Numerical simulation of polycrystalline aluminum alloy welded joints with micropores

Jiazheng Du1, Xiangchuan Nian1, Liya Liu1 and Wen Deng1

1Department of Engineering Mechanics, Beijing University of Technology, Beijing, 100124, China
*Corresponding author’s e-mail: djz@bjut.edu.cn

Abstract. Aluminum (Al) alloy welded structures are widely used in industry and daily life, while welded joints are easily produced defects, including macro and microscopic defects. It is a hot topic to study the effect of microscopic defects on the properties of welded joints. In this paper, a two-dimensional rate-dependent crystal plasticity model is established by using a numerical model, and then the mechanical behaviors of welded joints with micropores under tensile load is simulated in a mesoscale. The mechanical properties are described by varying the sizes and positions of micropores. The stress-strain response, equivalent plastic strain and equivalent stress distributions of polycrystalline Al alloy welded joints with different micropores are obtained. The results verify that those micropores have certain impact on the start of slip systems and the ability of resisting the deformation of polycrystalline joints. Compared with the positions of micropores, the sizes of micropores have a greater impact on the mechanical properties of the polycrystalline joints.

1. Introduction

At present, engineering and environmental issues mostly require lightweight and energy-saving structures. Because aluminium (Al) alloy has the characteristics of high specific strength, easy forming and environment friendly, it can meet the above requirements, which makes it widely used in industry and daily life, such as aerospace and high-speed rail. Welding is one of the most important ways to connect Al alloy in above-mentioned applications, but welding is prone to defects such as pores and inclusions. These defects often deteriorate the texture of welded joints and easily lead to welded joints fracture. With the improvement of welding technology, macroscopic defects have been greatly reduced. However, there are still many microscopic defects in welded joints, such as metallurgical pores [1], the reports on the effects of microscopic defects on welded joints are few, especially from the perspective of numerical simulation, which is essential issue of scientific and technical in the future [2].

Experiments indicate that the mechanical properties of welded joints are very uneven in various regions [3], in order to reveal the essential causes of this phenomenon, it must be from a microscopic point of view. But, there are still many problems based on traditional experience and experimental methods in a microscale or mesoscale. Studies have shown, the crystal plasticity finite element method (CPFEM) can solve above problems, a method combined by the crystal plasticity theory and the finite element method.

In the reports on CPFEM, more research has been done on single and bicrystal than on polycrystals. Orsini and Zikry [4] studied the growth of pores in FCC copper single crystals using rate-dependent crystal plasticity model. The results showed that the rotation and plastic slip of the crystal concentrated...
in the region between the pores. Schacht et al [5] simulated the voids evolution of three-dimensional single crystals with different initial orientations. The simulation results showed that the growth and deformation of voids were closely related to Crystal orientation. Asim et al [6] pointed out that tough failure in high-strength Al alloys occurred due to the evolution and accumulation of micropores. Numerical simulations of single crystal Al alloys (AA-5xxx) with different voids and orientations were performed using representative volume element (RVE) and the relationships among initial void size, void growth, plastic anisotropy and local size effects were predicted. Liu et al. [7] investigated the damage behavior of single crystal and bicrystal with voids under tensile load in a mesoscale by using a two-dimensional rate-dependent model. It is found some results by varying the initial orientations, void geometries, and loading conditions and indicated that mechanical properties of Al depend heavily on these factors. In the study on polycrystals, Si [8] developed a user-defined material constitutive law subroutine (UMAT), which simulated the plastic deformation of pure Al crystal in Abaqus, and verified the validity of programs. The geometrical model based on the Voronoi algorithm is used to simulate the actual shape of each grain, which proved the applicability of this method. However, there are few studies on Al alloy welded joints by CPFEM. Since Al alloy has undergone the welding process and its material properties have changed, which makes the welded joints with the typical characteristics of polycrystals. Therefore, this paper re-developed UMAT to realize numerical simulation of polycrystalline Al alloy welded joints with micropores. This not only provides a theoretical basis for the manufacture and safety evaluation of Al alloy welded joints, but also has great economic and time advantages.

2. The constitutive equation of CPFEM

In the analysis of finite deformation of single crystal materials, the total deformation gradient can be decomposed as

\[ F = F^e \cdot F^p \]  

in which, \( F^e \) denotes the gradient of elastic deformation and rigid rotation, \( F^p \) denotes the gradient of deformation caused by plasticity.

The velocity gradient is marked as \( L \), which can also be decomposed as

\[ L = \dot{F} \cdot F^{-1} = \dot{F}^e \cdot F^e + \dot{F}^p \cdot F^{-1} \cdot F^e = L^e + L^p \]  

The relationship between shear strain caused by slip and overall plastic deformation in each slip system is expressed as

\[ L^p = \sum_{a=1}^{N} \dot{\gamma}^a s^a \otimes n^a \]  

where, \( \dot{\gamma}^a \) is the slip rate on the \( a \)th slip system, \( s^a \otimes n^a \) denotes the Schmid tensor, \( N \) is the total number of activated slip systems.

The slip rate of slip system can be calculated according to the hardening equation.

\[ \dot{\gamma}^a = \dot{\gamma}_0^a \left[ \frac{\tau^a}{\tau_0^a} \right] \left[ \frac{\tau^a}{\tau_e^a} \right]^{m-1} \]  

where, \( \tau^a \) represents the shear stress on the \( a \)th slip system (Schmid stress), \( \dot{\gamma}_0^a \) represents the reference shear strain rate and \( m \) represents the rate sensitivity coefficient, \( \tau_e^a \) represents the reference shear stress, it can be expressed by
\[ \tau^\alpha_c = \sum_{\beta=1}^{m} h_{\alpha\beta} |\dot{\gamma}^\beta| \]  

in which, the hardening modulus \( h_{\alpha\beta} \) is

\[ h_{\alpha\beta} = q_{\alpha\beta} \left[ h_0 \left(1 - \frac{\tau^\beta}{\tau_s}\right)^{\alpha} \right] \]  

where, \( h_0 \) is the initial hardening rate, while \( \tau_s \) is the saturation flow stress and \( q_{\alpha\beta} \) denotes the latent hardening matrix.

Calculating single crystal model is the basis of calculating polycrystal model. The average Cauchy stress of polycrystals expressed by

\[ \langle \sigma \rangle = \sum_{k=1}^{N} \left( w_k \sigma_k \right) \]  

where, \( N \) is the total number of polycrystalline grains, \( w_k \) represents the volume of each grain as a percentage of the total volume, \( \sigma_k \) represents the Cauchy stress of the \( k \)th grain.

3. Simulation process

3.1. The preprocessing of finite element model

This paper used Voronoi cell to simulate a two-dimensional Al alloy welded joints to accurately express the grain morphology. We have independently developed some programs to quickly generate the 2D and 3D Voronoi models. In order to ensure the representativeness of the simulation, several models with different grain numbers had been simulated and finally adopted 45 grains, according to the principle of determining the number of crystal grains in the literature [9].

![Figure 1. Schematic diagram of the pores at two positions.](image)

To ensure the characteristics of the representative volume element, the boundary conditions were applied on the model shown in figure 2. During the simulation process, the maximum uniaxial tensile displacement was 20% of the side length, applied to the right border. The paper tested the sensitivity of elements, and when quantity of grid reaches a certain value, the results tend to be stable. Finally, about 2500 elements of CPE4R were established for those models.
3.2. Determination of material parameters

There are 8 parameters in the developed UMAT, as listed in Table 1 [10].

Table 1. The material parameters of CPFEM.

| Parameter | Value       |
|-----------|-------------|
| $C_{11}$  | 106.75 GPa  |
| $C_{12}$  | 60.41 GPa  |
| $C_{44}$  | 28.34 GPa  |
| $\dot{\gamma}_0$ | 0.001 s$^{-1}$ |
| $\tau_0$  | 0.02 GPa    |
| $\tau_s$  | 12.5 GPa    |
| $h_0$     | 75 GPa      |

In the table, $C_{11}$, $C_{12}$, and $C_{44}$ represent the linear elastic constants of the crystal, and $\tau_0$ represents the reference shear stress of the slip system $\alpha$ at $\dot{\gamma}_0 = 0$. The remaining parameters are the same as those in section 2.

4. Results and discussion

As shown in Figure 3, it is the stress-strain response and the equivalent stress distribution at four stages of welded joint without pore. For the elastic evolution stage, the slip system is not activated at this stage. Then polycrystals enter the yield stage, there is a clear yield point, 51.3 MPa, which shows that the slip system is activated at this time. Owing to the anisotropic characteristic of polycrystals, the overall stress distribution is extremely uneven. The maximum stress and strain appear at the lower left corner and the upper right corner. For the final stage, as a result of the interaction of polycrystals, a larger stress zone is formed in the region about 45° from the uniaxial tension direction. The stress on both sides of that region decreases gradually.

![Figure 3. Tensile response and equivalent stress distribution (No pore).](image)

(a) Equivalent plastic strain at $\varepsilon=0.14$.

(b) Equivalent plastic strain at $\varepsilon=0.2$.

![Figure 4. Equivalent plastic strain distributions (No pore).](image)

The equivalent plastic strain distributions at two stages was obtained, as illustrated in Figure 4. It is similar to the equivalent stress distribution. The equivalent plastic deformation begins to increase at the lower left corner and the upper right corner, and the slip system begins to start first at $\varepsilon=0.14$. Afterward, the slip system in the region at 45° to the loading direction begins to start at $\varepsilon=0.2$. It shows that these regions are the most vulnerable to failure.

Subsequently, we investigated a total of nine cases with pores, including pores of three sizes distributed in three positions. A comparison of the stress-strain response of ten cases (with/without pore) is shown in Figure 5. If there is a pore, the yield point is lower than that there is no pore, in other words, the slip system is easier to begin, and the ability of resisting the deformation is also deteriorated. When the strain is the same, the greater the magnitude of stress, the better the resistance to deformation. In the nine cases with pores, when the diameter of pore is 0.020 mm and it was located at the boundary, the yield point is the highest and the deformation resistance is the best, at this case, the performance of Al alloy welded joint is close to that without pore. And the effect of pore on the macro mechanical properties of the joints can be neglected, this conclusion is consistent with the literature [11]. On the contrary, when the diameter of pore is 0.050 mm and it was located near the boundary, the yield point is the lowest and the deformation resistance is the worst.

As the most concerned issues in many engineering cases is the factor causing the worst impact, so this paper takes the diameter of pore is 0.050 mm as an example to conduct a detailed study.
The stress-strain response at three positions of this pore is shown in figure 6. The yield point of polycrystals is the highest when the pore was located at the boundary, while the lowest was located near the boundary. Correspondingly, the ability of resisting the deformation at the boundary is the best, and the other two are a little worse and not very different.

When the pore was located near the boundary, the equivalent stress distribution at the final stage is shown in figure 7. The magnitude of stress around the left and right sides of the pore is low, called the shadow zone of stress, which is larger than formed by the other pores, and the width of the zone is almost equal to the diameter of pore, indicating that the bearing capacity of this zone is degraded and the mechanical properties are deteriorated. There is a maximum magnitude of stress at the lower left corner of the whole model and at the upper and lower sides of the pore.

The equivalent plastic strain distributions at two stages was obtained, as is shown in figure 8. Compared with no pore, the overall magnitude of equivalent plastic strain turns greater, and the slip systems in all regions of the crystal are generally activated, and most of the crystals are plastically deformed. The equivalent plastic strain begins to increase significantly on the upper side of pore at \( \varepsilon = 0.12 \). That magnitude of the upper side of pore continues to enlarge, then the region with larger magnitude extends to the boundary, in other regions have not changed any more.

5. Conclusions
This paper developed some programs based on Voronoi algorithm, which can generate polycrystalline geometry model. And CPFEM has been implemented in the Abaqus, by developing a UMAT, which based on a two-dimensional rate-dependent crystal plasticity model. The mechanical properties of polycrystalline Al alloy welded joints with micropores were simulated by developed subroutine. The conclusions are as follows:
(1) The stress distributions in the polycrystalline models are extremely uneven whether there is a pore or not. In the models with pores, the slip system is easier to begin than without pore, and the ability of resisting the deformation is also deteriorated. At the same time, shadow zone of stress will be formed around the pores, and the bearing capacity of the models will decrease.

(2) When the sizes of pores are the same, the process of pores movement from the center to the boundary, the properties of the models will gradually deteriorate, and the worst will be caused when the pores are located near the boundary, if continue to move will gradually improve. When the positions of pores are the same, the joints with the small pores have the better mechanical properties. Overall, compared with the positions of micropores, the sizes of micropores have a greater impact on the mechanical properties of the polycrystalline joints.

(3) Specifically, in the nine cases with pores, when the diameter of pore is 0.020mm and it was located at the boundary, the joint with the best mechanical properties, so in some cases it can be ignored. On the contrary, when the diameter of pore is 0.050mm and it was located near the boundary, the joint with the worst mechanical properties, and the slip systems in all regions of the polycrystalline begin to start universally.

References
[1] Song Z, Wu S C, Hu Y N, et al. (2018) The influence of metallurgical pores on fatigue behaviors of fusion welded aa7020 joints. Acta Metallurgica Sinica, 54(08): 1131-1140.
[2] Li X Y, Wu C S, Li W S. (2012) Study on the progress of welding science and technology in China. Journal of Mechanical Engineering, 48(06): 19-31.
[3] Du J Z, Zhao Z Y, Huang C, et al. (2017) Experimental study of mechanical properties of aluminum alloy welded joint. Journal of Experimental Mechanics, 32(06): 811-817.
[4] Orsini V.C., Zikry M.A. (2001) Void growth and interaction in crystalline materials. Int. J. Plast, 17(10): 1393–1417.
[5] Schacht T., Untermann N., Steck E. (2003) The influence of crystallographic orientation on the deformation behavior of single crystals containing microvoids. Int. J. Plasticity, 19(10): 1393–1417.
[6] Asim U., Siddiq M. A., Demiral M. (2017) Void growth in high strength aluminium alloy single crystals: a CPFEM based study. Model. Simul. Mater. Sci. Eng, 25(3): 35010.
[7] Liu L Y, Yang Q S, Zhang Y X, (2019) Plastic damage of additive manufactured aluminium with void defects. Mechanics Research Communications, 95: 45-51.
[8] Si L Y (2009) Simulation of the texture evolution during cold deformation of FCC metal with crystal plasticity FEM. Northeastern University, China.
[9] Luo J, Kang G Z (2013) Simulation to the cyclic deformation of polycrystalline aluminum alloy using crystal plasticity finite element method. International Journal of Computational Materials Science and Engineering, 02(03n04): 1350019.
[10] Roter F, Wang Y, Kuo J, et al. (2004) Comparison of single crystal simple shear deformation experiments with crystal plasticity finite element simulations. Adv. Eng. Mater, 6(8): 653–656.
[11] Mu P, Nadot Y, Nadot-Martin C, et al. (2014) Influence of casting defects on the fatigue behavior of cast aluminum AS7G06-T6. Int. J. Fatigue, 63(4): 97-109.