Effect of Crystal Orientation on Cyclic Plastic Behaviors of Partially Recrystallized Single Crystal Nickel-based Superalloy

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Abstract. Surface recrystallization (RX) is one of the main causes of fatigue failure of heavy gas turbine single crystal (SX) blade and thus a threat to safe long-time operation. Using crystal plasticity model, the effects of primary and secondary crystal orientation on the cyclic plastic deformation behaviors of recrystallized SX nickel-based superalloy was investigated via crystal plasticity finite element simulation. The results show that primary orientation has significant effect on the accumulated plastic shear stain $\gamma$ of the recrystallized SX superalloy: the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ occurs in SX matrix near RX transverse grain boundary; the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ of RX-SX system increases with increasing primary orientation ($\beta$); the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ at $\beta=15^\circ$ is 31.6% larger than that at $\beta=0^\circ$; the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ decreases first and then increases with the increasing of the secondary orientation ($\theta$) from 0° to 90°, with the lowest value of $\gamma_{\text{max}}$ at $\theta=43^\circ$, which is 1.4% smaller than that at $\theta=0^\circ$ and $\theta=90^\circ$.

The study shows that the crystal orientation can be optimized to reduce the effect of recrystallized grain on the fatigue property of SX nickel-based superalloy.

1. Introduction

Single crystal (SX) nickel-based superalloys have been widely used in aircraft turbines due to excellent high temperature fatigue and creep properties [1]. However, the absence of grain boundaries leads to anisotropic and crystallographic orientation dependent mechanical properties [2,3]. In most case, turbine blades are produced with the primary crystallographic orientation along airfoil stacking line. While the other two orientations are not controlled, named randomness orientation, and considered random variables. Although the primary crystallographic orientation is controlled in the manufacturing process of turbine blades, it is difficult to guarantee the airfoil stacking line align with the primary crystallographic orientation. Arakere et al. [3] studied the influence of variation in crystal orientation on blade stress and fatigue life. The result demonstrates that the control of primary crystallographic orientation has significant effect on a component’s resistance to fatigue crack growth. Wen et al. [4] studied the influence of loading direction on the three points bending creep and uniaxial tensile creep via three-dimensional finite element analysis. The results show that both of the
bending depth and deformation velocity associated with crystallographic orientation [001] are the largest among the three different orientations. Early study [5] assumes that secondary crystallographic orientation has no significant effect on the mechanical properties of SX nickel-based superalloys. However, subsequent studies show that secondary crystallographic orientation has significant effect on the fatigue life of SX nickel-based superalloys [6,7]. Kiyak et al. [6] reported that fatigue cracks grow about two times faster in the [100] direction than in the [110] direction in the Paris regime. He et al. [7] investigated the effects of secondary orientation on plastic deformation and fatigue crack initiation in a SX nickel-based superalloy. The result shows that specimens with different secondary orientation exhibit different crack initiation modes.

During manufacturing process or high temperature application, recrystallization (RX) layers may be formed on the surfaces of turbine components, e.g. leading and trailing edges due to susceptibility to environmental influence. Because the orientations of RX grains are inconsistent with that of single crystal matrix, the RX region is prone to be the initiation source of fatigue crack. The influences of RX grains on the properties of SX superalloys have been widely studied [8-9]. Ma et al. [10] investigated the influence of surface recrystallization on the low cycle fatigue behaviour of a SX superalloy, showing that fatigue life is significantly reduced by surface recrystallization. Zhang et al.[11] studied the fractured turbine blades and indicated that surface recrystallization can lead to the failure of superalloy blades. Therefore, recrystallization should be taken into consider in order to quantify the effect of crystallographic orientation on the strength and fatigue properties of SX superalloy. Up to now, the research about effect of primary orientation and secondary orientation on the cyclic plastic behavior and fatigue properties of recrystallized SX superalloy is rarely reported.

It is reported that fatigue crack is prone to initiate on the slip planes with maximum shear strain via slip band mechanism, or defects near surface or from grain boundaries due to local stress/strain mismatch [12-14]. In this paper, the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ is used to quantify fatigue crack incubation under cyclic loading condition. The influence of primary orientation and secondary orientation on the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ of recrystallized SX superalloy is investigated based on finite element analysis.

2. Crystal Plasticity Theory

The kinematics of crystal plasticity theory presented here is developed by Hill [15], Asaro and Rice [16,17]. The deformation of a crystalline material under external load consists of elastic deformation and inelastic deformation. The total deformation gradient $F$ can be separated into elastic and plastic part and given by

$$F = F^* \cdot F^p$$

where $F^*$ denotes the part of elastic deformation, $F^p$ denotes the part of plastic deformation. The rate of change of $F^p$ is related to shearing rate $\dot{\gamma}^{(a)}$ of a slip system as follow:

$$F^p \cdot F^{-1} = \sum_{\alpha} \dot{\gamma}^{(a)} S^{(a)} m^{(a)}$$

The shearing rate $\dot{\gamma}^{(a)}$ of a slip system can be expressed by the resolved shear stress $\tau^{(a)}$, in a rate-dependent way as

$$\dot{\gamma}^{(a)} = \dot{\alpha}^{(a)} f^{(a)} \left( \frac{\tau^{(a)}}{g^{(a)}} \right)$$

$$f^{(a)} (x) = x |x|^{n-1}$$
where $a^{(\alpha)}$ is the reference shearing rate on $\alpha$ slip system, $g^{(\alpha)}$ is the current strength of $\alpha$ slip system, and $n$ is the rate sensitivity exponent. $g^{(\alpha)}$ can be given by
\begin{equation}
  g^{(\alpha)} = h_{ap} \gamma^{(\beta)}
\end{equation}
where
\begin{equation}
  h_{ws} = h(\gamma) = h_0 \text{sech} \left( \frac{h_0 \gamma}{\tau_1 - \tau_0} \right)
\end{equation}
\begin{equation}
  \gamma = \sum_{\alpha} \int_{0}^{t} \gamma^{(\alpha)} \, dt
\end{equation}
\begin{equation}
  h_{ap} = q h(\gamma) \quad (\alpha \neq \beta)
\end{equation}
where $h_{ap}$ is latent hardening moduli, $q$ is latent hardening constant. For detailed in-depth review of the crystal plasticity theory, see the work of Huang [18].

3. Finite Element Simulation

3.1. Finite Element Model
The finite element geometry model of SX superalloy was constructed with carbide and two RX grains using the finite element software ABAQUS, as shown in Fig.1. A ABAQUS user-defined crystal plasticity material subroutine(UMAT) was used. The geometry of single crystal matrix is 400 μm high, 300 μm wide and 5 μm thick. The length (L) and width of two RX grains are both 100 μm. The carbide is ellipsoidal and the lengths of ellipsoidal semi-major and semi-minor axis are 30μm and 12μm, respectively. The typical finite element meshes are shown in Fig.2. 3D hexagonal linear incompatible element (C3D8I in ABAQUS) was used. The boundary conditions applied to the mesh on the top surface nodes of the mesh include a cyclically varying uniform displacement with a minimum value(-1.0μm) and a maximum value (1.0μm). load ratio is $R = -1$. In order to prevent rigid body movement, all nodes on the bottom surface of the mesh were fixed in the vertical (Y-axis) direction. The nodes at the bottom-left corner were fixed in the horizontal direction (X-axis).
3.2. Material Constants
The material parameters used in this model are derived from SX nickel-based superalloys PWA1480 and SRR99 [19], as shown in Table 1. $C_{11}$, $C_{12}$ and $C_{44}$ represent the elastic constants of the material in three different directions, respectively; $\dot{\alpha}$ is the reference shear strain rate in the slip system flow rule; $n$ is the rate sensitivity exponent; $h_0$, $\tau_0$ and $\tau_s$ are initial hardening modulus, initial yield stress and stage I stress, respectively. Details regarding these constants have been documented by Huang[18] and Feng et al. [19].

| Parameter | Value |
|-----------|-------|
| $C_{11}$ | 169536.0 MPa |
| $C_{12}$ | 107540.0 MPa |
| $C_{44}$ | 88105.7 MPa |
| $\dot{\alpha}$ | 0.001 |
| $n$ | 3.6 |
| $h_0$ | 548 MPa |
| $\tau_0$ | 100.64 MPa |
| $\tau_s$ | 60.64 MPa |
| $q$ | 1.0 |
| $c$ | 413300 MPa |
| $d$ | 1960 |

4. Definition of Primary Orientation and Secondary Orientation
In order to simplify the following discussion, the primary orientation is defined as $\beta$. The secondary orientation is defined as $\theta$, as shown in Fig.3. The orientations of the single crystal matrix and two RX grains are different in the local coordinate system. The orientations of two RX grains are constant. The orientations of the single crystal matrix and two RX grains in the local coordinate system at $\beta=0^\circ$ and $\theta=0^\circ$ are shown in Table 2.

| Local coordinate | Single crystal matrix | Grain1 | Grain2 |
|------------------|-----------------------|--------|--------|
| X' axis          | [100]                 | [100]  | [01-1] |
| Y' axis          | [010]                 | [011]  | [111]  |

Figure 3. Definition of (a) primary orientation $\beta$ (b) secondary orientation $\theta$

5. Results and Discussion
Figure 4 (a) and (b) show the distribution of Von Mises stress and accumulated plastic shear strain after five cycles at $\beta=0^\circ$ and $\theta=0^\circ$. It can be seen from Fig. 4(a) that the maximum Mises stress occurs in the RX grain and near the transverse boundary of RX grain. The reason is that dislocation slip is hindered and dislocation piles up at the transverse grain boundary of the RX grain, resulting in stress concentration. It can be seen from 4(b) that the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ is in the matrix. The reason may be that the region adjacent to the RX grains has larger hydrostatic pressure and plastic deformation is therefore reduced [20].

Fig.5 shows the dependence of the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ in recrystallization-single crystal system on primary orientation ($\beta$). The maximum accumulated plastic shear strain $\gamma_{\text{max}}$ increases with increasing of primary orientation ($\beta$). The influence of $\beta$ is remarkable and the
maximum accumulated plastic shear strain $\gamma_{\text{max}}$ at $\beta=15^\circ$ is 31.6% larger than that at $\beta=0^\circ$. In theory, this finite element model has better fatigue performance at $\beta=0^\circ$ than that at $\beta=15^\circ$. Hou et al. [21] studied the dependence of Mises stress, the maximum resolved shear stress and fatigue life of cooled blade on primary orientation based on finite element analysis method. The results show that the Mises stress and the maximum resolved shear stress increase with increasing of primary orientation($\beta$), similar to our result. However, the fatigue life decreases with increasing primary orientation($\beta$).

**Figure 4.** Distribution of the Mises stress and accumulated plastic shear strain after 5 cycles
(a) Mises stress (b) accumulated plastic shear strain

**Figure 5.** The dependence of the maximum accumulated plastic shear strain in recrystallization-single crystal system on primary orientation($\beta$)

The dependence of the maximum accumulated plastic shear strain $\gamma_{\text{max}}$ in recrystallization-single crystal system on secondary orientation ($\theta$) is shown in Fig. 6. The value at $\theta=0^\circ$ is the same as that of $\theta=90^\circ$ due to symmetry. The maximum accumulated plastic strain $\gamma_{\text{max}}$ at $43^\circ$ is the smallest, and it is 1.4% smaller than that at $0^\circ$ and $90^\circ$, even if the influence of secondary orientation ($\theta$) is not remarkable. It implies that the RX-SX system has better fatigue performance with $\theta=43^\circ$ than that at $0^\circ$.
and 90°. Hou et al. [21] also reported the influence of secondary orientation on Mises stress and the maximum resolved shear stress $\tau_{s\text{ max}}$ in single crystal blade, with the relative variation shown in Fig. 7. They noted that the influence of secondary orientation on fatigue life is much more obvious. The relative variations of creep displacement of blades studied by Yue Z F [22] are also shown in Fig. 7 for the sake of comparison. It can be seen that the mechanical response/deformation of single crystal reach an extreme value with secondary orientation of 40°-45°. Arakere et al. [3] analyzed the SX nickel base turbine blade models with different primary and secondary orientations by finite element method. They found that for $\theta=45\pm15$ degree cracks were arrested after some growth or did not initiate at all, indicating that these are preferential secondary orientations for optimal fatigue performance. It is consistent with the result we obtained here. Zhang Y. et al. [23] investigated the effect of secondary orientations on fatigue crack growth (FCG) behaviors of a SX nickel-based superalloy and proposed an energy release rate (G) coefficient model. The results show that secondary orientation of $\sim45°$ benefits the crack resistance and the proposed G coefficient model can effectively describe the difference of crack growth rates caused by different secondary orientations.

![Figure 6](image1.png)

**Figure 6.** The dependence of the maximum accumulated plastic shear strain in recrystallization-single crystal system on the secondary orientation ($\theta$) (a) range 0°-90° (b) range A

![Figure 7](image2.png)

**Figure 7.** Relative variation of maximum resolved shear stress $\tau_s$ [21], creep displacement [22], and maximum accumulated plastic shear strain $\gamma_{\text{max}}$ at different secondary orientations
6. Conclusions

By crystal plasticity finite element method, cyclic plastic deformation behaviors of recrystallized single crystal nickel-based superalloy were studied. The influences of primary orientation and secondary orientation on cyclic plasticity were examined. The following conclusions have been drawn:

1) The maximum accumulated plastic shear strain occurs in the matrix near the RX transverse grain boundary in recrystallization-single crystal system.

2) The influence of primary orientation (β) on the maximum accumulated plastic shear strain in the recrystallized single crystal superalloy is remarkable. The maximum accumulated plastic shear strain \( \gamma_{\text{max}} \) at \( \beta=15^\circ \) is 31.6% larger than that at \( \beta=0^\circ \).

3) The maximum accumulated plastic shear strain decreases first and then increases with the increase of secondary orientation from 0° to 90° in recrystallized single crystal superalloy. The maximum accumulated plastic strain \( \gamma_{\text{max}} \) at secondary orientation \( \theta=43^\circ \) is 1.4% smaller than that at 0° and 90°.

4) The maximum accumulated plastic shear strain \( \gamma_{\text{max}} \) reaches minimum value at \( \beta=0^\circ \) and \( \theta=43^\circ \). In other words, the corresponding primary orientation is [010], and the secondary orientation is [1.05 01], which corresponds to optimal fatigue performance due to low \( \gamma_{\text{max}} \).

References

[1] Suzuki S, Sakaguchi M, Inoue H. Temperature dependent fatigue crack propagation in a single crystal Ni-base superalloy affected by primary and secondary orientations[J]. Materials Science & Engineering A, 2018, 724.

[2] ZHOU Z J, WANG L, WANG D, et al. Effect of secondary orientation on room temperature tensile behaviors of Ni-base single crystal superalloys [J]. Materials Science & Engineering A, 2016, 659: 130-142.

[3] ARAKERE N K, SWANSON G. Effect of Crystal Orientation on Fatigue Failure of Single Crystal Nickel Base Turbine Blade Superalloys [J]. 2002, (78576): V004T001A004.

[4] Wen S, Zeng X, And Z K, et al. Investigation the effect of crystal orientation of nickel-based single crystal superalloys on bending creep tests [J]. Material wissenschaft Und Werkstofftechnik, 2014, 45(3).

[5] GEL M, DUHL D N, GIAMEI A F. The development of single crystal superalloy turbine blades; proceedings of the Superalloys, F, 1980 [C].

[6] FEDELICH B, KIYAK Y, MAY T, et al. Simulation of Crack Growth Under Low Cycle Fatigue at High Temperature in a Single Crystal Superalloy [J]. Engineering Fracture Mechanics, 2008, 75(8): 2418-2443.

[7] He Z, Qiu W, Fan Y N, et al. Effects of secondary orientation on fatigue crack initiation in a single crystal superalloy[J]. Fatigue & Fracture of Engineering Materials & Structures, 2017.

[8] Ma X, Shi H J. In situ SEM studies of the low cycle fatigue behavior of DZ4 superalloy at elevated temperature: Effect of partial recrystallization [J]. International Journal of Fatigue, 2014, 61: 255-263.

[9] Bing Z, Delin L, Chunhu T, et al. Influence of Surface Recrystallization on Intermediate-Temperature Stress Rupture Property and Fracture Behavior of Single Crystal Superalloy SRR99[J]. Journal of Aeronautical Materials, 2012, 55(6): 149–153.

[10] MA X, SHI H J, GU J, et al. Influence of surface recrystallization on the low cycle fatigue behaviour of a single crystal superalloy [J]. Fatigue & Fracture of Engineering Materials & Structures, 2015, 38(3): 340-351.

[11] ZHANG W F, GAO W, ZHAO A G, et al. Recrystallization and Fatigue Failure of Blades Made of a Directionally Solidified Alloy[J]. Acta Aeronautica et Astronautica Sinica, 2003, 24(4): 377-381.

[12] ABIKCHI M, BILLOT T, CR PIN J, et al. Fatigue life and initiation mechanisms in wrought Inconel 718 DA for different microstructures; proceedings of the 13th international
conference on fracture, Beijing, China, F 2013-06-16, 2013 [C].

[13] ZHU L, WU Z R, HU X T, et al. Investigation of small fatigue crack initiation and growth behaviour of nickel base superalloy GH4169 [J]. Fatigue & Fracture of Engineering Materials & Structures, 2016, 39(9): 1150-1160.

[14] JANG Y, JIN S, JEONG Y, et al. Fatigue Crack Initiation Mechanism for Cast 319-T7 Aluminum Alloy [J]. Metallurgical & Materials Transactions A, 2009, 40(7): 1579-1587.

[15] HILL R. On Constitutive Macro-Variables for Heterogeneous Solids at Finite Strain [J]. Proceedings of the Royal Society of London, 1972, 326(1565): 131-147.

[16] ASARO R J. Micromechanics of Crystals and Polycrystals [J]. Advances in Appl Mech, 1983, 23(08): 1-115.

[17] ASARO R J, RICE J R. Strain localization in ductile single crystals ☆ [J]. Journal of the Mechanics & Physics of Solids, 1977, 25(5): 309-338.

[18] HUANG Y. A User-Material Subroutine Incorporating Single Crystal Plasticity in the ABAQUS Finite Element Program [J]. 1991:

[19] LU F, ZHANG G, ZHANG K S. Discussion of cyclic plasticity and viscoplasticity of single crystal nickel-based superalloy in large strain analysis: comparison of anisotropic macroscopic model and crystallographic model [J]. International Journal of Mechanical Sciences, 2004, 46(8): 1157-1171.

[20] WANG, DANIEWICZ, S. R, et al. Three-dimensional finite element analysis using crystal plasticity for a parameter study of fatigue crack incubation in a 7075 aluminum alloy [J]. International Journal of Fatigue, 2009, 31(4): 659-667.

[21] HOU N X, GOU W X, WEN Z X, et al. The influence of crystal orientations on fatigue life of single crystal cooled turbine blade [J]. Materials Science & Engineering A, 2008, 492(1–2): 413-418.

[22] YUE Z F, LV Z Z, YANG Z G. Influence of deviation and randomness of crystallographic orientations on the strength and life of nickel-based single crystal superalloy turbine blades[J].Aerospace Power, 2003, 18(4): 477-480.

[23] ZHANG Y, QIU W, SHI H J, et al. Effects of secondary orientations on long fatigue crack growth in a single crystal superalloy [J]. Engineering Fracture Mechanics, 2015, 136: 172-184.