Science Press

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Trans. Nonferrous Met. Soc. China 16(2006) 753−759

Transactions of Nonferrous Metals Society of China

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Structure simulation in unidirectionally solidified turbine blade by dendrite envelope tracking model (Ⅱ): model validation and defects prediction

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Received 9 September 2005; accepted 29 November 2005

Abstract: The developed model was validated by the checking of grain preferential growth orientation and the solidification experiment with low melting point alloy of Sn-21%Bi(mole fraction). It was also applied to predict the structure defects (e.g. stray grain) of unidirectionally solidified turbine blade. The results show that the developed model is reliable and has the following abilities: 1) reduce the misorientation caused by the orthogonal mesh used in simulation; 2) well reproduce the growth competition among the different-preferential-direction grains with less than 10% relative error; 3) predict the structure defect of stray grain with the accuracy over 80%; 4) optimize the grain selector to better obtain a single crystal avoiding the multigrain defect; 5) simulate the structure evolution (nucleation and growth) of the directional and single crystal turbine blade.

Key words: unidirectional solidification; misorientation; stray grain; single crystal; turbine blade

1 Introduction

Commonly, a numerical model should be validated before application. Whether a simulation model for dendritic grain growth is reliable strongly depends on two aspects. 1) The model can effectively describe the anisotropy of grain growth. The misorientation phenomena of grain growth simulation caused by the calculation mesh is not allowed in order to get the reliable structure simulation results. 2) The model can correctly reproduce the competition phenomena during the growth of dendritic grains. The nucleation, growth kinetics, grain impingement should be considered in the numerical model to correctly describe the growth competition of grains. There are several numerical approaches to simulate the grain growth, such as cellular automaton (CA) [1−4], phase field [5−8]. They are working for different levels of grain growth. To capture the solid/liquid interface, the phase field method requires a very fine grid, leading to very high computational cost. Compared with the phase field method, the CA model can run on a much coarser grid, therefore introducing the misorientation of preferential direction by coarse meshwork. A decentered square/octahedron (2D/3D) growth algorithm was implemented in CA model for avoiding this problem. The algorithm is capable of simulating the dendritic grain growth with the <100> preferential directions either aligned or inclined with the grid. However this algorithm introduces more complex calculation for avoiding the misorientation.

One of the major problems encountered during the directional solidification and the single crystal growth is the formation of stray grains. Stray grains are heteroge-

Foundation item: Project(ICAST 11305054) supported by the NEDO of Japan; Project(20052176) supported by the Natural Science Foundation of Liaoning Province, China; Project supported by the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry
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neously nucleated with random orientations and hence may form high angle boundaries (HABs). HABs act as favorable locations for crack initiation, causing in-service failure. Therefore the stray grain is absolutely forbidden in the directional and single crystal turbine blade. The effects of various casting conditions and the remelting of dendrite fragments on the formation of stray grains have been experimentally investigated by prior authors[9−12]. It was found that stray grains grow from undesirable nuclei at specific locations in turbine blades, for example at the platform ends. Additionally, for producing a single crystal turbine blade, the design of grain selector is much more important to ensure a single grain survive finally to form a single crystal turbine blade[13, 14].

2 Model validation

2.1 Misorientation adjust

The misorientation caused by the orthogonal mesh often happens during the structure simulation. It is a key problem to be solved for correct describing the growth of grain especially a columnar grain. Fig.1(a) shows the Neumann neighborhood configuration which is commonly used for numerical simulation work. A grain growth simulation based on this neighborhood will lead to the misorientation problem, that is, the grain strongly tends to grow along the horizontal or vertical or diagonal directions. We rebuild the neighborhood configuration and increase the third neighborhood to make the neighborhood tend to a near circle distribution as shown in Fig.1(b).

After a cell has been solidified, a little fraction of envelope occupation (seeds) will be distributed from the current cell to its neighborhood. In order to reduce the misorientation problem, the little fraction to each neighboring cell is not the same, which depends on the angle between the envelope vector and the connecting line of current cell and its neighboring cell, as shown in Fig.2. The bigger the angle, the smaller the fraction of envelope is distributed.

In 3D case, the calculation will be heavy if the neighborhood configuration is set like Fig.1(b). Therefore, a dynamic selecting neighbor cells method according to the normal direction of interface is proposed as shown in Fig.3. Firstly, three reference surfaces and the corresponding neighbor cells configurations are predefined. Then the calculating dendrite envelope interface is compared with the reference surfaces according to the normal direction. Subsequently the corresponding neighboring cells are selected.

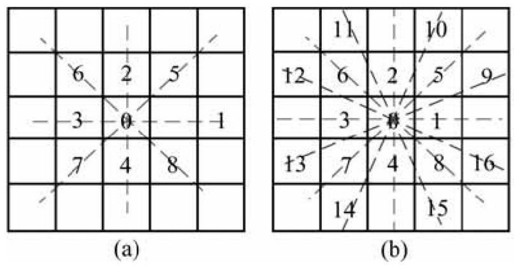

Fig.1 Neighborhood configuration: (a) Neumann type; (b) New type

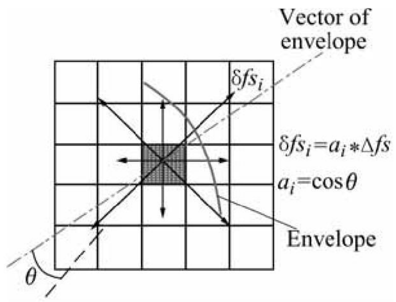

Fig.2 Distribution rule of little dendrite fraction (seeds)

Fig.4 shows three grains with 0˚, 45˚, and 22˚ preferential growth directions respectively. Two cases with/without adjusting misorientation are considered. It is seen that there is no misorientation for the 0˚and 45˚ preferential growth grains in both cases, whereas misorientation occurs for the 22˚ preferential growth grain in case of no misorientation adjusting (see Fig.4(a)).

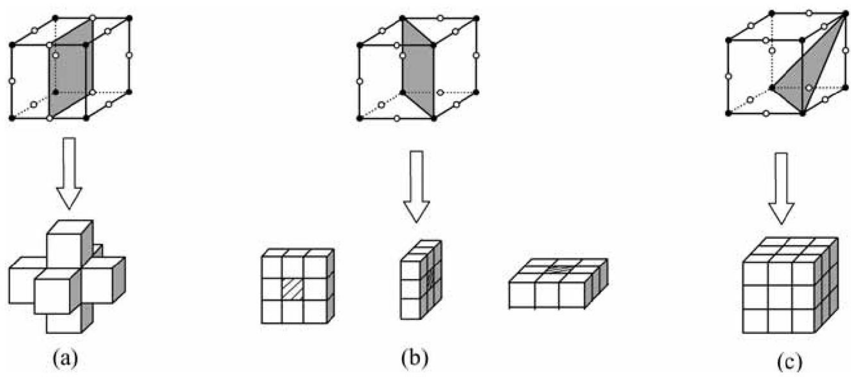

Fig.3 Schematic diagram of dynamic selecting neighbor cells: (a) Orthogonal surface; (b) Diagonal surface; (c) Inclined surface

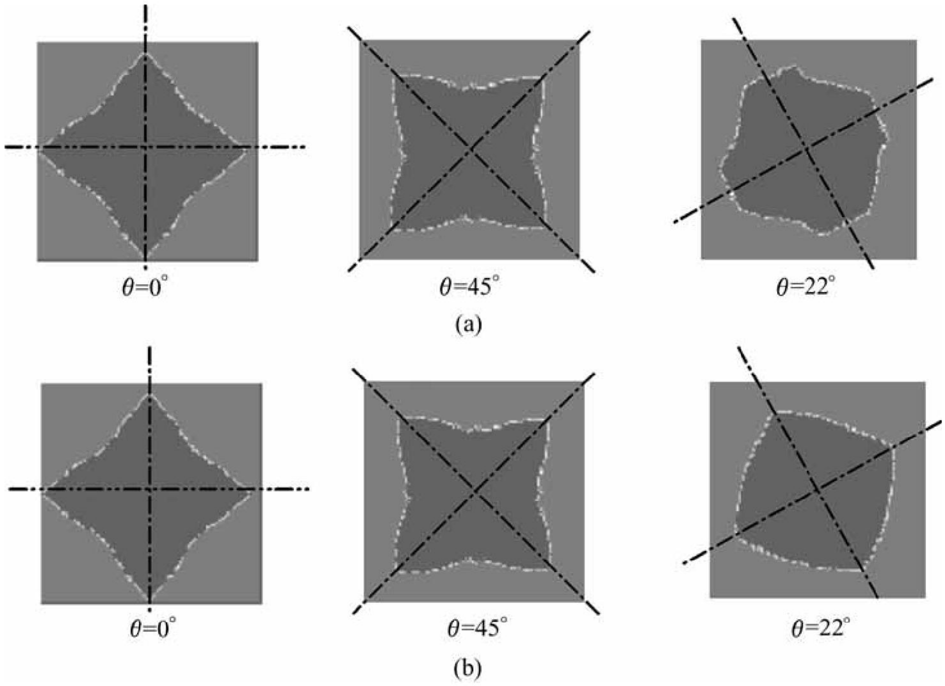

Fig.4 Misorientation test results: (a) Without adjusting misorientation; (b) With adjusting misorientation

By applying the misorientation adjusting algorithm above, the misorientation can be reduced to some extent (see Fig.4(b)).

Fig.5 shows a 3D view prediction of a single dendritic grain growing in a uniform temperature field by using the present grain growth algorithm. It is noted that the simulated grain shape coincides with the <100> directions well but not be misoriented by the axes of the calculation grid.

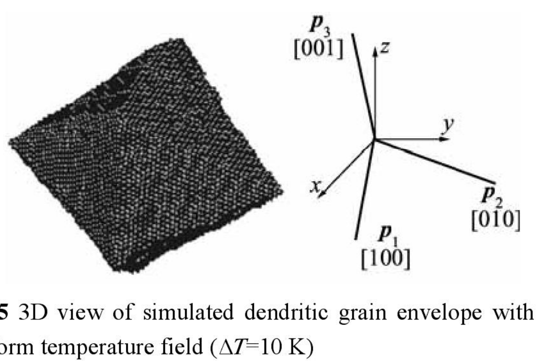

Fig.5 3D view of simulated dendritic grain envelope with an uniform temperature field (ΔT=10 K)

A unidirectionally solidified super alloy IN738LC (nickel base) turbine blade was calculated by using the dendrite envelope tracking model with the misorientation adjusting algorithm. Reasonable simulated results are obtained as shown in Fig.6.

2.2 Competition of grains growth

In order to further verify the developed model, a unidirectional grain growth experiment of Sn-21%Bi (mole fraction) alloy is implemented by using the X-ray imaging technique [15]. The evolution of grain growth, competition and impingement can be directly observed through a transparency mold as shown in Fig.7(a). The corresponding simulated results are shown in Fig.7(b). Good agreement can be concluded between them. By a quantitative analysis, the relative error of grain growth orientation between case (a) and case (b) is below 10%. The columnar grains whose preferential direction is closely parallel to the temperature gradient grow faster than those inclined to the temperature gradient. The faster growing grains hinder the growth of other grains hence win the competition of growth. It is obviously seen that four columnar grains survive after the growth com-

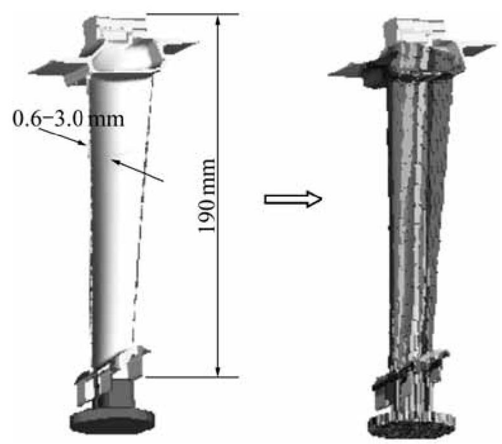

Fig.6 Turbine blade geometry shape and simulated solidification structure

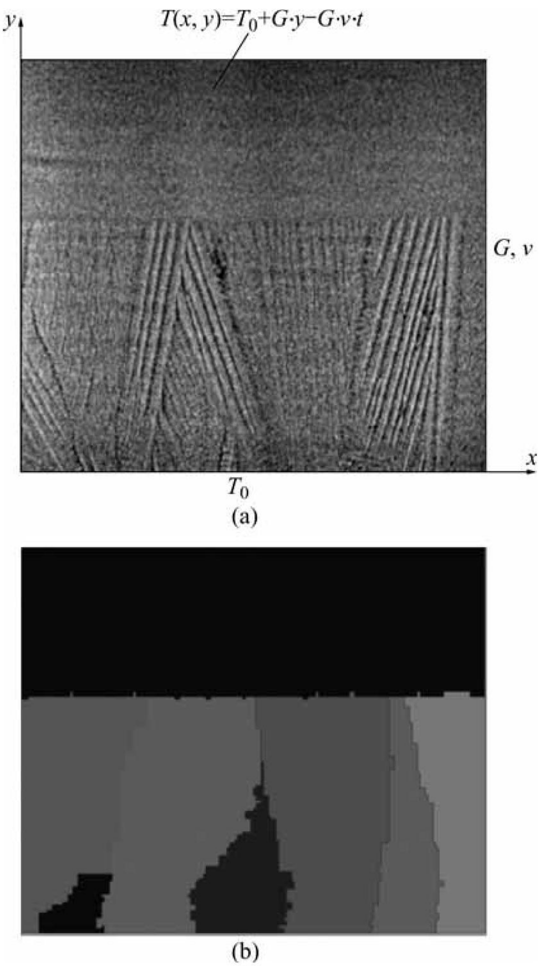

Fig.7 Comparison of experimental and simulated results: (a) Experimental results (Sn-21%Bi, mole fraction) (obtained by X-ray imaging technique); (b) Simulated results by dendrite envelope tracking model (G=3 ℃/mm, v=20 mm/h)

competition from both of Figs.7(a) and (b).

3 Prediction of structure defects

3.1 Stray grain

Stray grain is defined as a misorientated equiaxed grain nucleating in the front or interior of unidirectional solidification structures. The stray grain is a kind of defect which often occurs in a unidirectional solidification process and seriously reduces the production properties. Fig.8 shows a simple casting used in the experiment of MHI (Mitsubishi Heavy Industry). Fig.9 shows the corresponding experimental results obtained by MHI [16]. The stray grains are found in the surface of convex parts (2 stray grains in part Ⅲ and 5 in part Ⅱ) from their experiments. The simulated results by the present model are shown in Fig.10 and Fig.11. Similarly the stray grains are found in the vertex parts (3 stray grains in part Ⅲ and 6 in part Ⅱ). It is because that the high local under-cooling occurs in the vertex parts during the solidification. Please note that there are a lot of grains in part Ⅰ of Fig.10 which are called grain seeds formed by the grain generator. However Fig.9 only shows the stray grains but not all the grains. This is the reason why we don't see the grains in the part Ⅰ of Fig.9.

Another experiment of investment casting is implemented by IHI (Ishikawa Heavy Industry). Fig.12

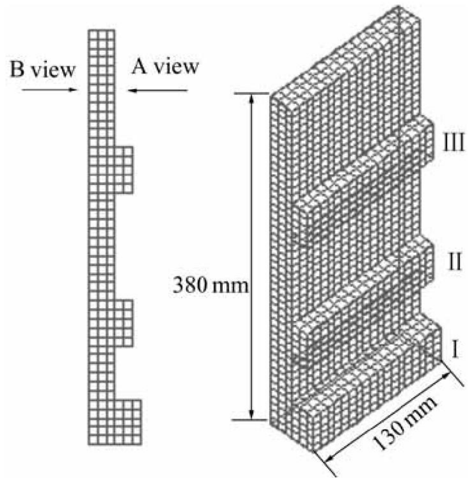

Fig.8 Geometry of sample casting

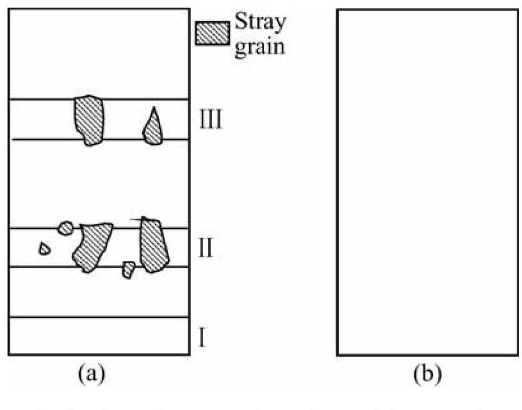

Fig.9 Distribution of stray grains observed by experiments of MHI withdrawal rate of 100 mm/h: (a) A view; (b) B view

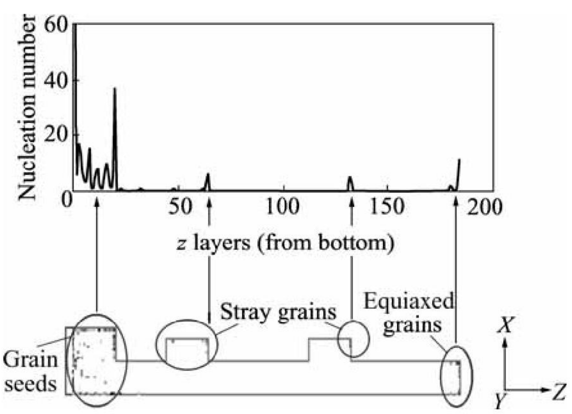

Fig.10 Curve of nucleation number and map of nucleation sites

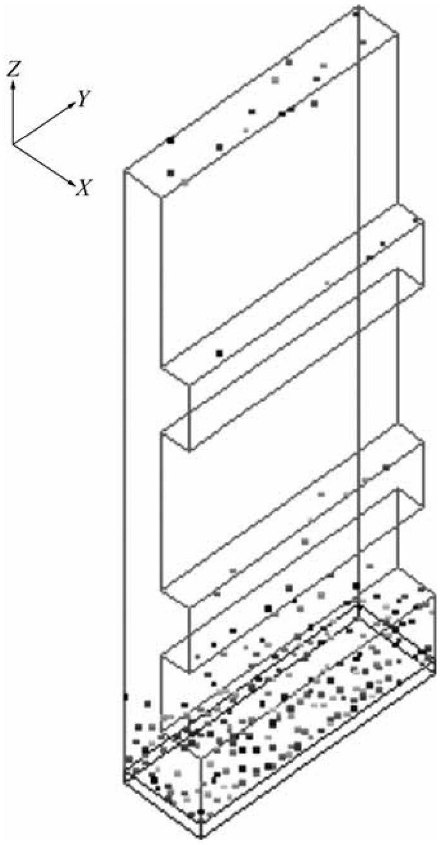

Fig.11 3D map of nucleation sites

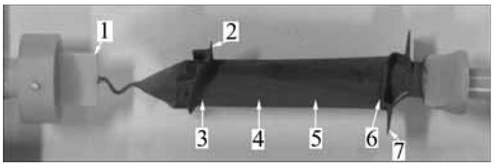

Fig.12 Turbine blade wax model and thermal couple positions from 1 to 7

shows a turbine blade wax model and the locations of thermal couples. The cooling curves of the experiment and the simulation are respectively shown in Figs.13(a) and (b). It is noted that Figs.13(a) and (b) are somehow compatible whereas relative large errors are also found by checking them in detail. The errors might be from: 1) simulation error of dendrite envelope tracking model; 2) measurement error of thermocouples; 3) the thermocouple positions used in simulation are not completely the same with the ones used in measurement. Since the temperature gradient is very high during the unidirectional solidification, a small error of position can cause a big error of temperature. Due to the difficulties and complexities of measurement, the measurement results of thermal couples 3, 5, 7 are interrupted.

Fig.14 shows the comparison of grain structure between the experiment and the simulation. Table 1 gives the checking list of comparison. Good agreement is found in case of 50 mm/h and 600 mm/h withdrawal rates. In case of 300 mm/h, stray grains appear in the turbine part of the experiment, whereas in the blade part of simulation. Totally, the prediction accuracy is over 80%. The reason for the prediction error is possibly that the flow calculation is not directly calculated but only done by an effective partition coefficient in the structure prediction solver. Table 2 shows the mesh information and calculation efficiency in case of the calculation for Fig.14.

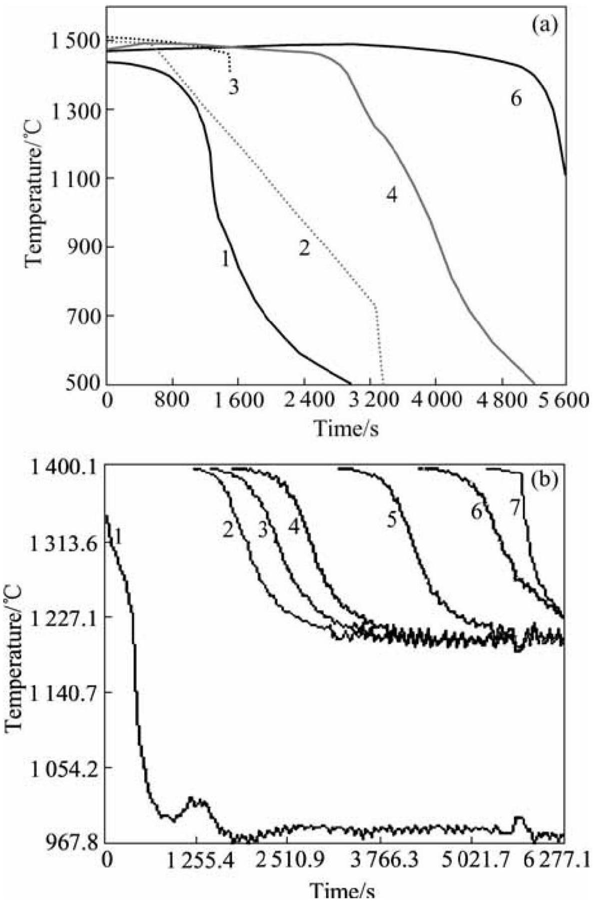

Fig.13 Temperature change of single crystal turbine blade during unidirectional solidification (pouring temperature: 1 520 ℃; mold preheating temperature: 1 520 ℃; withdrawal rate: 150 mm/h): (a) Measurement; (b) Simulation

Table 1 Checking list of comparison of turbine blade structure defects between experiment and simulation

Withdrawal rate/(mm·h^{-1})	Shoulder part	Blade part	Turbine part
50	Agreement	Agreement	Agreement
300	Agreement	Non-agreement	Non-agreement
600	Agreement	Agreement	Agreement

3.2 Grain selector (pig tail)

For producing a single crystal turbine blade, the design of grain selector is very important. Fig.15 shows two different type selectors used in the test experiments

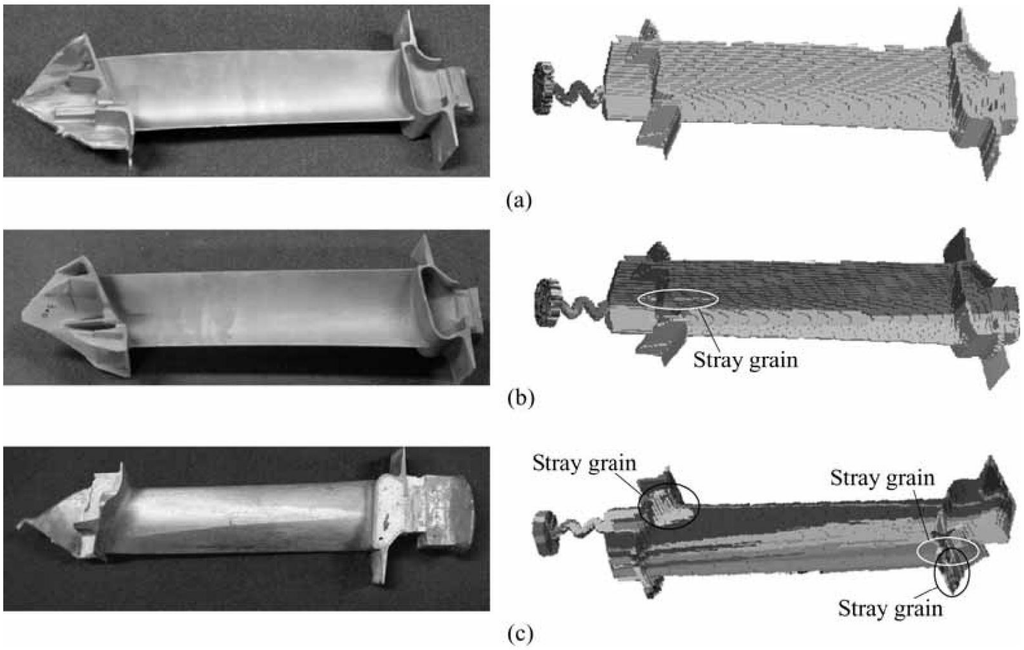

Fig.14 Comparison of grain structures between experimental results and simulated results: (a) 50 mm/h; (b) 300 mm/h; (c) 600 mm/h

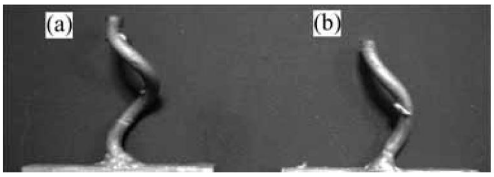

Fig.15 Two type selectors used in IHI experiment: (a) Type 1 (succeeded); (b) Type 2 (failed)

Table 2 Mesh information and calculation efficiency

Macro element size/mm	Total elements	Casting elements
1×1×1	1 026 000	38 553
Micro cell size/μm	Micro cells	CPU time/h
250×250×250	2 545 068	4
Memory	Computer profile	
120 M	CPU: P-IV 2.4 G; Memory: 1 G	

of IHI. The IHI experimental results are: it is successful to get a single crystal turbine blade with the type 1 selector selector but failed with the type 2 selector. The corresponding simulation work is implemented by using the present model. Fig.16 shows the geometry model used in the simulation. The simulated grain structures are shown in Fig.17. A single crystal with type 1 selector and a columnar structure with type 2 selector are obtained, showing good agreement with the experimental results. It is noted that a lot of grains generate in the bottom chill plate and then pass through the grain selectors. Only one grain finally survives after type 1 selector (see Fig.17(a)) forming a single crystal turbine blade, and several grains survives after type 2 selector (see Fig.17(b)) forming a

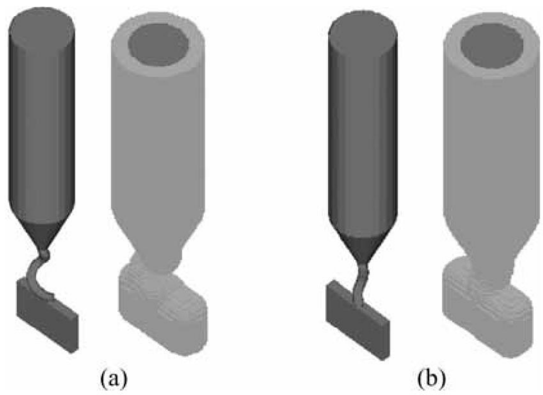

Fig.16 Geometry models used in simulation: (a) Type 1 selector (simple); (b) Type 2 selector (complex)

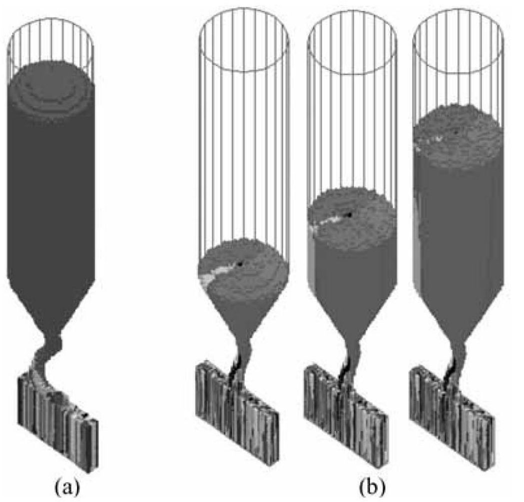

Fig.17 Simulated grain structures with two type selectors: (a) Type 1 selector (f_s =0.8); (b) Type 2 selector (f_s=0.3, 0.6, 0.8)

columnar structure turbine blade. The helix of type 1 selector is higher and more curved as compared with that of type 2 selector. This means type 1 selector has stronger ability for selecting the grains. It ensures that only one grain can pass through the selection to be a unique grain seed for forming the single crystal turbine blade.

4 Conclusions

The dendrite envelope tracking model was validated in this work. The developed model can correctly reproduce the growth competition of different-preferential-direction grains. The relative error of simulated grain orientation is less than 10% as compared with the experimental results. The developed model was applied to predict the solidification structure of unidirectionally solidified turbine blade and structure defects. The prediction accuracy of stray grain defect is over 80%. The developed model is also very helpful to optimize the design of grain selector for producing the single crystal turbine blade. It is owing to the numerical model having the ability to reproduce the grain selection effectively. In a summary, the dendrite envelope tracking model is a promising and reliable structure-simulation-tool.

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(Edited by LI Xiang-qun)