Numerical Simulation of Grain Growth of Directionally Solidified DZ4125 Alloy under Varied Blade Orientations

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The ProCAST simulation software is used to simulate the temperature field and the mushy zone of the blade under different blade orientations, and then grain growth was investigated based on them. It is found that the temperature field and the mushy zone of the blade samples in the parallel orientation are stably horizontally distributed at the same height, while the perpendicular orientation has a degree of inclination. In the heat preservation zone, the sample temperature close to the furnace wall is higher than that of the sample temperature near the center (referred to here as the Center-Side), and the temperature field is inclined upwards. However, in the cooling zone, the temperature field is inclined downwards because the temperature near the furnace wall (referred to here as the Wall-Side) is lower than that of the Center-Side. The grain growth of the blades with parallel orientation is superior as single crystal blade castings are formed. The blade samples in a perpendicular orientation have a certain heterocrystal tendency. The grain growth of the mutated cross-section of the blade samples is summarized using variable cross-section samples. Heterocrystals are used to be formed at the edge plate of complex structure, the mutation section and the end of spiral crystal separator. [doi:10.2320/materials.2020.02.012]

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Keywords: orientation relationship, directional solidification, temperature field, mushy zone, grain growth

1. Introduction

Ni-based superalloy are used for turbine blades of aircraft jet engines because of their excellent creastress rupture, thermo mechanical fatigue capabilities.1) Directional Solidification (DS) technology is widely utilized for manufacturing components with columnar or single crystal structure that align a particular crystallographic axis to the growth direction to improve the high temperature properties of nickel superalloy.2–4) However, the grain defects of different degrees was caused by uneven heat exchange with the furnace wall due to the complex structure of the blade during the directional solidification process. Numerical simulation, a technology can directly reflect the directional solidification process which has been increasingly applied to the development of single-crystal superalloy turbine blades.5)

Many researchers have studied the temperature field and grain growth of blades formed with directional solidification. Using the CA-FD method, Lee et al.6) simulated the dendritic growth process under different parameters and studied the adverse effects of blade mutations cross-section on the growth of a single crystal. Kermanpur and Varahram et al.7) simulated the grain growth of a single crystal turbine blade under the condition of liquid metal cooling directional solidification process using the CA-FE method. In particular, the influence of process parameters on the growth and defects of single-crystal tissue was examined. Yu et al.8) established a radiation heat transfer model between the blade and the furnace wall, which accounted for the influence of the geometric size of the furnace body. The temperature field distribution of the blade was then simulated under different drawing speeds. Gao9) studied the directional solidification temperature field of a nickel-based single crystal blade. The results showed that when the drawing speed reached a certain value, the blade isotherm became concave, and inclined to the thin side of the blade. Yang et al.10) studied the temperature field of the blade platform during the directional solidification process and found that the probability of heterocrystal grains formation increased with the increased isotherm inclination angle. Liang et al.11) studied the directional solidification process under the condition of a single blade and predicted the microstructure of a single crystal. Process parameters such as drawing speed were considered in the model. The results indicate that the isothermal curvature at the solid-liquid interface front increases with increased drawing speed, and the temperature gradient increases accordingly. Saitou and Hirata12) used a two-dimensional model to calculate the relationship between the shape of the solid-liquid interface and the growth conditions in the HRS directional solidification furnace. It was pointed out that the solid-liquid interface presented a certain curvature in the stable stage. Yu et al.13,14) used commercial finite element analysis software to study the directional solidification process and the associated temperature field of a single crystal blade. In addition, the relationship between temperature gradient and casting defects, such as heterocrystal grain was examined from a macroscopic perspective. The key to successful directional solidification technology is to control the influence of radiative heat transfer on the temperature field in order to obtain a well-organized single crystal blade. However, the majority of research focused on the directional solidification process parameters rarely mention the influence of blade orientation on the directional solidification temperature field, which further affects the grain growth.

In this paper, the three-dimensional CAD program SolidWorks is used to set the blade sample model with different orientations. The blade temperature field, the mushy zone and grain growth at different blade orientations are calculated by the ProCAST simulation software during the directional solidification process. The present paper focuses on the evolution of the grains at the complex mutation cross-section of the blade platform and uses a simplified model to explain the formation of heterocrystal grains in order to
provide a theoretical basis for the preparation of optimal blade products.

2. Experimental Setup and Procedure

A simple model is established to simulate the directional solidification process, as shown in Fig. 1. The model includes a graphite sleeve, a heat insulation baffle, a water-cooled ring, and a water-cooled copper plate under the sample. The graphite sleeve with 450/400 mm (inside/outside diameter), and 500 mm in height is used to heat and insulate the model. In the actual industrial production process, shielding of the surrounding magnetic field is also one of its important roles. The heat insulation baffle blocks the heat exchange between the upper heat preservation zone and the lower cooling zone. The thickness of the baffle is 25 mm. The figure shows the simply structures of the water-cooled ring and water-cooled copper plate which circulate cooling water internally and play an important role in the directional solidification apparatus.

In order to study the effect of blade orientation in the directional solidification furnace on the grain growth, two groups of models were created and are referred to here as parallel orientation and perpendicular orientation. These orientations are shown in Fig. 2. The blade bodies are 110 mm high and 40 mm wide, and the samples are spaced 90° apart. Figure 2(a) shows the perpendicular orientation assembly. The blade bodies are held relatively perpendicular to the graphite sleeve. Figure 2(b) shows the parallel orientation assembly. In this case, the blade body is relatively parallel to the graphite sleeve, and the different positions in the same height of the blade body are approximately the same as the furnace wall distance.

The superalloy used in this paper is DZ4125, a nickel-based directionally solidified superalloy which is widely used in China. DZ4125 has excellent high-temperature oxidation resistance, creep resistance, and rupture life. The specific alloy components and their mass fraction are given in Table 1.

The pouring temperature was fixed at 1550°C and was heated in 1550°C, holding for 180 s with a withdraw velocity of 5 mm/min. The water-cooled ring and the water-cooled copper plate in the cooling zone were held at a constant temperature of 20°C. The molded shell, casting, and water-cooled copper plate move simultaneously during the drawing process. The model was divided into total 467161 grids by using MeshCAST module in the ProCAST simulation software. The size of the grid unit in important parts is 2 mm, such as the blades. In less important regions, the grid size was 10 mm × 10 mm × 10 mm. The physical parameters of DZ4125 alloy are imported into the material database of ProCAST, the main physical properties of the DZ4125 superalloy (15) are shown in Table 2.

![Fig. 1 Schematic diagram of the simplified model of directional solidification.](image1)

![Fig. 2 Schematic diagram of different blade orientations.](image2)

Table 1 Chemical composition of nickel-based directionally solidified superalloy DZ4125.

<table>
<thead>
<tr>
<th>Element</th>
<th>Cr</th>
<th>Co</th>
<th>W</th>
<th>Mo</th>
<th>Al</th>
<th>Ti</th>
<th>Ta</th>
<th>Hf</th>
<th>B</th>
<th>C</th>
<th>Ni</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass fraction, %</td>
<td>8.68</td>
<td>9.80</td>
<td>7.08</td>
<td>2.12</td>
<td>5.24</td>
<td>0.94</td>
<td>3.68</td>
<td>1.52</td>
<td>0.012</td>
<td>0.09</td>
<td>Bal</td>
</tr>
</tbody>
</table>
3. Calculation Method

In the process of directional solidification drawing, the heat transfer is mainly divided into two forms. One is the local contact heat transfer between the water-cooled copper plate and the mullite structural shell. The other is the radiative heat transfer between the sample column and other components, including other sample columns, heating furnace walls, and the water-cooled ring. In the heat transfer process, the energy conservation law must be satisfied. The mathematical representation of the heat transfer model is:

\[ \frac{\partial T}{\partial t} = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \rho L \frac{\partial f_s}{\partial t} + Q_{\text{net}} \]  

(1)

where \( \rho \) is the material density, \( c \) is the specific heat capacity of the material, \( T \) is the material temperature, \( t \) is time, \( \lambda \) is the thermal conductivity of the material, \( L \) is the latent heat of the material crystallization, and \( f_s \) is the solid fraction. It can be seen from eq. (1) that the heat transfer process is composed of three parts, the contact heat conduction term, the internal heat source term caused by latent heat of crystallization, and the \( Q_{\text{net}} \) radiative heat transfer term.

Radiative heat transfer is the core problem in the whole process of the directional solidification process. According to the Stefan-Boltzmann law, the radiant heat transfer between the surfaces of a gray body is:

\[ Q_{\text{net}} = \frac{\pi}{4} \cdot \frac{A_1 \sigma (T_s^4 - T_l^4)}{\varepsilon_1} \]  

(2)

where, \( \varepsilon_1 \) in eq. (2) can be expressed as:

\[ \varepsilon_1 = \frac{C_V}{A_1} \int \int A_1 A_2 \cos \theta_2 \cos \theta_1 \frac{1}{\pi R^2} dA_1 dA_2 \]  

(3)

In these equations, \( \sigma \) is the Stefan Boltzmann constant, \( A_1, A_2 \) is the gray body surface area, \( C_V \) is the visible coefficient on gray body surface (0 is invisible, 1 is visible), \( \theta \) is the angle between the normal line of gray body surface and the center line of the surfaces, \( R \) is the center distance between two surfaces, \( f_s \) is radiation angle coefficient, \( T_1, T_2 \) is the surface temperature, and \( \varepsilon_1 \) is the surface element grayscale.

The preferred orientation of the DZ4125 dendrite growth was \((100)\). The CAFE module in the ProCAST simulation software was used to establish the grain growth model. The Rappaz model of continuous nucleation is consistent with a normal distribution used by the grain nucleation. The grain density at the solid-liquid interface front was characterized by a Gaussian distribution function:

\[ \frac{dn}{d(\Delta T)} = n_{\text{max}} \frac{1}{\sqrt{2\pi} \Delta T_{\sigma}} \exp \left[ -\frac{1}{2} \left( \frac{\Delta T - \Delta T_{\sigma}}{\Delta T_{\sigma}} \right)^2 \right] \]  

(4)

where, \( n \) is the nucleation density, \( n_{\text{max}} \) is the maximum nucleation density, \( \Delta T \) is the undercooling, \( \Delta T_{\sigma} \) is the standard deviation of the undercooling distribution, \( \Delta T_{\sigma} \) is the average nucleation undercooling.

The number of grains for a certain degree of undercooling can be calculated using eq. (5):

\[ n(\Delta T_{\sigma}) = \int_{0}^{\Delta T_{\sigma}} \frac{dn}{d(\Delta T)} d(\Delta T) \]  

(5)

where \( \Delta T_{\sigma} \) is the level of undercooling.

A kinetic model of grain growth was established at the solid-liquid interface, namely the dendrite tip growth front. The model was composed of four parts which can be expressed as:

\[ \Delta T = \Delta T_{c} + \Delta T_{r} + \Delta T_{k} + \Delta T_{i} \]  

(6)

Table 2 Directionally solidified superalloy DZ4125 main thermophysical parameters.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquidus temperature, ( T_e ), K</td>
<td>1617</td>
</tr>
<tr>
<td>Solidus temperature, ( T_l ), K</td>
<td>1508</td>
</tr>
<tr>
<td>Density, ( \rho ), kg/m³</td>
<td>8350</td>
</tr>
<tr>
<td>Heat coefficient in liquid, ( K_L ), W/(m·K)</td>
<td>5.0×10⁹</td>
</tr>
<tr>
<td>The maximum density of nuclei, ( n_{\text{max}} )</td>
<td>1.2×10⁹</td>
</tr>
<tr>
<td>The standard deviation of ( \Delta T ), K</td>
<td>1</td>
</tr>
<tr>
<td>The average nucleation undercooling, ( \Delta \bar{T} ), K</td>
<td>3</td>
</tr>
<tr>
<td>Alloy latent heat, ( \Delta H ), J/kg</td>
<td>99200</td>
</tr>
<tr>
<td>Specific heat, ( c_p ), J/(kg·K)</td>
<td>960</td>
</tr>
<tr>
<td>Diffusion coefficient in liquid, ( D_L ), m²/s</td>
<td>5.0×10⁹</td>
</tr>
<tr>
<td>Gibbs-Thomson coefficient, ( \Gamma ), m·K</td>
<td>2.41×10⁻⁷</td>
</tr>
<tr>
<td>( a_2 ), m/(s·K³)</td>
<td>7.93×10⁻⁸</td>
</tr>
<tr>
<td>( a_3 ), m/(s·K³)</td>
<td>1.09×10⁻⁸</td>
</tr>
</tbody>
</table>
where, $\Delta T_c$ is the component undercooling; $\Delta T_r$ is the curvature undercooling, $\Delta T_d$ is the dynamic undercooling, $\Delta T_t$ is the thermodynamic undercooling.

The cell capture method was used for grain growth, and the kinetic growth model was integrated to obtain the following polynomial:

$$v = a_2 \Delta T^2 + a_3 \Delta T^3$$  \hspace{1cm} (7)

where $v$ is the dendrite tip growth rate, $a_2$ and $a_3$ are grain growth coefficients.

4. Results and Discussion

4.1 Effects of different blade orientation on temperature field and mushy zone

Figure 3 contains a schematic diagram of the temperature field of two different orientations at the same time and solidification fraction. For the perpendicular orientation in Fig. 3(a), the temperature field at the upper part of the blade and at the lower part of the blade are inclined in different directions. For the parallel orientation shown in Fig. 3(b), the temperature field isotherm tends to stabilize and flatten. Moreover, under closer examination of the complex structure of the blade platform, the inclined temperature field of the perpendicular orientation case results in different temperature fields at the mutation cross-section, which is apt to generate defects. The overall temperature field at the platform of the parallel orientation has a smooth transition, especially at the complex structure of the blade body.

To examine the perpendicular orientation of the temperature field inclination, a simplified model was established using a cylindrical sample. Here, the sample is a round bar with a diameter of 18 mm, a height of 110 mm. The number of modules is 4. The other simulation conditions are the same as those used for the blade sample simulations. The simulation results are shown in Fig. 4.

The temperature field distribution of the cylindrical sample passing through the heat insulation baffle was selected. It was found that in the upper part of the heat insulation baffle, known as the heat insulation zone, the temperature of the Wall-Side was higher than the Center-Side. For this reason, the temperature field presents an upward inclination. In the cooling zone, the temperature of the Wall-Side sample is lower than that of the Center-Side, and the temperature field is inclined downward. In order to clearly explain the distribution of the temperature field, the radiation dissipation angle is used.

In the process of directional solidification, the sample cooling is primarily achieved in two ways: First, the water-cooled copper plate provides an upward cooling effect, but due to the barrier of the mullite structure and the small structure of the spiral grain selector, the cooling effect is very small. The second cooling effect is provided by the water-cooled ring. The water-cooled temperature of 20–30°C is always maintained by the water-cooled ring and therefore has a large temperature difference with the sample resulting in a good radiative cooling effect. In the calculation of radiative heat transfer, the selected temperature measurement point is visually separated from the water-cooled copper plate and the heat insulation baffle. The visible included angle is called the radiative heat dissipation angle. The larger the radiation angle, the stronger the radiation ability. As shown in Fig. 5, two points A and B at the same height above the heat insulation baffle are selected. By drawing the angle between the heat insulation baffle and the water-cooled copper plate, it is found that the angle $\alpha < \beta$. Therefore, the radiative heat dissipation capacity at point A is lower than that of point B,
which causes the temperature near point A to be higher than at point B. Under the heat insulation baffle, the parallel points C and D are examined. The angle between the heat insulation baffle and the cooling copper plate is such that $\gamma > \delta$. As a result, the temperature near Point C is lower than the temperature at point D.

In a similar fashion, the more uniform temperature field of the parallel orientation can be explained. In this case, the blade surface of the parallel orientation is parallel to the furnace wall, and all points on the same horizontal surface are equidistant from the furnace wall. Therefore, the radiation heat transfer angle formed through the water-cooled ring is the same resulting in consistent heat transfer. Additionally, since the blade is relatively thin, the heat transfer difference in thickness could be ignored.

Aiming at the mushy zone of the blade sample, the complex structure of the blade was studied. Due to the inclination of the temperature field in the perpendicular orientation, the advancing direction of the mushy zone deviates from the preferred orientation. This effect becomes increasingly obvious in the complex structure of the blade. The mushy zone of the different blade orientation is shown in Fig. 6, when the solidification fraction is 28.3%. Here, the solid-liquid interface moves to the complex structure of the blade. When the blade is in the perpendicular orientation, the mushy zone has an inclined angle. This indicates that the Center-Side mutation cross-section solidifies earlier than the Wall-Side mutation cross-section, damaging the overall structure of the blade. This can also lead to the formation of heterocrystal grains or change the growth direction of the columnar crystals. In the parallel blade orientation, the mushy zone moves more stable in the complex structure. In this case, the distance from each point on the plane to the water-cooled ring is equal. As a result, no obvious uneven heat dissipation phenomenon, leading to improved results.

### 4.2 Grain growth behavior of different blade orientation

The study of the blade temperature field and mushy zone provides a reference for exploring the blade grain growth behavior. The fluctuation of the temperature field and the mushy zone affects the grain formation and growth, particularly in the mutation cross-section. Therefore, the grain growth status of the different orientations was studied. Two types of grain growth models were observed for the perpendicular and parallel blade orientations with the variable insulation temperature of 1550°C. The simulation results are shown in Fig. 7. The results show that the tendency of heterocrystal grains to form is increased in the blade samples with a perpendicular orientation. Because the temperature field and mushy zone of the blade sample of the perpendicular orientation have a certain inclination, there are different temperature gradients at a given height, which facilitates the formation of heterocrystal grains. Particularly at the mutation cross-section of blades, heterocrystal nucleation occurs more readily. For the parallel orientation, no heterocrystal tendency was observed at the complex platform or the mutation cross-section of the blade. This is because the temperature field distribution of the blade sample with parallel orientation is relatively stable without excessive inclination. The original grains screened from the end of the spiral grain selector gradually grow in the direction of heat flux until the complete blade casting is filled.

In order to demonstrate the growth behavior of the grains at the mutation cross-section more clearly, a variable cross-section sample was introduced for detailed analysis. The structure of the variable cross-section sample is similar to that of the cylindrical sample. Following a transition section, the main body of the variable section sample is cuboid, there is a variable cross-section platform every 20 mm. The widths of
these variable-sections platform are 3, 6, 9, 12 mm from bottom to top, and the thickness of the variable cross-section platform is equal to 5 mm. The sample height is equal to the cylindrical sample.

Figure 8 shows one of the variable cross-section platforms of the sample (platform width is 6 mm and thickness is 5 mm). The time taken by dendrites on the Center-Side to grow from the initial point A to the inflection point of the variable cross-section platform is given by \( t_1 \). The filling time of the original secondary transverse dendrites from the inflection point of the variable-section platform to Point B is \( t_2 \). When the liquidus is at the position shown in Fig. 8(a), point B at the platform is not nucleated due to insufficient undercooling. The time interval where Point B changes from liquidus temperature to grain nucleation is \( t_3 \). The following relationships exist: When \( t_1 + t_2 < t_3 \), the time taken for the original grain to grow from Point A to the fully filled variable-section platform is less than the time taken for the undercooled heterocrystal nucleation. Therefore, no heterocrystal grains are generated, and the original grain continues to grow. When \( t_1 + t_2 > t_3 \), the nucleation time from the liquidus to the new grain at Point B is faster than the time required for the original grain to fill the variable cross-section platform. Therefore, the heterocrystal grains at the variable-section platform continue to grow along the direction of heat flux. During the competitive growth of the original grains, some of the heterocrystal grains are replaced by the original grains, and conversely, some of the heterocrystal grains replace the original grains. Figure 8(b) shows a schematic diagram of the heterocrystal grains growth in the variable cross-section platform.

Figure 9 is a schematic diagram of the grain growth in the second section of the variable cross-section sample. When the grain growth is close to the variable cross-section platform, the sample trunk is completely filled by the original grain, as shown in Fig. 9(a). As the drawing process continues, the original grains grow in the direction of the heat flux and reach the second variable cross-section platform. As shown in Fig. 9(b), the original grains grow at the variable cross-section platform corner opposite from the furnace wall.

As the process continues, many new heterocrystal nucleations occur at the corners of the platform, as shown in Fig. 9(c). These heterocrystal grains grow gradually, and there is competitive growth between the heterocrystal grains until the variable cross-section platform is completely filled together with the original grains, as shown in Fig. 9(f). In the subsequent directional solidification process, the Wall-Side platform is filled with original grains. Because the temperature field is inclined from the Wall-Side to Center-Side, there is no possibility of heterocrystal nucleation and growth on this platform. During this process, the heterocrystal grains from the Center-Side pass through the upper surface of the platform and enter the sample trunk, competing with the original grains for growth. This part of the process is shown in Fig. 9(g). As the directional solidification continues, the heterocrystal grains gradually replace the original grain, as shown in Fig. 9(h).

4.3 Position of heterocrystal grains in the blade

Simulation software was used to simulate the grain growth of the blade samples. The selected samples were arranged in a perpendicular orientation, and the results are shown in
Fig. 10. In order to better express the position where heterocrystal grains are likely to be formed, the tendency of heterocrystal formation was increased by reducing the heat insulation temperature to 1530°C. The left side of the blade sample is the Center-Side, and the right side is the near furnace wall side. As shown in Fig. 10(a), Point A is located on the complex structure platform of the blade. Due to the inclination of the temperature field, alloy liquid undercooling nucleation first occurs on the Center-Side, forming the heterocrystal grains. The same behavior also exists at the mutation cross-section at Point B. In Fig. 10(b), the newly formed heterocrystal grain gradually replaces the original grain and fills in the blade. At Point C, at the end of the spiral grain selector, multiple grains grow together due to the poor crystal screening of the selector. Therefore, there are three positions on the blade where the heterocrystal grains easily generate: the complex structure platform, the mutation cross-section, and the end of the spiral grain selector.

5. Conclusions

(1) The temperature field and mushy zone of blades under different orientations were simulated and calculated. A relatively stable temperature field and mushy zone of the blade sample with parallel orientation were easily obtained at the same horizontal height. Conversely, the
temperature field blade sample with a perpendicular orientation had a certain inclination.

(2) Based on a radiative heat transfer calculations and the heat dissipation angle, the temperature field and relative position between the sample and the furnace body were analyzed. In the heat insulation zone, it was found that the sample surface temperature at a given height was higher on the Wall-Side than the Center-Side. In the cooling zone, the sample surface temperature at Center-Side was higher than Wall-Side.

(3) For the parallel orientation, the blade sample easily obtains a complete single crystal structure. This is a result of the stable temperature field and mushy zone in the parallel orientation. Using a variable cross-section sample, the grain growth behavior in the directional solidification process was further studied, and the growth state of the original grain passing through the variable-section platform is summarized. The heterocrystal formation positions of blade samples were analyzed. It was found that the most likely positions of heterocrystal grains formation are the complex structure platform, the mutation cross-section, and the end of the spiral grain selector.

Acknowledgments

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