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Distributions of BCC, FCC, and HCP structures in Al-Co composite materials

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The structural configurations of atoms constituting materials are one of the fundamental factors in the study of the physical properties of materials. Presented in this paper is a mathematical and computational methodology based on Euclidean Voronoi diagrams to efficiently classify a given atomic structure of an Al-Co composite material into groups of atoms with *BCC, FCC,* and *HCP* crystal structures. In this paper, the presented mathematical theory has been applied to analyze a multi-layer atomic structure with a geometric perspective so that the best conditions for thin film growth can be found.

Key words: Crystal Structure, Voronoi Diagram, Geometric Algorithm, Composite Material.

Introduction

Techniques to understand and control microscopic systems are important because they provide ways to control material properties. For instance, the defects in geometric arrangements of atoms in a material have critical influences on mechanical behavior such as the distribution of strain and mechanical strength [1, 2]. The electronic and chemical characteristics of materials also change by the existence of impurities in the material. For example, impurities enhance the mechanical characteristics of materials by protecting the material from the possible propagations of cracks and dislocations [3, 4].

The followings are important geometric factors affecting the material properties: While pores, dislocations, cracks, and grain boundaries affect the material properties on a microscale the arrangement of atoms, the order of stacks, and lattice mismatches influence them in on a nanoscale.

For the investigation of the above properties, therefore, a method to model grains based on a theory of geometry has become inevitable since it can provide an effective and efficient tool which can analyze facts and phenomena of materials where it is very difficult to do experiments. Among possible tools, molecular dynamics handles the movement of atoms using their potentials and is usually adopted as a simulation tool to replace experiments for the arrangements and movements of atoms, crystal growth, the propagation of grain boundaries, etc.

Voronoi diagrams have diversely been used as an atomic simulation tools like molecular dynamics in material science. One of the fields of using a Voronoi diagram is to make substrates consisting of a poly-crystalline structure. Each crystallite has its particular structure and orientation, however, there are nearly no relationship among the crystallites. Hence, the space between the crystallites with a different structure and orientation should be filled under a reasonable assumption so that a Voronoi diagram may be introduced to make the substrate. Moreover, there are applications for spatial problems. For example, analyzing the distributions of voids and investigating the structure of grains [2, 5-9] are examples of these. We found an interesting study using a Voronoi diagram to study the distribution of voids in a porous material [30].

Presented in this paper is a computational algorithm with a few geometric conditions on the fundamental three crystal structures: Body-Centered Cubic (*BCC*), Face-Centered Cubic (*FCC*), and Hexagonal Closed-Packed (*HCP*). Note that the geometric conditions for these three crystal structures are described in our previous paper [22]. Based on the geometric observations, a powerful and well-known computational tool called a Voronoi diagram and its use are introduced in this paper. Finally, the result of the structural extraction from an Al-Co composite material are presented and a few experiments are described. We want to note that a group of Russian scientists lead by Medvedev has been working on a similar problem with a slightly different perspective [10-15]. As early as 1987, Medvedev developed a theory to extract local geometric structures among nearly atoms using Voronoi diagram [15].

Euclidean Voronoi Diagram of atoms

Suppose that a finite number of distinct geometric entities, which we call *generators*, are given in a space.

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If we allocate all locations in this space with the closest member among the generators with respect to the Euclidean distance, the partition of the space into a number of regions results. Such a partition is a tessellation of the space and called the Euclidean Voronoi diagram of the given generators where each region is called a Voronoi region [24].

The most critical part of the process is to locate the neighboring atoms for a given atom and we take advantage of an Euclidean Voronoi diagram of atoms constituting the material. The computation of a Voronoi diagram can be done by a library such as CGAL [35]. In CGAL, the neighboring generators for a given generator are found by using a tetrahedron in 3D space. Note that each tetrahedron has four generators. Hence, if the neighboring tetrahedrons with a given generator for a particular tetrahedron are found, all neighboring generators are located for a given generator. After computing a Voronoi diagram, it is quite easy to find information from among the neighbors so that the computation of distance and angular conditions in the crystal structure extraction can be efficiently performed [17, 18].

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 [19-21], 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.

Extraction of Crystal Structures

For extraction of crystal structures, the needs of a Voronoi diagram are essential to search the neighboring atoms next to a particular atom extracted by a certain crystal structure. Hence, the efficiency of a Voronoi diagram for extracting crystal structures from just the location of atoms is as follows.

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 a linear time of the number of neighbors. In a planar case of a Delaunay triangulation, for example, a triangle next to a particular triangle can be found in a constant time. In 3D, similar observation holds and a neighboring tetrahedron for a particular tetrahedron can be located in a constant time. Therefore, a neighborhood search for a given 3D atomic structure can be very efficiently done once its Voronoi diagram is computed [21, 29, 31, 32].

In [22], the geometric conditions inherent to BCC, FCC, and HCP crystal structures have been presented. In report, an atom in a BCC structure should satisfy 28 angular conditions with 3 distinct angles, while a FCC structure has 66 angular conditions with 4 distinct angles. On the other hand, a HCP structure requires 66 angular conditions with 6 distinct angles. All three crystal structures have distance conditions with an identical distance between atoms.

To extract the crystal structures from substrates obtained from MD simulations, the Voronoi diagram for each substrate is computed so that the neighboring atoms for a particular atom can be efficiently located. Once the neighbors are located, the angular and distance conditions as summarized in the above are checked to see if they satisfy them. The following pseudocode summarizes the algorithm to extract grains with different crystal structures from substrates.

Experiments of crystal structure extraction

The algorithm explained in the previous section was implemented and tested against material data sets obtained from molecular dynamics simulations and the test results are given as follows.

Model data file description

To create a material data set, the embedded-atom method (EAM) based on interatomic potentials, as explained in [36], was utilized. In the present study, we have employed the potential developed by Pasianot and Savino for Co-Co [37], and Voter and Chen potential for Al-Al [38]. The pair potential of Co-Al was obtained by a linear combination of the effective pair interactions given by the following formula [39].

$$V_{CoAl}^{eff}(a+bx)=A[xV_{CoAl}^{eff}(c+dx)+(1-x)V_{CoAl}^{eff}(e+fx)] \quad (1)$$

where $0 \le x \le 1$ denotes the interpolation distance between two atoms and the parameters a, b, c, d, e and f are listed in Table 1. The Co-Co, Al-Al and Co-Al potentials employed showed good agreements with the experimental values for the pure elements as well as those for the intermetallic properties between atoms.

The substrate produced contained 1,440 atoms with planes normal to the surface forming ten layers of (001) planes containing 144 atoms each. The dimensions of the substrate were $12a_0 \times 6a_0 \times 5a_0$, where a_0 was the bulk lattice constant for the surface normal to the z direction. Periodic boundary conditions were utilized in the x and y directions. To mimic a surface, the position of the bottom-most two layers was fixed and the

Table 1. Parameters for Co-Al interatomic pair potential. Energies are in eV, distances in Å

a	b	c	d	e	f	Å
1.690	4.0	1.910996	3.643984	1.75373	3.509799	1.0909091

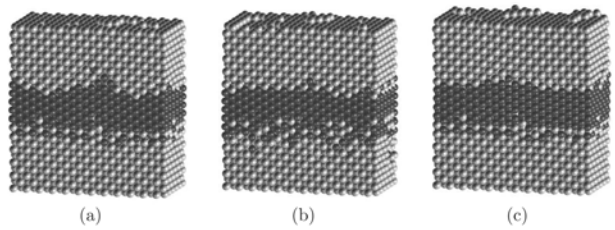

Fig. 1. (a) K_i=0.1 eV. (b) K_i=3.0 eV. (c) Modulate K_i.

substrate was kept at 300 K using the atom-velocity-rescaling method. The adatoms were randomly positioned in the xy plane at a distance of 30 Å from the substrate surface. The initial velocity of each incident atom can be calculated from the incident energy by the following expression:

$$V_{adatom}=\sqrt{\frac{2K_i}{M}} \quad (2)$$

where K_i represents the initial kinetic energy and M is the atomic mass. The MD time step was set to 1 femto-second (fs), and the system was fully relaxed for each additional adatom in the limit of 5 pico-second (ps). The XMD 2.5.32 code of Rifkin was utilized for the MD simulation [40].

Figure 1(a), (b), and (c) illustrate the substrates produced by the molecular dynamics software with parameters K_i=0.1 eV, 3.0 eV, and a modulated K_i between both 0.1 and 3.0 eV's, respectively. Among 5,458 atoms (Al: 3,627, Co: 1,831) constituting the substrates, shown in grey colors are Al atoms and dark grey colors are Co atoms.

In Fig. 1(a), the initial layer *Layer*-1 consisting of Al atoms are given. Then, Co atoms were deposited with K_i=0.1 eV to form a second layer *Layer*-2. After some number of Co atoms were deposited, the third layer *Layer*-3 was created by depositing Al atoms with an identical K_i condition. Note that the interface between *Layer*-1 and *Layer*-2 was relatively smooth while the other interface was rather bumpy.

On the other hand, Fig. 1(b) shows the opposite case. When K_i is 3.0 eV, the first interface was rather fluctuating while the second interface was relatively smooth.

The phenomenon in Fig. 1(a) is explained by "Transient mobility" and "Downward funnelling" models proposed for describing layer-by-layer growth and "Steering effects" which are induced by a strong attraction force between the adatom and substrate. "Steering effects" were proposed for explaining the surface roughening with the low incident energy [25-27]. On the other hand, the roughness on the first interface in Fig. 1(b) is explained by an "Impact cascade diffusion" model. This model suggest that the impacting atom knocks out adatoms on the surface with high incident energy for layer-by-layer growth [28].

The objective of this experiment was to find a condition that produced rather smooth interface in both case. Hence, we experimented with a third substrate by combining both experiments. Consider Fig. 1(c) which consists of two layers *Layer*-1 and *Layer*-2, instead of three. We first deposited half of the Co atoms with K_i= 0.1 eV on the given initial Al atoms at the bottom. Then, the other half of the Co atoms and all the Al atoms on the top were deposited with K_i=3.0 eV. The result turned out to give rather smooth interfaces for both cases.

The experiments for an Al-Co composite material

We have run the program implementing the presented algorithm through three substrates above. Shown in Fig. 2(a) and (b) are the substrate with K=0.1 eV and the extracted crystal structures, respectively. In Fig. 2(b), the black, gray, and white atoms illustrate the grains with structures in BCC, FCC, and HCP, respectively. This particular grain boundary was computed using the angular tolerance of 0.15 radians and the distance tolerance of 0.15 Å. As expected, we can see the BCC structure in between FCC and HCP structures. Shown in Fig. 2(c) is the distribution of atoms in BCC, FCC, and HCP structures with respect to the different values of tolerances for angles and distances among atoms. Figures 3 and 4 show similar experiments with

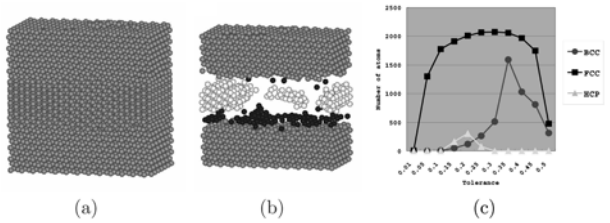

Fig. 2. (a) K=0.1 eV. (b) Black: BCC, Gray: FCC, White: HCP, and Gray: NONE. (c) Frequency.

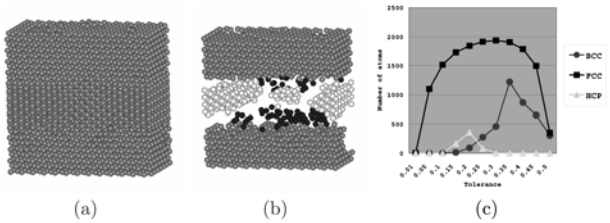

Fig. 3. (a) K=3.0 eV. (b) Black: BCC, Gray: FCC, White: HCP, and Gray: NONE. (c) Frequency.

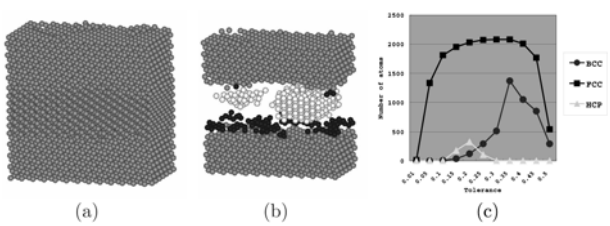

Fig. 4. (a) Modulate K. (b) Black: BCC, Gray: FCC, White: HCP, and Gray: NONE. (c) Frequency.

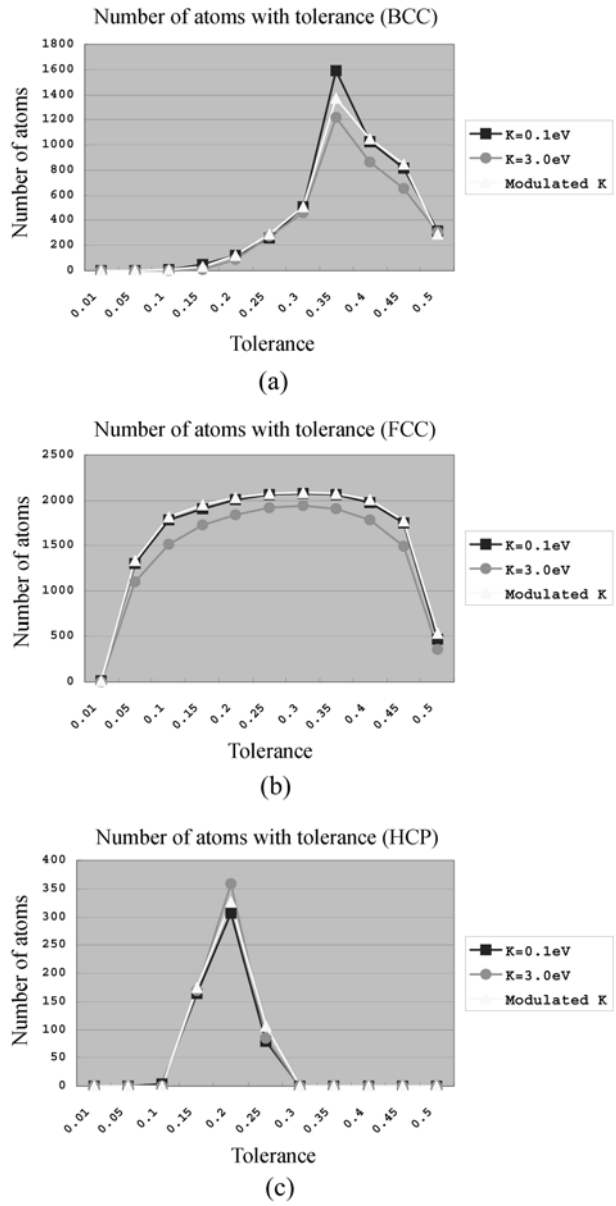

Fig. 5. (a) K_i=0.1 eV. (b) K_i=3.0 eV. (c) *Modulate* K_i: The tolerance of angle and distance is identical.

substrates with K=3.0 eV and the modulate.

Using the above-described substrates, we have tested our theory using various values of tolerances for the extraction of grain boundaries. Shown in Fig. 5 are the frequencies of each grain plotted in one graph. Fig. 5(a), (b), and (c) are the frequencies of BCC, FCC, and HCP structures.

Figure 5 shows that the distance and angular tolerances when most of atoms are 0.35 Å and 0.35 rad under K_i=0.1 eV, 3.0 eV, and *Modulated* K_i, respectively. When K_i is 0.1 eV which means the low incident energy, 1,589 *BCC* atoms are extracted as the highest peak. In Fig. 5(b), the number of *FCC* atoms are nearly the same with both 0.1 eV and *Modulated* K_i and the number of *FCC* atoms are found under the 3.0 eV condition is smaller than the others, in general. Shown in Fig. 5(c) is the frequency of *HCP* atoms extracted under the three energy conditions. The largest number of *HCP* atoms is 358 when the energy condition is 3.0 eV. The computing environment used in the experiment is as follows: Pentium IV with 2GH clock speed and 512 MB of main memory.

Conclusion

This paper has presented a theory to extract grains satisfying the crystal structures of BCC, FCC, and HCP. Based on a few geometric observations and Euclidean Voronoi diagrams discussed in our earlier paper [22], a number of substrates consisting of Al and Co atoms produced via MD simulations were tested.

The technique presented has been applied to find an appropriate process parameters for investigating the optimal conditions for appropriate geometric properties of the atomic structure in multi-layer composite materials such as thin films. Based on experiments, we have given statistics characterizing the spatial properties of given substrates consisting of Al and Co atoms.

The advantages of the proposed technique stems from the powerful geometric properties of Voronoi diagram of atoms. Once a Voronoi diagram is available, isolating neighbors of a particular atom can be efficiently done so that the geometric conditions among them can be performed easily as well.

The theory presented can be, in future, applied to characterize grains with *B*2, *L*11, *L*12, and other structures. In addition, the grain boundaries and properties of a material can be also analyzed under the circumstances of different conditions of temperature, stress, shock wave, and so on.

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