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Simulation of grain selection during single crystal casting of a Ni-base superalloy

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ABSTRACT

The grain selection process during single crystal casting of a Ni-base superalloy DD403 in spiral grain selector is simulated by a macro-scale ProCAST coupled a meso-scale Cellular Automaton Finite Element (CAFE) model. And the simulation results are validated by experimental observations. It is found that the grain orientations can be optimized in starter block and the length of starter block could be reduced to about 26.0 mm. A single crystal can be rapidly selected after the solidification front climbing 400° along the spiral passage. It is proposed that the coupling effect of the heat flow direction, the preferred growth direction and the geometrical restriction of spiral wall makes contribution to the crystal selection in spiral passage. An investigation into the grain orientation selection in grain selectors with different geometries reveals that crystal orientation can be optimized by increasing the length of starter block or decreasing its width. However, no obvious relationship is found between the crystal orientation and the parameters of spiral passage.

1. Introduction

Ni-base single-crystal (SX) superalloys are extensively used as blades in aero-engines and industry gas turbines for its excellent high temperature strength and creep resistance [1–5]. The superior mechanical properties of Ni-base superalloys are derived largely from the microstructure and crystal orientation [6–11]. One benefit of SX blades is that the creep life of SX blades can be improved significantly due to the removal of grain boundaries that exist in a polycrystalline morphology, such as equiaxed or columnar [12–17]. Another benefit of SX blades is that the preferred $\langle 001 \rangle$ crystallographic solidification direction, which coincides with the minimum in Young's modulus, is oriented parallel to the casting axis [18,19]. However, a slight deviation of axial orientation from $\langle 001 \rangle$ direction can result in a significant decrease in creep performance [11]. Consequently, it is of great importance to direct the $\langle 001 \rangle$ of the SX as close as possible to the axial orientation during SX casting to improve the creep resistance along the longitudinal direction of a SX blade.

In general, the single crystal structure is produced through competitive grain growth by directional solidification technology [20]. Mostly, the grain boundaries are removed entirely by adding a 'grain selector' to the very base of the wax mould, typically in the form of a spiral grain selector, which consists of a starter block and a spiral selector [21], see Fig. 1.

To improve the production efficiency and yield rate of SX blades, numerous efforts on the grain selection during SX casting have been made over the last few decades by simulations and experiments [22–26]. The simulation analysis taking into account the shape of a two-dimensional (2-D) "pigtail" by Esaka et al. [22] revealed that the evolutions of grain structures and crystal orientations during SX casting significantly depend on the geometries of the starter block (length L and width D, see Fig. 2). The yield rate of well-oriented single crystal increases with increasing the ratio of the length to the width of starter block. However, the increase of starter block length inevitably decreases the height of spiral during the production of turbine blades. Besides, a simplified 2-D model is not sufficient to investigate the grain selection in 3-D spirals.

Recently, Dai et al. [23] simulated and analyzed the competitive growth and grain selection in the selector with emphasis on the geometric parameters of the spiral (spiral angle θ, spiral thickness d_T and spiral rotation diameter D_s, see Fig. 2), using a coupled ProCAST&CAFE model. The results showed that the grain selection in spiral become more efficient with the decreasing of the spiral angle or spiral thickness, or increasing the spiral rotation diameter. However, the grain orientations cannot be optimized during the selection process in the spiral. While the results of Meng et al. [24] showed that the grain orientation could be further optimized

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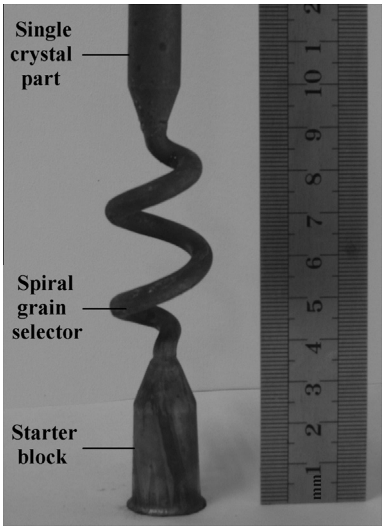

Fig. 1. Photograph of a single crystal sample with a spiral grain selector after macro-etching.

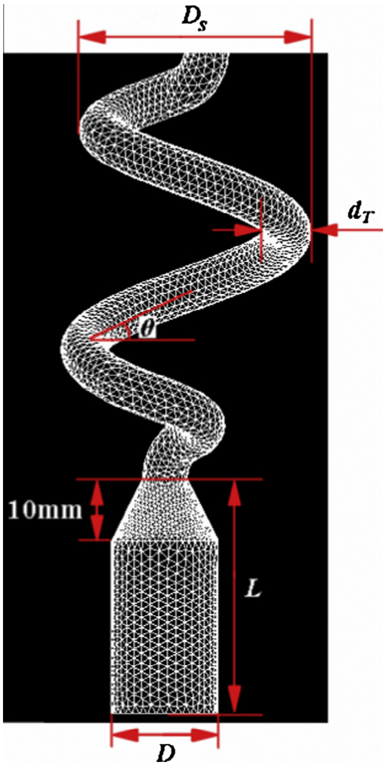

Fig. 2. Schematic diagram of starter block and spiral grain selector showing the parameters used in this study.

Table 1
Parameters of starter block designed in this study.

Group 1									
L/mm	5	10	20	30	35	40	50	60	
D/mm				15					
Group 2									
D/mm	5	10	15	20	25	30	35	40	50
L/mm				35					

Table 2
Parameters of spiral grain selector designed in this study.

Group 1												
θ/°	15	20	25	30	35	40	45	50	55	60	65	70
d_T/mm						5						
D_s/mm						25						
Group 2												
θ/°						30						
d_T/mm	2	3	4	5	6	7	8	9				
D_s/mm						25						
Group 3												
θ/°						30						
d_T /mm						5						
D_s /mm	17	20	23	25	27	31	35	41				

during the competitive growth in the spiral, in the case of that the spiral angle are larger than about 50°. Due to the contradictory conclusions above, it is necessary to get further insight into the relationship between the crystal orientation and the geometries of the spiral grain selector.

Furthermore, to enhance the understanding of grain selection and to provide the capability to design and optimize a spiral grain selector for newly developed alloys and components, it is of interest to investigate the mechanism of grain selection in the spiral passage for the attempt to improve the efficiency and reliability of the grain selector. Dai et al. [25] proposed that the geometrical restriction is a dominant factor in the process of grain selection. Gao et al. [26] observed the competitive dendritic growth in spiral passage by experimental methods and verified that the geometrical blocking of narrow passage attributes to the grain selection. Nevertheless, research on the mechanism of grain selection in the spiral should not be limited to the geometrical restriction. It has been established that the competitive growth during directional solidification depends on the relative orientation of grains and their relation with the direction of maximum temperature gradient (the direction of heat flow) [27]. And that the crystal orientation determines the dendritic growth direction, while the growth direction of cellular crystal almost depends on the heat flow direction [28]. In view of the dominant role that the heat flow plays in the competitive grain growth during directional solidification, it is speculated that the heat flow also makes contribution to the grain selection in the spiral passage. However, little attention has been paid to the influence of heat flow on the competitive growth and grain selection in the spiral passage.

Based on such facts, this article is devoted to investigate the relationship between the crystal orientations and the geometries of the grain selector. In addition, the influence of heat flow will be taken into account when analyzing the mechanism of grain selection in the spiral passage. The SX casting process is simulated by a coupled ProCAST&CAFE model. The geometries of the starter block and the spirals grain selector designed in this study are shown in Tables 1 and 2, respectively.

2. Experimental procedure

The material used in this study was the first generation SX Ni-base superalloy DD403. The chemical composition of DD403 is listed in Table 3. The SX castings were performed using a modified Bridgman directional casting furnace schematically shown in Fig. 3. It consisted of a vacuum-induction melting unit, a thermal retardation unit and a cooling zone. Prior to casting, the ceramic mould was mounted on a water-cooled copper chill plate and the furnace chamber was evacuated to a partial pressure of approximately 10^{-3} bar. Then, the mould was preheated to 1550 °C above the melting point of DD403 alloy by graphite heating elements. After melting of the ingot, the charge was poured into the preheated mould at the pouring temperature of 1460 °C and held for 2 min to stabilize the melt. Finally, the ceramic mould was withdrawn from the furnace at a pre-determined withdrawal velocity of 100 μm/s.