Surface Slip Deformation Characteristics of Nickel-Base Single Crystal Thin Plates With Film Cooling Holes

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Abstract
In this study, tensile tests at room temperature and observations of slip bands on the free surface of a nickel-based single-crystal thin plate with densely distributed film cooling holes were performed. The deformation of the slip system at the edge of the cooling hole and between the holes was analyzed. Numerical simulation predictions were conducted based on the plasticity theory of crystals, and the comparison with the experimental results showed good consistency. Based on the simulation and experimental results, the nucleation and propagation direction of the edge cracks were analyzed by means of crystallography. The results showed that the fracture surface was mainly attributed to slipping, and the slip traces were approximately in two directions, namely [011] and [01–1], both of which were 45° to the stress axis. The maximum values of the resolved shear stress around the cooling hole were attained at 82.5°, 112.5°, 247.5°, and 277.5°, which corresponded to \( \tau_2 \), \( \tau_8 \), \( \tau_{10} \), and \( \tau_6 \).

Index Terms
Ni-based single crystal, film cooling holes, crystal plasticity, slip deformation, micro crack initiation.

I. INTRODUCTION
In actual working conditions, turbine blades are often subjected to the combined effects of centrifugal force and thermal stress. In order to improve the cooling performance of the blades, large numbers of cooling holes are often used in the design [1]–[3]. As a consequence, the area around the cooling holes is often the place where cracks nucleate and expand. Early research showed that in tensile fracture, the single crystal slips along the {111} plane, which is composed of 12 slip systems. Studies have shown that the slip accumulation on the slip band was the major cause of crack nucleation, and crack growth was related to plastic deformation near the crack [4]–[10]. In addition, crack nucleation is closely related to shear stress on the 12 slip systems. This demonstrated that the internal sliding mode of the single crystal alloy under load is directly related to crack initiation and the expansion mode of the material. Consequently, it is necessary to conduct an in-depth study on the sliding characteristics around film holes to understand the elastic-plastic behavior of the blades with densely distributed film cooling holes.

Thus far, the research on the surface sliding phenomenon of nickel-based single crystals under multi-axial stress has been mainly focused on the notched and CT specimens. Relevant experiments on CT specimens were performed by Floriot [11], [12], and the plastic strain field at the crack tip was analyzed combining the crystal plasticity theory and numerical simulation [13]–[16]. Previous researchers analyzed the slip band in the deformation process using the three-dimensional elastic anisotropy theory combined with experiments, revealing the plastic evolution law of the double-notched nickel-based single crystal under different random orientations [17]–[21]. Wilson et al. and Shibanuma et al. studied the structure of the body-centered cubic single crystal and analyzed the local deformation law near the crack tip [22], [23]. These experimental studies combined with theoretical analysis have laid the foundation for future scholars to analyze the plastic evolution of single-crystal alloys. However, in spite of the theoretical basis and solid experimental results, there are few reports on the
influence of film-cooling hole structures on the elastoplasticity of nickel-based single-crystal alloys. Zhang studied the mechanical characteristics of Ni-based single crystal superalloy samples with densely arranged air film holes [24], [25]. Combined with the crystal plasticity theory, a feasible equivalent method was given. Nonetheless, such results were restrictive as the effect of the number of holes was not considered. Some researchers conducted tensile tests along the [001] orientation on a nickel-based single-crystal sample with a single hole. They observed the evolution of stress and strain around the hole, as well as the slip band distribution. Combined with the plastic theory of single crystal, numerical calculations were conducted that revealed satisfactory results [26]–[28]. Zhou performed room temperature tensile tests on the nickel-based single crystal alloy with a hole in the center along various orientations and observed the strain field distribution in the sample in real-time through the ARAMIS system [29], [30].

At present, there are few types of studies on the plastic evolution of nickel-based single crystal alloys with densely distributed film holes under unidirectional load. There are evident differences between the densely distributed film hole structure and the notch structure, as well as between the CT structure and the single-hole structure in the elastoplastic behavior. Due to the different arrangements of film holes, the multi-hole interference could take effect between the cooling holes, which complicates the stress-strain field. In this paper, tensile tests at room temperature were performed on a plate specimen with densely distributed film cooling holes, and slip band observations were performed on the free surface of the specimen. The motion of the slip system at the edge of the cooling hole and between the holes was analyzed. Combined with the crystal plasticity theory, a numerical simulation of the model was performed, whose results were compared with the experimental observations.

**II. MATERIALS AND EXPERIMENTAL DETAILS**

The test material used was the second-generation nickel-based single crystal superalloy DD6, whose main chemical composition is shown in Table 1. All the casting materials for the round bar were obtained from the Institute of Aeronautical Materials, and they were subjected to standard heat treatment (1290° × 1 h + 1300° × 2 h + 1315° × 4 h/AC + 1120° × 4 h/AC + 870° × 32 h/AC). After heat treatment, the deflection angle of the sample was within 10° and the casting direction was [001]. As shown in Figure 1, the material was processed into thin plates and perforated samples were prepared. The total length of the sample was 100 mm with the gauge length being 25 mm. Besides, 14 round holes, each with a diameter of 0.4 mm, were processed in the middle. The horizontal distance (perpendicular to the stress axis) between the two round holes was 1 mm and the vertical direction was 0.96 mm. The film holes were fabricated by electrostream machining. The tensile tests on the DD6 plate with and without holes were performed at room temperature with a tensile rate of 0.2 mm/min.

**TABLE 1.** Chemical composition of DD6 single crystal superalloy (wt %).

| Element | Cr | Co | W | Al | Ta | Re | Mo | Ni | C | Nb | Hf |
|---------|----|----|---|----|----|----|----|----|---|----|----|
| %       | 4.0 | 9.0 | 8.0 | 5.7 | 7.0 | 2.2 | 2.0 | surplus | 0.05 | 1.0 | 1.0 |

**III. CRYSTAL PLASTICITY THEORY**

**A. CONSTITUTIVE EQUATIONS**

In this paper, the strain-rate-dependent crystal slip theory and the lattice rotation effects were considered, both of which were embedded into the general finite element software subroutine using the tangent coefficient method.

The total deformation gradient \( F \) of a crystal can be expressed as follows:

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

(1)

where \( F^e \) represents the deformation gradient caused by lattice distortion and rigid rotation. Accordingly, the slip direction \( m^{(\alpha)} \) can be expressed as follows:

\[
m^{(\alpha)} = F^e m^{(\alpha)}
\]  

(2)

Furthermore, the slip plane normal vector \( n^{(\alpha)} \) is expressed as follows:

\[
n^{(\alpha)} = \left( (F^e)^{-1} \right)^T n^{(\alpha)}
\]  

(3)

The velocity gradient can be decomposed into parts corresponding to the slip and lattice distortion and the rotation of the rigid body, respectively.

\[
L = FF^{-1} = L^e + L^p
\]  

(4)

Accordingly, \( L \) can be written as follows:

\[
L = D + W
\]  

(5)

where \( D \) and \( W \) are the symmetric rate of the stretching and spin tensors, respectively.

The following expression can be obtained due to plastic deformation occurs by dislocation slip:

\[
L_p = \sum_{\alpha=1}^{N} P^{(\alpha)} \psi^{(\alpha)}
\]  

(6)
where $\gamma''$ is the slipping rate of the $\alpha$ slip systems, the Schmidt tensor $P^{(\alpha)}$ is defined as

$$P^{(\alpha)} = \frac{1}{2} (m^{(\alpha)} \otimes n^{(\alpha)} + n^{(\alpha)} \otimes m^{(\alpha)})$$  \hspace{1cm} (7)$$

where $m^{(\alpha)}$ and $n^{(\alpha)}$ are the unit vectors of the slip direction and that of the normal direction of the slip plane before deformation, respectively.

Defining $\sigma$ the Cauchy stress tensor, and $\tau$ the weighted Cauchy stress tensor, and then we have

$$\tau = (\det F) \sigma$$  \hspace{1cm} (8)$$

and

$$T = F^t \tau F^{-1}$$  \hspace{1cm} (9)$$

Furthermore, the resolved shear stress of the slip system is expressed as follows:

$$\tau^{(\alpha)} = P^{(\alpha)} : T$$  \hspace{1cm} (10)$$

In consideration of the rate dependence, the resolved shear strain rate $\gamma''$ follows the hardening equation of power function as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left[ \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right]^{\frac{1}{m} - 1}$$  \hspace{1cm} (11)$$

where $g^{(\alpha)}$ is the slip system strength or resistance to shear, $\gamma''$ is the reference shear strain rate, and $m$ is the strain rate sensitivity index. When $m = 0$, the shear stress is independent of the strain rate.

When $\gamma(\alpha) = 0$, assuming the initial value of $g^{(\alpha)}$ being $\tau_0$, the evolution of $g^{(\alpha)}$ is determined from the following formula:

$$\dot{g}^{(\alpha)} = \sum_{\beta=1}^{N} h_{\alpha\beta} \left| \dot{\gamma}^{(\alpha)} \right|$$  \hspace{1cm} (12)$$

where $h_{\alpha\beta}$ is the hardening coefficient, which determines the hardening of the slip system $\alpha$ caused by the shearing in the slip system $\beta$ and $h_{\alpha\beta}$ is a function of $\gamma$.

Thus, $\gamma = \sum_{\beta=1}^{N} \left| \gamma^{(\alpha)} \right|$ is the cumulative slip strain.

In the numerical calculation, the tangent coefficient increment method was used and accordingly, equation (7) was rewritten as:

$$\Delta \gamma^{(\alpha)} = \gamma^{(\alpha)} (t + \Delta t) - \gamma^{(\alpha)} (t)$$  \hspace{1cm} (13)$$

Furthermore, $h_{\alpha\beta}$ is the extreme of potential hardening, while $h_{\beta}$ is the single hardening rate, expressed as

$$h_{\beta} = h_0 \left[ 1 - \frac{g^{(\alpha)}}{\tau_s} \right]$$  \hspace{1cm} (14)$$

where $h_0$ is the hardening modulus, $\tau_s$ and $\beta$ are the model parameters.

The above constitutive model is incorporated into the finite element ABAQUS user subroutine UMAT [10], and the calculation flow-chart is shown in Figure 2.

**FIGURE 2.** Calculation flow-chart of the crystal plasticity theory.

### B. FINITE ELEMENT MODEL AND MATERIAL PARAMETERS

According to the tensile test results, the finite element model was established, as shown in Figure 3. The specific size was consistent with that of the real sample, and the middle gauge segment was taken as the research object. Stress was applied along the [001] direction, and the direction perpendicular to the model surface was [100]. The load was applied to one end of the model, while the other end was constrained.
The finite element mesh is shown in Figure 3. To increase the accuracy of the calculation results, the mesh near each cooling hole was refined. Finally, the finite element model composed of 51807 nodes and 41616 C3D8 elements (linear hexahedral element).

The tensile properties of DD6 nickel-based single crystal superalloy and the model parameters obtained from [31] are listed in Table 2.

In this paper, the slip directions of the twelve slip systems of the octahedron were defined, as shown in Table 3.

### IV. RESULTS AND DISCUSSION

#### A. EXPERIMENTAL RESULTS

The yield stress of the DD6 plate at room temperature was 796 MPa, and the Schmid factor of the [001] oriented slip system was 0.4082. The critical resolved shear stress of the DD6 single crystal was 325 MPa.

Figure 4 (a) and (b) show the slip traces near the hole edge after fracture. Figure 4 (c) displays the slip traces near the fracture edge of the sample. It can be seen from the figure that the fracture surface was generated by the slip plane. The angle between each fracture surface and the stress axis was $45^\circ$. 

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The finite element model and mesh generation.

**TABLE 2.** Basic parameters used in the CPFEA simulations.

| Symbol | Value          |
|--------|----------------|
| $\sigma$ | 796 MPa         |
| CRSS   | 325 MPa         |
| E      | 131500 MPa      |
| G      | 155070 MPa      |
| $\mu$  | 0.344           |
| $\gamma_0/s^{0.5}$ | 0.003          |
| m      | 0.02            |
| $h_0/t_0$ | 1.2            |
| $\tau_0/t_0$ | 1.17           |
| $\beta$ | 1.3             |

**TABLE 3.** Definition of the slip systems used in the crystal plasticity model.

| SS No. | Slip plane | Slip direction | SS No. | Slip plane | Slip direction |
|--------|------------|----------------|--------|------------|----------------|
| 1      | (111)      | [10-1]         | 7      | (1-1-1)    | [110]          |
| 2      | (111)      | [0-11]         | 8      | (1-1-1)    | [0-11]         |
| 3      | (111)      | [1-10]         | 9      | (1-1-1)    | [011]          |
| 4      | (-11-1)    | [10-1]         | 10     | (-11-1)    | [011]          |
| 5      | (-11-1)    | [110]          | 11     | (-11-1)    | [101]          |
| 6      | (-11-1)    | [011]          | 12     | (-11-1)    | [1-10]         |

Figure 4. Slip trace of a flat plate with film cooling holes.
The fracture surface shown in Figure 4 (c) is particularly distinct with each fracture surface showing a slip plane perpendicular to the fracture plane. The fractured planes were intersected, and the crack propagated along the slip trace at the intersections. Figure 4 (d) shows the distribution of the slip trace on the surface of the specimen when the specimen with film holes was stretched to the yield. From the figure, we can see that due to the multi-hole interference effect between each hole, four sets of slip bands symmetrically distributed around each hole, which was also the area where the specimen experienced relatively larger stress and strain.

Figure 5(a) shows the original morphology of hole 1 marked in Figure 4, and Figure 5(b) shows the morphology of the hole when the specimen gets into the yield stage during tensile test. It can be seen that the hole changed from a circular to an elliptical shape along the loading direction. The deformation degree of the hole depends on its position with the fracture path. The further away from the fracture path, the smaller deformation degree of the hole is.

**FIGURE 6.** Slip trace around the film holes.

**FIGURE 7.** Maximum octahedral shear stress distribution.

**FIGURE 8.** Resolved shear stress along the circumference of the hole.

Figure 6 is an enlarged view showing the initiation of the slip trace around the hole edge. We can see that because of the complex stress state around the hole edge, multiple slip systems active at the same time, and the slip traces roughly followed two directions, namely, [011] and [01−1], both of which are inclined 45° to the direction of the tensile stress. These two slip directions corresponded to two groups of slip planes, namely, {11−1}, {1−11}, and {111}, {111}. In the place where the hole edge was completely perpendicular to the stress axis, i.e., the place where the specimen was damaged and the axial stress was the largest during the tensile process, we can see that numerous cavities and micro-cracks were generated. Furthermore, these cavities and micro-cracks initiated from the slip trace and propagated along the direction of the slip traces, as shown in the red box in Figure 6.

**B. RESULTS OF THE NUMERICAL CALCULATION**

In the process of the finite element simulation, the load followed the actual load spectrum, and the stress was 5.5 kN. Figure 7 shows the distribution chart of the maximum calculated octahedral resolved shear stress on the free surface of the sample. We can see considerable stress concentration along a certain vector direction between the holes, and a large stress gradient appearing around the hole; also, the stress along the loading direction was quite low. Along with the directions that are 82.5°, 112.5°, 247.5° and 277.5° to the external stress, relatively large stress exists. These places and directions were likely to be the crack initiation and crack propagation directions during fracture.

Figure 8 shows the variation in the 12 types of resolved shear stress of the octahedron along the circumference of the cooling hole at different angles. As shown in Figure 8, the maximum value of the resolved shear stress appeared at 82.5°, 112.5°, 247.5°, and 277.5°, which corresponded to a resolved shear stress of τ2, τ8, τ10, and τ6. According
TABLE 4. Prediction of the initiation of the slip system on the surface.

| θ     | τ_{max} | Slip System       |
|-------|---------|-------------------|
| 0°–13°| τ_6     | (-1 1 0) [0 1 1]  |
| 13°–17°| τ_4    | (-1 1 0) [0 1 1]  |
| 17°–51°| τ_11   | (-1 1 0) [1 0 1]  |
| 51°–90°| τ_2    | (1 1 1) [0 1 1]   |
| 90°–129°| τ_8   | (1 1 1) [0 1 1]   |
| 129°–163°| τ_4  | (-1 1 0) [0 1 1]  |
| 163°–172.5°| τ_10 | (-1 1 0) [0 1 1]  |
| 172.5°–180°| τ_2  | (1 1 1) [0 1 1]   |
| 180°–187.5°| τ_6  | (-1 1 0) [0 1 1]  |
| 187.5°–197°| τ_8  | (1 1 1) [0 1 1]   |
| 197°–231°| τ_1  | (1 1 1) [0 1 1]   |
| 231°–270°| τ_10 | (-1 1 0) [0 1 1]  |
| 270°–309°| τ_6  | (-1 1 0) [0 1 1]  |
| 309°–343°| τ_9  | (1 1 1) [0 1 1]   |
| 343°–347°| τ_1  | (1 1 1) [0 1 1]   |
| 347°–360°| τ_2  | (1 1 1) [0 1 1]   |

to the test results, the critical resolved shear stress of the DD6 single crystal was 325 MPa, i.e., when the resolved shear stress of a certain slip system exceeded 325 MPa, the slip trace appeared on the sample surface, as shown by the dotted line in Figure 8. From the figure, we can predict the startup of the sliding system. In the range of 0°–43°, each type of shear stress did not exceed the critical resolved shear stress. In the range of 43°–51°, 51°–90°, 90°–129°, and 129°–138°, the first sliding system to active was \( \tau_{11} \), \( \tau_2 \), \( \tau_8 \), and \( \tau_4 \), respectively. At 180°, the resolved shear stress showed a symmetrical distribution. However, the slip systems in action were not symmetrical due to anisotropy. In the range of 231°–270°, the first sliding slip system to active was \( \tau_{10} \), while that in the range of 270°–309° was \( \tau_6 \). Notably, in the actual observation, the observed slip trace was limited by the main slip system. Although with the increase in the load, the resolved shear stress of other slip systems will exceed the critical resolved shear stress, the main slip system was more evident on the sample surface [26].

Based on the results shown in Figure 8, Table 4 shows the prediction of the initiation of the slip system on the sample surface around the holes. Compared with the experimental observations shown in Figure 8, the prediction results appear to be generally accurate. Two slip systems around the hole, namely, \( \tau_2 \) at 82.5° and \( \tau_8 \) at 112.5° that were of 45° and 135° to the stress axis, respectively, were more distinct than other slip systems.

C. DISCUSSION

Figure 9 displays the distribution diagram of the deformation of the slip systems around the cooling holes and the direction of the slip trace drawn according to the numerical simulation results. Figure 10 shows the distribution diagram of the real slip trace around the hole observed in the experiment when the sample was strained to the yield stress. The comparison shows that the predicted results were in good agreement with the experimental ones.

As shown in Figure 10, the distribution of the slip band around the hole is not the same as the predicted value, which is mainly reflected in the distribution of the slip bands that were inclined 90°–270° to the hole-edge of the film hole. According to the predicted values, the slip system 8 should be the first to active between 90° and 129°, and the slip
system 10 should be the first to active between 231° and 270°. However, in actual observation, the slip traces corresponding to the slip systems 8 and 10 were not clearly visible.

The features of other slip systems could also be observed in these two areas and were in the opposite direction to the slip traces of slip systems 8 and 10. This was mainly due to the fact that although the stress distribution at the hole...
edge showed that $\tau 8$ and $\tau 10$ reach the maximum at $112.5^\circ$ and $247.5^\circ$, respectively, the main slip system was within a very small range of the hole edge. On the other hand, there existed a much larger area where other slip systems could experience larger stress, and these slip systems were more likely to become the primary slip systems, as can be seen on the free surface of the sample with a larger area (Figure 10). Furthermore, no-slip system was observed between $0^\circ$ and $51^\circ$, $129^\circ$ and $231^\circ$, and $309^\circ$ and $360^\circ$, primarily because these two areas were low-stress areas, and the stress did not reach the critical value. The threshold values for the initiation of slip are shown in the finite element calculation results in Figure 7.

Figure 11 shows the initiation of the slip systems around the hole at the position with the maximum resolved shear stress. The first system to slip at $82.5^\circ$ was slip system 2 along the $[\text{011}]$ direction and $\{\text{111}\}$ slip plane. The first system to slip at $112.5^\circ$ was slip system 2 along the $[\text{011}]$ direction and $\{\text{111}\}$ slip plane. The first system to slip at $247.5^\circ$ was slip system 10 along the $[\text{011}]$ direction and $\{\text{111}\}$ slip plane. The first system to slip at $277.5^\circ$ was slip system 4 along the $[\text{011}]$ direction and $\{\text{111}\}$ slip plane. The increase in tensile stress, other potential slip systems could also start to slip.

Figure 12 shows the distribution of the resolved shear stress (left image) and strain (right image) of the slip system between the film holes at the area marked in Figure 7. According to the numerical calculation results, the prediction diagram of the initiation of the slip system on the free surface of the sample under the multi-hole interference effect can be drawn, which was combined with the actual observation results to Figure 13. It is worth noting that there will be multiple slip systems in the corresponding area in the figure, which does not mean that these slip systems were initiated at the same time in this area. Instead, it indicated that these slip systems were the main slip systems in this area, while other slip systems could also be activated with the increase in stress. It can be seen from Figure 13 that the predicted results were in good agreement with the experimental observations.

V. CONCLUSION

In this paper, the distribution of slip bands and the activation of slip systems on the free surface of a nickel-based single-crystal thin plate with densely distributed film cooling holes are studied by experiments and numerical simulation. The fracture morphology shows four sets of slip bands symmetrically distributed around each hole, due to the multi-hole interference effect. The slip traces extend in the $[\text{011}]$ and $[\text{01}−\text{1}]$ directions corresponding to the activation of $\{\text{11}−\text{1}\}$ or $\{\text{1}−\text{11}\}$ and $\{\text{111}\}$ or $\{−\text{111}\}$ slip plane, on which the crack propagated and formed the fracture surface.

Crystal plastic finite element method was used to predict the initial active slip systems and distribution of slip bands successfully. The finite element result shows the maximum resolved shear stress around the cooling holes appeared at the positions $82.5^\circ$, $112.5^\circ$, $247.5^\circ$, and $277.5^\circ$, which corresponded to the resolved shear stresses of $\tau 2$, $\tau 8$, $\tau 10$, and $\tau 6$.

The predicted results around and between holes were in good agreement with the experimental observations.

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