2.5.32 with Al and Co atoms constituting the substrate [20, 22]. In the substrate, there are 3,627 Al and 1,831 Co atoms, respectively. Note that Al and Co atoms are known to form FCC and HCP structure in general, and the radii of Al and Co are 1.43 Å and 1.25 Å, respectively. As the initial condition for XMD run, the inter-atomic distances between Al atoms was set at 2.86 Å, between Co atoms was set at 2.51 Å, and the distance between Al and Co atoms was set at 2.68 Å, respectively.

Using the above lemmas and Voronoi diagram, the grains with three crystal structures are extracted and some statistics are obtained. For example, Fig. 6(a) shows the input substrate and Fig. 6(b) shows the extracted structures of *BCC* in a black color, *FCC* in a gray color, and *HCP* in a white color. Note that the atoms which do not belong to any crsytal structure are not shown in the Fig. 6(b).

Since the angles and distances are represented in floating numbers, it is inevitable to employ tolerances when numbers are compared to test. More importantly, the vibration of atoms also requires the concept of tolerances as well. In the current experiment, we adopted the value of 0.15 for both angular tolerance (in radians) and distance tolerance. Note that 0.15 radian is approximately 9^o.

Conclusions

In this paper, for the classification of three crystal structures from an arbitrary material, the Voronoi diagram as a powerful tool for analyzing spatial attributes was presented. Especially, the useful property of searching a neighbor in a Delaunay tessellation, which is a dual of Voronoi diagram, is applied. Also,the distinct number and value of angles for each crystal structure (*BCC*, *FCC*, and *HCP*) are introduced by lemmas. Therefore, using the properties based on angular distribution of each crystal structure and its Voronoi diagram, the crystal structure extraction can be applied to analyze the structure of material and information on grains quantitatively from the location of atoms in 3D space.

For the future work, there are more observations for other crystal structures and we can analyze the grain boundary of a material under the parameters such a temperature, stress, shock waves, and etc.

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