비정질금속에서 일반적 보로노이 해석에 의한 오차
Common errors of Voronoi tessellation technique for metallic glasses

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1. Introduction

The Voronoi tessellation technique in computational studies is the most common tool to analyze the internal structures of metallic glasses, while neutron diffraction is used in experimental studies. So far, most of approaches about atomic structure using Voronoi tessellation technique have inherent error for the metallic glasses studies because of the atomic radius difference of the atomic elements.

It is possible to define the convex polyhedron occupied by half-plane between each point and its neighbor points, using the ordinary Voronoi tessellation technique. However, bisection cannot depict the exact plane to represent the atomic structure because of the atom radius difference in the various compositions of materials. It produces errors of atomic volume, the number of faces, polyhedron distribution, atomic stress, atomistic elastic constant and so on.

2. Radical Plane Method

In the ordinary Voronoi tessellation technique, the location of the vertex can be derived by the equation of sphere as follows:

$$(x_i - x_v)^2 + (y_i - y_v)^2 + (z_i - z_v)^2 = L_c^2 \quad (1)$$

where (x_i,y_i,z_i) are the coordinates of each atom, (x_v,y_v,z_v) are the coordinates of the vertex and L_c is the distance from the vertex to the center of any atom.

In radical plane method, polyhedron plane is located on the position proportional to the atomic radii. The location for the vertex also can be derived by a very similar form with eq. (1) as follows:

$$(x_i - x_v)^2 + (y_i - y_v)^2 + (z_i - z_v)^2 - r_i^2 = L_c^2 \quad (2)$$

where, r_i and L_t are the radius of each atom and the distance between the vertex and the tangential point, respectively. Similar to the ordinary Voronoi tessellation technique, in radical plane method, there must be no atoms with a smaller distance than L_t.

3. Computational Model Setup

Modeled binary systems consist of different composition of fictitious A atoms and B atoms. Molecular dynamics study using modified Lennard-Jones potential is adopted under periodic boundary condition and constant pressure condition. The A atom is originally modeled as Zr atom. B atom also is modeled as a fictitious atom with smaller atomic radius than A atom. The size ratio of A atom to B atom and total number of atom, is fixed as 0.55 and 2000, respectively. The composition of the binary system is changed to describe the effect of element composition from $A_{20}B_{80}$ to $A_{80}B_{20}$. Finally constructed models are $A_{20}B_{80}$, $A_{40}B_{60}$, $A_{50}B_{50}$, $A_{60}B_{40}$ and $A_{80}B_{20}$.

To get amorphous structure, the system is fully heated to 5000K for 235ps, relaxed for 1000ps and cooled to 300K for 4700ps with periodic boundary condition and a cooling rate 10^{12}K/s. During the process, Parinello-Rahman method is applied to keep constant pressure. Finally, we obtain the models with amorphous structure.

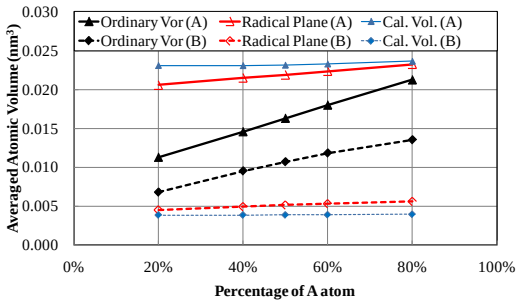

Fig.1. Averaged atomic volume measured by ordinary Voronoi tessellation technique and radical plane method. Calculated volume depicts the volume per atom based on the radius ratio of B atom to A atom.

4. Results and Discussion

To calculate the averaged atomic volume, whole model volumes for each composition are measured. Then, the atomic volume is calculated under the assumption that atomic volume of B atom is around 6 times smaller than that of A atom because the atomic radius ratio of B atom to A atom is 0.55. Based on the calculation, calculated atomic volume denoted by blue line with small solid marks in Fig. 1 has almost constant value for various compositions. However, averaged atomic volume by the ordinary Voronoi tessellation technique is clearly proportional to the percentage of bigger atom (A atom). In radical plane method, the proportion is relatively much smaller or negligible. Especially, for the case of A80B20, (80% on abscissa of Fig.1), the error percentage of B atom measured by the ordinary Voronoi tessellation technique, is around 250%. As can be expected from atomic volume distribution, for the case of A50B50, the volume for both atoms includes a lot of errors.

To know the atomic structure, Voronoi polyhedron index is often analyzed. Voronoi index measured by ordinary Voronoi tessellation technique and radical plane method is depicted in Fig. 2. Some Voronoi polyhedron often found in CuZr or NiZr metallic glasses such as a trigonal prism capped with three half-octahedron (0 3 6 0 0 0), and Archimedian antiprism capped with two half-octahedra (0 2 8 0 0 0), and a tetragonal dodecahedron (0 4 4 0 0 0), are

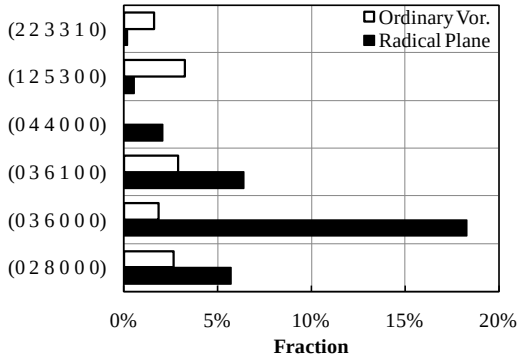

Fig. 2. Voronoi polyhedron index for $A_{50}B_{50}$ model.

measured. As seen in Fig. 2, the fraction of (0 3 6 0 0 0) structure is exceedingly increased from 2% to 18% when the analytical way is changed from ordinary Voronoi tessellation technique to radical plane method. The fraction of (0 2 8 0 0 0) is also increased from 3% to 6%. Some other structure such as (1 2 5 3 0 0) structure is going down. Consequently, the structure analyzed by ordinary Voronoi tessellation technique is not matched with that by radical plane method, at all.

5. Conclusion

In this work, the ordinary Voronoi tessellation technique and the radical plane method considering the size of atoms are compared as the composition of models is changed. Consequently, the error between two analytical ways is exceedingly large. And it is not just a quantity matter. It can affect to the whole analysis, for example, Voronoi polyhedron index. Voronoi analysis without considering the size difference of atoms leads to totally incorrect results.

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Reference

1. Voronoi GF. J Reine Angew Math 1908;134:198
2. Gellatly BJ, Finney JL. J Mol Biol 1982;161:305
3. Park J, Shibutani Y. Intermetallics 2007;15:187