Entrepreneurship and Innovation
2025, VOL. 9, NO. 1, 88-91
DOI: 10.47297/wspeiWSP2516-253516.20250901

Algorithmic analysis of the microstructure of aluminum alloy

Chang Liang

National Technical University, Kharkiv, Ukraine, 61000

ABSTRACT
In this paper, the microstructure and mechanical properties of aluminum alloy materials were studied. The microstructure simulation program of Voronoi algorithm was written with Python, and the program was imported into ABAQUS finite element software to establish the grain model of aluminum alloy. The finite element model of grain structure was established. The results show that the stress concentration coefficient of a single inclusion particle decreases first and then increases with the increase of elastic modulus. Compared with a single inclusion particle, the stress concentration of two inclusion particles will increase, and the shape, quantity and distribution of inclusion particles have influence on the microstructure stress concentration.

KEYWORDS
aluminum alloy; Voronoi; microstructure; python

1 Introduction

From the damage of structural materials, people gradually realize that the damage or fracture phenomenon of materials comes from the micro-scale or micro-scale of materials, and any factors affecting the microstructure of metal materials will affect the macroscopic mechanical properties of materials. In order to better understand the mechanical properties of aluminum alloy materials used in aircraft and clarify the damage and failure mechanism, it is necessary to conduct research on both macroscopic mechanics and microscopic mechanics[1].

With the deepening of people's understanding of the nature of material fracture failure, the limitations of the application of fracture mechanics have also been understood: fracture mechanics cannot describe the process of damage initiation and evolution until the emergence of macroscopic cracks[2]. Predecessors have done a lot of research work on the microscopic test analysis of aluminum alloy, Liao *et al.*[3] studied the microstructure and the distribution of microscopic inclusion particles. McDowell *et al.*[4] studied the sensitivity of polycrystalline microstructure formed by fatigue cracks, providing a basis for the microstructure anti-fatigue design and the reduction of crack nucleation sites. Li *et al.*[5] studied 2026 aluminum alloy and found that crack nucleation is directly related to the second phase particles containing iron. Wang *et al.*[6] experimentally studied the microscopic failure mechanism of cast MG-Al series alloys by SEM in-situ observation method.

2 Algorithm of microstructure of aluminum alloy

Voronoi graph generation algorithm is shown in Figure 1. Figure 2 shows the Voronoi diagram generated by using a Python program to generate 100 random points.

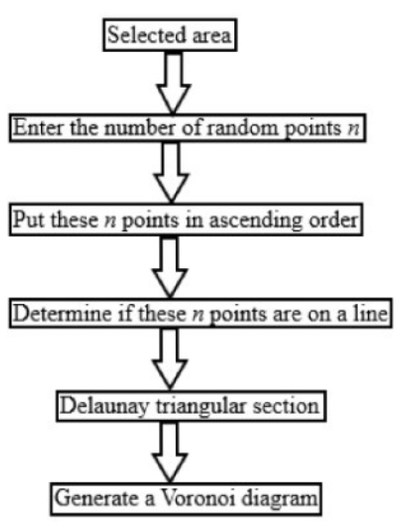

Figure 1 Generation algorithm of Voronoi diagram

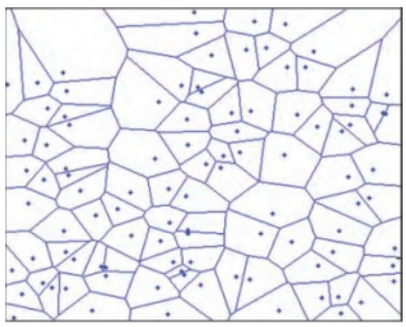

Figure 2 Voronoi diagram

According to the statistical grain size of aluminum alloy, the grain size distribution function of aluminum alloy is obtained. Combined with Voronoi diagram, the two-dimensional grain model of aluminum alloy polycrystal is established. The polycrystalline microstructure of metal materials generated by Voronoi algorithm is consistent with the actual microstructure of the actual structure. The difference between the orientation of grains and the orientation of adjacent grains has a great influence on the initiation of short cracks. The Voronoi diagram can only be used to simulate the initial number and location of crystal nuclei, but it cannot be used to simulate the orientation of grains. The orientation of grain has great randomness. Therefore, in the microstructure diagram shown in Figure 2, the orientation of the grains is randomly generated and determined.

3 The cohesion relationship between grains

Cohesive Zone Model (CZM) can describe the cohesive force and frictional slip between interfaces. The initiation and propagation of intergranular microcracks are expressed in an explicit form by CZM, which conforms to the law of intergranular force. CZM can reflect both the Forward Region of crack and the Wake Region of crack that inhibits crack growth. Especially for elastoviscoplastic materials, the failure does not occur instantaneously after the maximum stress, so it is physically reasonable to use CZM to reflect the continuous progressive fracture process.

The two-dimensional six-node cohesive element selected in this paper is composed of two three-node quadratic isoparametric line segments. When the adjacent elements are deformed by the force, there is relative displacement between the interfaces, and cohesion is generated.

4 Finite element model

4.1 Assumptions of the model

The determination of grain size is the first problem to be solved in modeling grain size scale. Using the cohesive force model and the relevant knowledge of continuum mechanics, the following assumptions are made:

1) Aluminum alloy grains were generated according to Voronoi method, and the microscopic grain size of aluminum alloy was statistically analyzed, and the grain size of the simulation was 53μm;

2) The mechanical relationship between grains is defined as the relationship between displacement and driving force in the cohesive region model, and the finite element method based on the theory of continuous mechanics is applied to the mechanical analysis of grain size, so as to carry out finite element analysis;

3) Material parameters do not change with the change of research scale.

4.2 Grain size model

According to the proposed Voronoi algorithm, Voronoi polygons containing elliptical inclusion particles are generated in the grain scale model, and each Voronoi polygon is considered to be a continuum. Then, the model is meshing, and the parameters such as element type and material properties are unchanged. The geometry information of Voronoi diagram is obtained by programming related programs in Python, and the microstructure simulation program of Voronoi method is written. The *inp* file was written with Python scripting language and imported into ABAQUS software to establish the grain model of aluminum alloy. The geometric information part of the model was established using the pre-processing module CAE of ABAQUS finite element simulation software, and the ABAQUS input file of the aluminum alloy microscopic model was obtained by combining Python program. The finite element calculation module STANDARD of ABAQUS was used for simulation analysis and calculation. The final visualization results are analyzed by ABAQUS post-processing module.

4.3 Model grid and boundary conditions

According to the above assumptions, geometric parameters and boundary conditions, the model element type is quadrilateral plane strain element. Figure 3(b) shows the grain model with 2304 divided elements, and it can be seen that the grid division is relatively rough compared with the grain boundaries. In order to meet the linear grain boundary, the mesh needs to be further refined during calculation, but the corresponding calculation time will also increase. The total number of units divided by the microstructure model calculated in this paper is 36,864. The boundary conditions for simulating the stress distribution under unidirectional tension are as follows: AB edges are fixed and constrained, CB and DA remain flat and CD is subjected to uniform displacement.

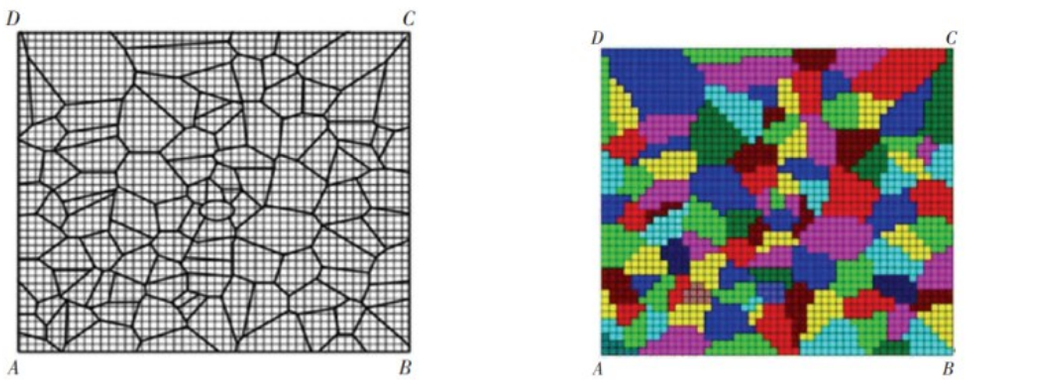

Figure 3 Finite element model for micro grain scale

The grain orientation is determined by random number to ensure that the aluminum alloy is the same material. When the influence of inclusion particles on microscopic stress concentration is investigated, the elastic modulus of inclusion particles is assumed to be variable and the elastic modulus of matrix is assumed to be constant. It is assumed that the elastic modulus of the inclusion particle is smaller than that of the matrix when the stress between the inclusion particle and the matrix is investigated. Among them, the material parameters of the matrix are elastic modulus E and Poisson's ratio v. The bilinear cohesion relation adopted in this paper includes three parameters: the normal displacement and tangential displacement δ_n^0 and δ_t^0 corresponding to the cohesive force when the normal and tangential directions are the maximum values, or the initial linear modulus; The maximum normal stress and tangential stress of cohesion σ_{max} and τ_{max}; Critical opening normal displacement and critical opening tangential displacement and or normal breaking energy critical values $\varphi_n^c = 1/2{\cdot}\sigma_{max}\delta_n^c$, $\varphi_t^c = 1/2{\cdot}\tau_{max}\delta_t^c$ and tangential breaking energy critical values are shown in Table 1 and Table 2.

Table 1 Material parameter of computed model

parameter	*E/GPa*	*v*
substrate	69.58	0.33
particle	57.00	0.32

Table 2 Grain boundaries parameter of computed model

Grain boundary parameter	$\sigma_{max} = \tau_{max}/GPa$	$\delta_n^0 = \delta_t^0/\mu m$	$\delta_n^c = \delta_t^c/\mu m$
grain boundary	0.5	0.3	0.1
Particle Grain boundary	0.1	0.3	0.1

5 Conclusion

The stress concentration coefficient of a single inclusion particle decreases first and then increases with the increase of elastic modulus. Compared with a single inclusion particle, the stress concentration of two inclusion particles will increase. When d/r is close to 2, the stress concentration coefficient increases significantly. When d/r is around 6, the stress concentration coefficient basically returns to the size of the single inclusion particle.

The microstructure of aluminum alloy containing inclusions (second phase particles) is simulated by Voronoi diagram algorithm. Using the cohesive stress-displacement relationship in the cohesive force model to describe the mechanical relations between grains and between grains and inclusion particles, the finite element analysis of microstructure of aluminum alloy is realized. The influence of the shape, quantity and distribution of the inclusion particles on the microstructure stress concentration is obtained by finite element model analysis.

Funding

Heilongjiang Provincial Department of Education basic research funds basic research project (No. 2023-KYYWF-0580).

References

[1] Bian G, Chen Y, et al. Microstructural mechanism fatigue crack nucleation and propagation of 2A12 aluminum alloy[J]. Chinese Journal of Materials Research, 2012:26(5):521-526.

[2] Liu D, Xie Y, et al. Influence of process parameters creep age forming formability of 7075 aluminum alloy sheet[J]. Materials Science and Technology, 2015:23(3):50-56.

[3] Liao M. Probabilistic modeling of fatigue related microstructural parameters in alloys[J]. Engineering Failure Mechanics, 2009:76, 668-680.

[4] Mcdowell D L, Dunne F P E. Microstructure-sensitive computational modeling of fatigue crack formation[J]. International Journal of Fatigue, 2010, 32(9):1521-1542.

[5] Li J X, Zhai T, et al. Four-point-bend fatigue of AA2026 aluminum alloys[J]. Metallurgical and Materials Transactions A, 2005, 36: 2529-2549.

[6] Wang X, Tang B, et al. In-site observation technology and application of fatigue crack initiation and propagation for cast magnesium alloys[J]. Materials for Mechanical Engineer. 2006:30(2):1-5.