Numerical Simulation and Experimental Study of Spiral Grain Selection Process for Single Crystal Superalloys II: Spiral Section Postprint

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Abstract

The spiral grain selector is a critical component for manufacturing single-crystal blades and ensuring crystal integrity, consisting primarily of a seed section and a spiral section. This study investigates the role of the spiral section in the grain selection process. Based on metallographic and EBSD experimental results, it is revealed that during competitive grain growth, the competitive advantage of grains is collectively determined by the orientation of their secondary dendrite arms and their initial position distribution characteristics. Two geometric constraint mechanisms underlying the grain selection process are proposed: the competition-promoting effect of secondary dendrite arms in the horizontal direction and the constraint effect of primary dendrite arms in the vertical direction. These two models successfully elucidate the role of the spiral section in grain selection. The competitive grain growth process within the spiral section is simulated using a modified cellular automaton (MCA) technique. The evolution of grain structure and crystal orientation during directional solidification is examined and compared with experimental results, demonstrating good agreement. Based on the combined simulation and experimental investigations, the influence of spiral parameters on grain selection behavior and the associated mechanisms are established, leading to the proposal of design criteria for the spiral section of grain selectors.

Full Text

Numerical Simulation and Experimental Study on Grain Selection Process of Single Crystal Superalloy II. Spiral Part

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ABSTRACT

The spiral selector is the key part for producing single crystal (SX) blades and ensures the integrity of crystal, which mainly includes starter block and spiral part. In this paper, the influence of spiral part on the grain selection process was studied. Both of the metallography results and EBSD results proved that the prior location and the special orientation of the second dendrite arms were important for the grains competitive growth during the directional solidification process. Based on the experimental results, two geometrical restrict mechanisms of grain selection were proposed. They were the competitive stimulating effect on the second dendrite arms in horizontal direction, which was resulted from the spiral arc shape, and the growing blocking effect on the primary dendrites in vertical direction, which was resulted from the take-off angle of the spiral part. These models could successfully explain the grain selecting effects of the spiral part. The modified cellular automaton (MCA) technology was used to simulate the grains' competitive growth in spiral part. The changes of grains structure and orientation as the grain growing on were studied. The simulated and experimental results were compared and agreed well. Based on the simulated and experimental results, Influences of structural parameters on the grain selection behavior were proposed. The criteria for designing spiral part were also presented.

KEY WORDS numerical simulation, grain selection behavior, grain orientation, EBSD

Directionally solidified single crystal turbine blades obtain their single crystal structure through grain selectors. The structure of the grain selector directly affects the selection efficiency and consequently influences product yield. Traditional grain selectors include various configurations such as constriction type, deflection type, inclination type, and spiral type [1]. The main difference among these four types lies in the selector section (the part above the starter block of the selector). The spiral selector is widely adopted due to its superior grain selection effectiveness. However, the spiral selector involves numerous design parameters and complex spatial geometry, which increases the difficulty of research.

In recent years, numerical simulation technology has become an important tool for grain selector research. Directional solidification simulation developed rapidly in the 1990s, based on fundamental solidification theory [2, 3], dendrite growth theory [4-6], and research on superalloy materials [7, 8]. Among these, Gandin and Rappaz et al. [9-13] employed the cellular automaton (CA) combined with finite element (FE) method to simulate the temperature field and microstructure evolution during directional solidification, and developed the directional solidification module of the commercial software ProCAST. Chinese researchers [14-18] have subsequently conducted related work on directional solidification simulation, among which references [14-16, 19, 20] used the cellular automaton-finite difference (CA-FD) method to simulate the temperature field and microstructure during directional solidification.

Numerous studies on grain selection have been conducted by scholars worldwide. Carter et al. [21] investigated the important influence of the spiral section on dendrite secondary arm orientation. Esaka et al. [22] employed simulation methods to analyze the effects of structural parameters of a two-dimensional simplified spiral selector on grain selection efficiency. Epishin et al. [23] experimentally studied the evolution of grain competition at different cross-sections of the spiral selector. Seo et al. [24] used ProCAST software to simulate the grain selection process of a three-deflection-angle selector and compared it with experimental results. Pan et al. [25, 26] studied the grain distribution at cross-sections of the spiral part using numerical simulation combined with EBSD experiments. Dai et al. [27-29] used ProCAST software to simulate spiral selectors with different structures, compared with experiments, and obtained qualitative rules regarding the effects of some parameters on grain selection. Jiang et al. [30] studied the grain selection process of Ni3Al-based superalloys. Meng et al. [31, 32] used ProCAST software to simulate spiral selectors with different parameters and compared the results with experiments. Gao et al. [33] used EBSD experimental technology to observe and analyze the characteristics of grain competitive growth at cross-sections of the spiral part, and pointed out that the blocking effect of the narrow channel of the spiral selector is the main reason for grain selection.

In this study, the CA-FD method was adopted to independently develop a numerical simulation program for directional solidification of single crystal blades, and the single crystal grain selection process was simulated. An EBSD experimental scheme was designed to analyze the grain structure and orientation characteristics at cross-sections of the spiral part, the influence laws and mechanisms of spiral parameters on grain selection behavior were obtained, and design criteria for the spiral section of the grain selector were proposed.

1.1 Spiral Structure Design and Experimental Scheme

The structure of the spiral selector can be divided into three parts: starter block, spiral part, and transition section. Among these, the structural design of the spiral part is critical to the grain selection effect, as shown in Figure 1 [Figure 1: see original paper].

The main structural parameters of the spiral part include: spiral pitch hs, spiral diameter ds, take-off angle , and spiral line diameter dw. The pitch hs, spiral diameter ds, and take-off angle satisfy the relationship (1): s tan

[Figure 2: see original paper] Molding pattern of the spiral selector (a) Molding pattern (top view) (b) picture of the wax pattern

Cross-sectional analysis was performed on the spiral part of the selector. One horizontal section was taken every 90° increase in spiral rotation angle. Metallographic (OM) analysis was conducted using a Zeiss (Axio Imager A1m) metallographic microscope. Samples were prepared by mechanical polishing and observed using EBSD with a JEOL 6301F field emission scanning electron microscope. The positions of each section are shown in Figure 3 [Figure 3: see original paper]. The heights of the sections from the top surface of the starter block are listed in Table 2 .

Table 2 Corresponding table of height (distance between the top surface of starter block and the position where the corresponding section was cut) and sections in the spiral part (dw=5 mm)

Section	Height, mm
S1	
S2	
S3	
S4	
S5	
S6	

[Figure 3: see original paper] Schematic of the sections' positions of the spiral part (S1—S6: the sections of different heights; h1—h6: the corresponding heights of sections.)

1.2.1 Metallographic and EBSD Orientation Imaging Results

Generally, the orientation angle of grains entering the spiral part is less than 15°. In this case, different grains are difficult to distinguish by primary arm orientation, thus requiring consideration of secondary arm orientation differences to identify different grains. Figure 4 [Figure 4: see original paper] shows the experimental microstructure results at different cross-sections of the spiral part. As seen in Figure 4b, when grains grow into the spiral part, their number is relatively large; the secondary arms of grains near the lower edge and inner side of the cross-section undergo lateral growth. As the solidification process proceeds, the secondary arms of these grains further grow laterally, while the number and size of grains near the upper edge and outer side of the spiral decrease through competition, as shown in Figures 4c and 4d. With continued solidification, eventually only one grain wins the competition and grows into a single crystal.

[Figure 4: see original paper] Experimental results of microstructures at different sections in spiral part of G1 (a) S1 (b) S2 (c) S3 (d) S4 (e) S5 (f) S6

Figure 5 [Figure 5: see original paper] shows the EBSD grain orientation imaging maps at different cross-sections of the spiral part. At the transition section, grain boundaries are clear and numerous, as shown in Figure 5a. When grains grow into the spiral part, grains at the lower edge and inner side of the spiral expand rapidly, and the finally selected single crystal structure occupies the entire cross-sectional area, as shown in Figure 5f.

[Figure 5: see original paper] EBSD grains' orientation images of different sections in spiral part of G2 (a) S1 (b) S2 (c) S3 (d) S4 (e) S5 (f) S6

1.2.2 Grain Growth Characteristic Analysis

(1) Competitive Grain Growth at the Lower Edge of the Spiral

During the spiral grain selection process, grains at the lower edge of the spiral exhibit extended growth, as shown in Figures 4 and 5. Figure 6 [Figure 6: see original paper] illustrates the lateral expansion process of grains at the lower edge of the spiral. The secondary arms of the spiral lower edge expand and grow along the [100] and [010] directions. Differently oriented dendrites exhibit different growth lengths in the secondary arm directions, showing obvious competitive growth. As seen in Figure 6a, grains A and B grow simultaneously along the [100] direction, and there is a certain angle between their secondary arm crystal orientations, resulting in competition. When the grains continue to grow and the spiral rotates 90°, the grain growth result is shown in Figure 6b. At this point, both grains A and B have increased in size. The secondary arm growth of grain A along one direction stops, while the secondary arm along the [010] direction grows rapidly and completely occupies the upper edge of the spiral. The [100] direction secondary arm of grain B is blocked by the arc side wall and stops growing. As shown in Figure 6, grain A is closer to the lower edge and inner side of the spiral, thus having obvious positional advantages that facilitate the extended growth of grain secondary arms. Grain B, being closer to the outer side of the spiral, lacks spatial advantages and is eventually eliminated.

Based on the above analysis, the metallographic experimental results and EBSD orientation imaging results demonstrate that the spiral section promotes secondary arm competition in the horizontal direction through its curved geometry, leading to the elimination of some grains and completing the grain selection process. Grains near the lower edge and inner side of the spiral have significant positional advantages in competitive growth and are easily selected to grow into the final single crystal structure.

(2) Competitive Elimination of Grains at the Upper Edge of the Spiral

As shown in Figure 5, the extended growth of secondary arms of grains at the lower edge of the spiral is a factor in the rapid elimination of other grains. However, research reveals that the number of grains at the upper edge of the spiral and the cross-sectional area occupied by grains also change with the spiral ascent process. Figure 7 [Figure 7: see original paper] shows the comparison of {001} crystal plane pole figures between the upper edge region and lower edge region of the spiral. It can be seen that the elimination process of stray grains at the lower edge of the spiral is relatively fast, and by the time it reaches section S4, only one grain remains. The elimination process of stray grains at the upper edge of the spiral is slower, and even when reaching section S6, only one grain remains. Moreover, as shown in Figure 5f, when reaching section S6, a single crystal structure has already formed.

The above analysis indicates that there is also a certain grain competitive elimination effect at the upper edge of the spiral, but its elimination rate for stray grains is slower than that at the lower edge.

[Figure 6: see original paper] Extending growth at the lower edge of spiral part (a) S2 (b) S3

[Figure 7: see original paper] Pole figures of {001} crystal face at upper edges and lower edges of spiral

2. Spiral Segment Grain Competition Growth Mechanism

Based on the above experimental results, obvious extended growth of secondary arms of grains occurred at the lower edge and inner side of the spiral cross-section, leading to the elimination of some grains through competition; the growth of grains near the upper edge and outer side of the spiral was restricted and partially eliminated. Summarizing these experimental observations, two important grain selection mechanisms of the spiral selector are proposed.

2.1 Crystal Geometry Restriction Growth Mechanism I—Horizontal Secondary Arm Competition Promotion Effect

When grains enter the spiral section, the angle between their optimal orientation and the z-direction (opposite to heat flow) is relatively small, generally less than 15° [25], and grain competition growth in this direction is weakened. The main role of the spiral section is to provide geometric restriction conditions that promote competitive growth of secondary arms to achieve single crystal selection.

To illustrate the grain secondary arm competition growth and selection mechanism in the horizontal direction, a two-dimensional top-down projection of the spiral section is made. Figure 8 [Figure 8: see original paper] shows the 2D projected schematic diagram of grain secondary arm competition growth in the spiral part, where bold lines represent the marginal lines of cross-sections obtained by horizontally cutting the three-dimensional solid.

[Figure 8: see original paper] The 2D projected schematic diagram of grains second dendrite arm competition growth in spiral part (a) the positions of sections (b) schematic of grain competition

During solidification, after grains complete competitive growth in the starter block and enter the transition section, a certain number of grains remain. The optimal growth direction [001] of these grains forms a small angle with the z-direction, but their secondary arms, i.e., the [010] and [100] directions, are randomly distributed. The width of the spiral line (dw) hinders other grains near the outer side and front of the spiral from continuing to grow along the spiral channel, giving grain   a spatial advantage in competitive growth. Therefore, grain   has a larger size, as shown in section B of Figure 8b.

These grains continue to grow and enter the spiral section, as shown in section A of Figure 8b. Grains near the lower edge of the spiral begin rapid growth of secondary arms along the [010] and [100] directions, but due to the restriction of the arc geometry, secondary arm growth of some grains is limited. An intense grain competition growth process occurs during this stage. Grains , , and   in Figure 8 undergo secondary arm competition growth.

As grains continue to grow and the spiral ascends and rotates 90°, secondary arms of grains near the lower edge grow fully and grain size increases, as shown for grains   and   in section B of Figure 8b. Grain   is closer to the lower edge and inner side of the spiral and has the largest grain size. The main reasons are: on one hand, grain   is near the lower edge and inner side of the spiral and needs to extend a smaller distance forward to reach the solidification front, thus having a time advantage in competitive growth; on the other hand, the already grown dendrites of grain   penetrate through the spiral line width. As solidification proceeds, grain   continues to grow, while the growth of grain   is completely blocked by grain   and the arc geometry. When growth reaches section C in Figure 8b, grain   has completely occupied the lower edge of the spiral, while grain on the outer side of the spiral is eliminated through competitive growth. Furthermore, when grain growth reaches section D in Figure 8b, grain may occupy the entire cross-section, forming a single crystal structure.

The above model successfully explains that the spiral section promotes competitive growth of grain secondary arms in the horizontal direction by providing arc-shaped geometric restriction conditions. The model also indicates that grains near the lower edge and inner side of the spiral have geometric advantages in competitive growth and are more easily selected to grow into the final single crystal structure.

This model identifies grain secondary arm orientation, position distribution, and the horizontal arc structure of the spiral section as factors affecting the grain selection process, representing a summary and refinement of existing experimental results.

2.2 Crystal Geometry Restriction Growth Mechanism II–Vertical Primary Arm Restriction Effect

The spiral selector mainly provides geometric restriction conditions for grain growth through the design of the take-off angle, achieving the elimination of some grains. Its longitudinal grain selection behavior is similar to that of an inclined type selector [22].

Figure 9 [Figure 9: see original paper] shows the 2D schematic diagram of crystal restriction and elimination for spiral selectors with different take-off angles. When the spiral take-off angle is larger (1), grains and are eliminated at the same growth height H. As shown in Figure 9b, when the take-off angle decreases to 2, grains - are all eliminated at the same growth height H, leaving only grain able to continue growing. When the take-off angle decreases to 3, grains - are all eliminated at the same growth height H, and the growth of grain is also inhibited, with only its side branches continuing to grow. In Figure 9c, when the growth height reaches h (h<H), grains - have already been eliminated, leaving only grain able to continue growing.

The above analysis demonstrates that the geometric restriction conditions provided by the spiral take-off angle are directly related to the inclination degree of the spiral boundary and the bottom diameter a. For the two-dimensional case, when H>a · tan is satisfied, the geometric restriction and elimination effect of the spiral take-off angle will be fully realized, and only grains near the lower edge of the spiral (such as grain) will be selected. For actual three-dimensional conditions, hs>H should be satisfied; however, due to the complex structure of the spiral rotation angle and the inclined distribution of the temperature field during solidification, the growth velocity of dendrites at different angles varies, affecting the grain selection efficiency. Therefore, the provided pitch hs should also be much larger than dw · tan to satisfy the conditions for successfully selecting a single crystal structure.

[Figure 9: see original paper] Schematic diagram of geometry restricting and obsoleting effect of spiral take-off angle (1, 2, 3—different take-off angles; H—a certain growth height; h—the height that grains — were eliminated by competition growth; a—the width of growth passageway in 2D) (a) Inclined growing channel with the angle of (b) inclined growing channel with the angle of (c) inclined growing channel with the angle of

The vertical primary arm restriction effect is another important mechanism of grain competitive growth in the spiral section. This model explains the influence of the relationship between spiral take-off angle ( ), pitch (hs), and spiral line diameter (dw) on grain selection efficiency, and indicates that the initial positional advantage of grains (such as grain near the lower edge) is key to being selected in competition. The model successfully explains the experimental variation process of grain competitive growth at the upper edge of the spiral shown in Figures 5 and 7.

In summary, the horizontal secondary arm competition promotion effect and the vertical primary arm restriction effect are two important geometric restriction mechanisms of spiral grain selection. They explain how the spiral section promotes dendrite secondary arm competition through arc structure conditions in the horizontal direction and restricts dendrite primary arms through the spiral take-off angle in the vertical direction. The actual spiral selector is a superposition of these two mechanisms, and rational design of the spiral arc diameter (ds), spiral take-off angle ( ), pitch (hs), and spiral line diameter (dw) directly affects the spiral grain selection efficiency.

2.3 Modeling Based on Spiral Segment Grain Competition Growth Mechanism

The cellular automaton (CA) method simulates microstructure evolution by defining a series of rules reflecting short-range or long-range interactions between cells.

In this work, a modified cellular automaton method (MCA) was adopted, considering the above crystal geometry restriction growth mechanisms I and II, to perform computer numerical simulation of the spiral grain selection process.

The grain selection effect of the spiral section is mainly geometric structure restriction; therefore, appropriately selecting the mesh size for microstructure simulation is key to reasonably reflecting the spiral grain selection mechanism. The CA model for microstructure evolution during solidification can be described by equation (2):

$$\zeta_{ijk}^{t+n} = f(\zeta_{ijk}^{t}, x_{ijk}^{t}, \Gamma, L, M, N)$$

In equation (2), ζ_{ijk}^{t} is the state variable value of cell (i, j, k) at time t; $f(x)$ is the transformation rule defined by the cellular automaton; x_{ijk}^{t} is the specific physical quantity of cell (i, j, k) at time t, which may be T (temperature), ΔT (temperature change), C (solute), V (volume), etc.; Γ represents the size of the temporal domain; L, M, N represent the size of the spatial domain; Γ, L, M, N are all positive integers.

For finite difference (FD), a regular hexahedron unit is selected as the cell. Let Ψ be the parameter coupling different dimensions.

$$\Psi = L \times M \times N$$

In equation (3), when $\Psi \leq 1$, the composed domain is the von Neumann cell type; when $\Psi \leq 2$, the composed domain is the Moore type; when $\Psi \leq 3$, the composed domain includes all adjacent cells. The CA model is applicable to multi-scale systems, and the specific applicable scale is determined by the integer units in equation (3). Define l_δ as the discrete unit spatial step. In simulation calculations, considering the effects of all neighboring cells (when $\Psi \leq 3$), the microscopic interaction length l_Ψ satisfies the following condition:

$$l_\Psi \leq \lambda_1$$

where λ_1 is the primary dendrite arm spacing. Based on the above analysis, under geometric structure restriction conditions, selecting a reasonable mesh size is key to reflecting the spiral grain selection process. Therefore, the microscopic interaction length in simulation should satisfy condition (5). Consequently, the simulation mesh unit step length is approximately $l_\delta \approx \lambda_1/3$. In actual directional solidification, the average dendrite spacing λ_1 is about 0.3 mm [34]; in this study, the measured average dendrite spacing is 0.32 mm (as shown in Figure 4). Therefore, the discrete unit spatial step length l_δ for simulating the geometric restriction growth process of spiral grain selection is approximately 10^{-4} m.

[Figure 10: see original paper] Simulation results of grain structure of different sections in spiral part of G1 (a) S1 (b) S2 (c) S3 (d) S4 (e) S5 (f) S6

3.1 Simulation and Experimental Comparison of Spiral Segment Crystal Growth

In this study, crystal growth in the spiral selector was simulated, with results shown in Figure 10. The simulation employed a macro-micro coupling algorithm, where the macroscopic temperature field mesh unit size was 0.6 mm × 0.6 mm × 0.6 mm, and the microscopic microstructure calculation used a mesh unit size of 0.15 mm × 0.15 mm × 0.15 mm. The material was the domestic second-generation single crystal superalloy DD6. The basic parameters used in the simulation are listed in Table 3 .

Table 3 The thermophysical parameters of DD6 superalloy [25, 35]

Parameters	Value
Liquidus, K	
Solidus, K	
Specific heat, kJ/(kg · K)	
Density, kg/m^3	
Latent heat, kJ/kg	

As can be seen from Figures 5 and 10, the simulation results basically reflect the actual competitive growth process in the spiral section of the spiral selector. The experimental results can clearly reveal the morphology and spacing characteristics of primary dendrites, as well as the extended growth characteristics of secondary arms. The simulation can clearly reflect the competitive distribution of different grains and demonstrate the dynamic growth process of grains under spiral geometric restriction conditions.

Figure 11 [Figure 11: see original paper] shows the orientation imaging maps of different grains. It can be seen that when grains enter the transition section, the angle between the grain [001] orientation and the z-direction is less than 15°. When the section position height exceeds 14.5 mm, the angle has approached 0°, and the orientation of the selected grain meets the requirements.

[Figure 11: see original paper] Simulation results of angles between [001] orientation and z direction of some sections in spiral (a) S1 (b) S3 (c) S5

3.2 Simulation Study on Influence of Spiral Structural Parameters on Grain Selection

Simulation technology was used to study the relationship between spiral structural parameters and grain selection. As shown in Figures 10 and 11, numerous grains enter the spiral section, and the angle between the grain [001] orientation and the z-direction (opposite to heat flow) is within 15°. The requirements for selector design are twofold: (1) the angle between the obtained single crystal orientation and the z-direction should be less than 15°; (2) the position where the single crystal forms should not be too high (generally within 1-2 times hs).

Regarding requirement (1), based on previous research results on the starter block, when directional solidification conditions are appropriate, grains entering the spiral section basically meet the standard. When the [001] orientation satisfies the condition, the secondary arms in the [010] and [100] directions become key factors affecting the grain selection process and directly determine the position where the single crystal forms.

Table 4 lists the structural parameters of spiral selectors used in the simulation calculations, where all selectors adopt a two-turn spiral structure. Considering the random distribution characteristics of secondary arms, 10 calculations were performed for each parameter set in the table, and the height of single crystal formation and single crystal orientation values were statistically analyzed.

Table 4 The structure parameters of spiral selectors for simulation calculation (dw=5 mm, hs=14 mm)

Group	ds, mm	, deg
M1	8	
M2	10	
M3	12	
M4	14	

Figures 12 [Figure 12: see original paper] and 13 [Figure 13: see original paper] show the temperature field and mushy zone distribution during solidification for spiral selectors with different structural parameters. The temperature field distribution basically conforms to the one-dimensional heat transfer characteristics of directional solidification. However, in Figure 13c, the mushy zone distribution is relatively wide, and an anomalous temperature field distribution region appears, shown by the black frame. In such anomalous temperature field regions, stray grain nucleation and growth are highly likely to occur, which is detrimental to the single crystal selection process. The appearance of this region is related to many factors, including spiral section structural design and withdrawal rate. It is mainly caused by excessive spiral turns and small take-off angle, resulting in poor unidirectional heat dissipation conditions; simultaneously, radiation from the lower cooling zone can also directly radiate and cool this region, causing local undercooling.

Therefore, excessive spiral turns and small take-off angles are unfavorable for the grain selection process. In design, the number of spiral turns should be minimized based on the principle of selecting a single crystal structure.

[Figure 12: see original paper] The simulation results of directional solidification temperature fields of M2 group (a)30%, 630 s (b)50%, 840 s (c)65%, 1200 s (d)75%, 1350 s

[Figure 13: see original paper] The changes of mushy zone during the directional solidification process of M2 group (a)30%, 630 s (b)50%, 840 s (c)65%, 1200 s (d)75%, 1350 s

Figure 14 [Figure 14: see original paper] shows the simulation results of microstructure evolution during directional solidification of the M2 group. The figure presents the microstructure distribution at solidification fractions of 30%, 50%, 65%, and 75%. When the solidification fraction exceeds 50%, crystal growth reaches the spiral section and the secondary arm competition growth process begins. As seen in Figure 14c, grains near the inner side of the spiral have obvious advantages in competitive growth, thereby eliminating other grains and eventually growing into a single crystal structure.

[Figure 14: see original paper] The simulation results of directional solidification microstructure growth of M2 group (a)30%, 630 s (b)50%, 840 s (c) 65%, 1200 s (d)75%, 1350 s

A comparative analysis of solidification microstructure simulation results for spiral selectors with different spiral diameters ds is shown in Figure 15 [Figure 15: see original paper]. After grains enter the spiral section, due to different ds parameters, the competitive growth conditions vary, and the position height where the single crystal structure appears differs. It can be seen from the figure that as ds increases, the position height of single crystal formation gradually decreases.

[Figure 15: see original paper] The simulation results of directional solidification microstructure growth of spiral selector with different parameters (a) ds=8 mm (b) ds=10 mm (c) ds=12 mm (d) ds=14 mm

Considering the random distribution characteristics of grain secondary arms, multiple simulation calculations were performed for spiral selectors with different ds values, and the position of single crystal formation was statistically analyzed. Figure 16 [Figure 16: see original paper] shows the analysis of single crystal formation height position. The figure contains multiple arc curves, where the arc radius equals ds/2. The arc angle range is determined by the following steps: first, determine the single crystal appearance position in the spiral selector, then measure the spiral rotation angle from the starting position of the spiral section to this position, recorded as the single crystal formation angle; based on the single crystal formation angle and radius, determine the corresponding points for each experimental result in Figure 16, thus forming the arc range shown in the figure. The arc radius indicates that when ds differs in the spiral section, the single crystal formation position (corresponding to the single crystal formation angle) varies; the arc range indicates the possible range of single crystal appearance positions for spiral selectors with different ds.

[Figure 16: see original paper] The height of single crystal formed

The single crystal formation position exhibits the following characteristics: (1) As ds increases, the single crystal formation angle decreases, corresponding to a lower position. When ds increases from 8 mm to 14 mm, the average single crystal formation angle decreases from 314.9° (corresponding height of 12.2 mm) to 204.6° (corresponding height of 8.0 mm). Figure 17 [Figure 17: see original paper] shows the linear relationship between the average single crystal formation angle and ds.

The cause analysis of characteristic (1) is as follows: Under constant hs conditions, when ds increases, according to equation (1), the spiral take-off angle decreases. According to crystal geometry restriction growth mechanism I, increasing ds promotes competitive growth of grain secondary arms in the horizontal direction, accelerating grain elimination and lowering the single crystal formation height position. On the other hand, according to crystal geometry restriction growth mechanism II, decreasing strengthens the geometric restriction and elimination effect in the vertical direction, also lowering the single crystal formation height position. Therefore, when hs is constant, increasing ds or decreasing will both strengthen the geometric restriction growth effect and lower the single crystal formation height position.

(2) As ds increases, the range of single crystal formation angles widens. When ds increases from 8 mm to 14 mm, the single crystal formation angle range increases from 93.4° to 155.3°, as shown in Figure 16. Therefore, when ds is larger, the stability of the single crystal formation height position is poorer.

The cause analysis of characteristic (2) is as follows: Analysis based on crystal geometry restriction growth mechanisms I and II reveals that grain competitive advantage is a comprehensive manifestation of positional advantage and secondary arm orientation advantage. When ds increases, the horizontal secondary arm competition promotion effect (mechanism I) is strengthened, and grains with secondary arm orientation advantages may rapidly block other grains and form single crystal structures at lower positions. Simultaneously, the vertical primary arm restriction effect (mechanism II) is strengthened, and grains with positional advantages may grow rapidly and form single crystal structures at lower positions. Random phenomena under these two mechanisms coexist, strengthening the randomness characteristics of grain competitive growth, thus resulting in a significantly wider single crystal formation angle range. Conversely, when ds is smaller, the strengthening effects of both mechanisms are simultaneously weakened, and only grains with both secondary arm growth advantages and initial positional distribution advantages can eliminate other grains to form single crystal structures. Therefore, the randomness of the grain selection process is weakened, and the single crystal formation angle range becomes narrower.

[Figure 17: see original paper] Relationship chart between ds and the single crystal average appearing height

4. Conclusions

(1) Using EBSD and metallographic experimental techniques, the grain structure and orientation at different height positions of the spiral selector were obtained, and the crystal competitive growth behavior during the spiral grain selection process was analyzed. It was pointed out that grains with positional and orientation advantages are more easily selected in competition. Based on experimental results, two important mechanisms of grain geometry restriction growth were proposed, fundamentally explaining that the horizontal secondary arm competition promotion effect (mechanism I) and the vertical primary arm restriction effect (mechanism II) are the main working mechanisms of the spiral section.

(2) Based on the grain geometry restriction growth mechanisms, mathematical modeling analysis was conducted and the simulation scale was reasonably selected. Simulation calculations were performed for spiral selectors with different spiral diameter parameters, obtaining results for temperature field, mushy zone, and microstructure distribution during directional

solidification at different solidification percentages. From the temperature field perspective, it was pointed out that the structure of the spiral section would disrupt the one-dimensional heat transfer characteristics, and excessive spiral turns are unfavorable for selecting single crystal structures. Meanwhile, through numerous simulation results, the influence of spiral diameter variation on single crystal formation height position was statistically analyzed. Combined with crystal geometry restriction growth mechanisms, it was indicated that increasing spiral diameter strengthens the grain selection effect and lowers the single crystal formation height position, thus allowing appropriate reduction of spiral turns. However, increasing spiral diameter also strengthens the randomness of grain competitive advantages, expanding the possible formation position range of grains. Actual spiral section design should comprehensively consider both effects.

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