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Structure simulation in unidirectionally solidified turbine blade by dendrite envelope tracking model(I): numerical modeling

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Abstract: A 3D dendrite envelope tracking model was developed for estimating the solidification structure of unidirectionally solidified turbine blade. The normal vector of dendrite envelope was estimated by the gradient of dendrite volume fraction, and growth velocity of the dendrite envelope (dendrite tips) was calculated with considering the anisotropy of grain growth. The solute redistribution at dendrite envelope was calculated by introducing an effective solute partition coefficient(k_e). Simulation results show that the solute-build-up due to the rejection at envelope affects grain competition and consequently the solidification structure. The lower value of k_e leads to more waved dendrite growth front and higher solute rejection. The model was applied to predict the structure of turbine-blade-shape samples showing good ability to reproduce the columnar and single grain structures.

Key words: turbine blade; dendrite envelope tracking model; structure simulation; unidirectional solidification

1 Introduction

Unidirectional solidification technology is used to get special properties of casting, for example, to get the turbine blades with columnar or single crystal structures. Several modelling approaches have been carried out for the structure defects prediction and process optimization during unidirectional solidification. They can be classified into two categories: one is analytical approach, which predicts grain defects based on the process parameters, mainly the thermal gradient, G, and the velocity of the isotherms, v. The curves or windows in G—v diagrams show the limits between reliable and inappropriate casting conditions[1]. The other one is numerical approach, which predicts structures based on the grain nucleation-growth simulation, for example, GANDIN and RAPPAZ et al[2−5] have done much work to predict the unidirectional solidification structure by using cellular automaton-finite element (CAFE) method and have obtained some reasonable results. LI et al[6] applied CA model to simulate the equiaxed grains of turbine blade. WANG et al[7,8] developed a cellular automaton-monte carlo(CAMC) coupling model to simulate the dendritic grain growth. The CAMC model has both advantages of probabilistic and deterministic models. XU and LIU et al[9] developed the dendritic grain growth model based on the dendrite shape function. The models above were applied in the scale of grain and have no comprehensive consideration of the effect of solutal field on the grain growth. Several other models are used for simulating the dendrite morphology. NASTAC[10] developed a liquid/solid interface tracking model to simulate the evolution of unidirectional solidification structure. ZHU and HONG et al[11] developed a Modified Cellular Automaton model for simulating the dendritic growth. LI et al[12,13] simulated the dendrites of directional solidification by using phase field model.

In the present study, the solutal field is implicitly involved for the estimation of the dendrite growth rate, while thermal field is explicitly calculated. However, solute-build-up in liquid phase occurs and can affect grain competition and nucleation ahead of the growing

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dendrites under some solidification conditions. For example, solute can transfer from the mushy zone by diffusion or convection in unidirectional solidification with rather low growth rate. Therefore, it is valuable to discuss the effect of solute reject from the mushy zone on the solidification structure. This paper firstly presents a tracking model of the dendrite envelope and the solute redistribution calculation at the dendrite envelope. Then the model is applied to simulate the solidification structure of the turbine-blade-shape castings. The effect of the solute rejection at the envelope on solidification structure is discussed finally.

2 Model description

As shown in Fig.1, the calculation domain is enmeshed with micro cells, of which geometry is square(2D) or cubic (3D). The cells are classified as three groups in terms of dendrite envelope position. One is 'liquid cell'that contains only the liquid phase. Another is 'envelope cell'that contains the dendrite envelope interface. The other is 'solidifying cell' in which the dendrite envelope interface has already passed. Therefore, the 'solidifying cell' is partially or completely solidified. The envelope interfaces in each 'envelope cell' are tracked at each time step by calculating the interface parameters: the normal vector $\boldsymbol{n}$, the normal velocity $\boldsymbol{v}_n$, and the interface area s. The angle α, between the preferential growth direction $\boldsymbol{p}$, and the interface normal direction $\boldsymbol{n}$, is introduced in the present method for considering the growth anisotropy of dendrite. The state of cell is changed from 'liquid' to 'envelope' and 'solidifying' with the proceeding of grain nucleation and growth.

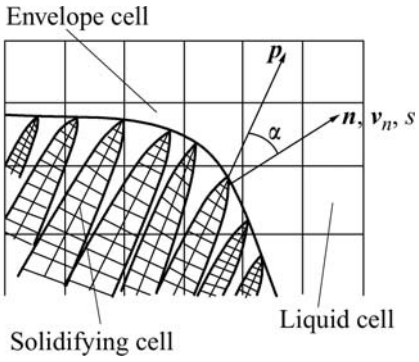

Fig.1 Schematic diagram of dendrite envelope tracking method

3 Solute calculation and nucleation simulation

The governing discrete equation for the solute diffusion in liquid is derived with the direct finite difference method(DFDM)[14] and expressed as

$$V \cdot (c_i^{t+\Delta t} - c_i^t) = D_1 \cdot S_{ij} \cdot \Delta t \sum_j \left(\frac{c_j^t - c_i^t}{a}\right) \quad (1)$$

where v is cell volume, c is solute concentration, D_1 is solute diffusion coefficient in the liquid phase, S is surface area, Δt is time step, a is cell size, the subscripts i, j denote the current cell and its neighbor cell, respectively.

The solute redistribution at the dendrite envelope is done by introducing an effective solute partition coefficient, k_e. It is defined as

$$k_e = \frac{\bar{c}_{\text{env-in}}}{\bar{c}_{\text{env-out}}} \quad (2)$$

where $\bar{c}_{\text{env-in}}$ and $\bar{c}_{\text{env-out}}$ are the average concentration inside and outside of the dendrite envelope, respectively. It should be pointed out that the effective solute partition coefficient is neither the equilibrium partition coefficient nor the effective partition coefficient at the solid/liquid interface.

When the dendrite volume fraction (volume occupying ratio) in an 'envelope cell' is increased by Δf_e due to the grain nucleation and growth, the amount of solute rejected from the 'envelope cell', Δc_r, is given by

$$\Delta c_r = V \cdot \Delta f_e \cdot (1 - k_e) \cdot \bar{c}_{\text{env-out}} \quad (3)$$

This rejected solute is distributed to the neighboring liquid cells of the "envelope cell" uniformly.

Definition of the undercooling for the grain growth and the nucleation should be noted, since solutal field is involved in this model. The undercooling is defined as temperature deviation from the liquidus temperature with respect to the solute concentration at the interface. Therefore, the undercooling, ΔT is calculated by

$$\Delta T = T_1 + m(c_1 - c_0) - T \quad (4)$$

where c_0 is initial concentration of the alloy, T_1 is the liquidus temperature at the initial concentration, m is the liquidus slope, and c_l is the liquid concentration.

Heterogeneous nucleation was calculated by using the instantaneous model proposed by RAPPAZ et al[15]. The nuclei density at a given undercooling was calculated with the integral of Gaussian distribution. Two sets of Gaussian distribution parameters were separately used for the mold wall and melt bulk to characterize their different nucleation ability. Once a cell nucleates, a random integer that represents the crystallographic orientation is given to the cell. The state of the nucleated cell is changed from 'liquid' to 'envelope'.

4 Dendrite envelope tracking algorithm

As shown in Fig.1, the normal vector $\boldsymbol{n}(n_x, n_y, n_z)$ is

calculated with the dendrite volume fraction gradient[16]

$$n_x = -\frac{\partial f_e}{\partial x}, n_y = -\frac{\partial f_e}{\partial y}, n_z = -\frac{\partial f_e}{\partial z} \quad (5)$$

As shown in Fig.2, the six preferential <100> growth directions of each orientation are described with the three vectors $\boldsymbol{p}_1$, $\boldsymbol{p}_2$, $\boldsymbol{p}_3$, which are generated with three Euler angles, θ, ψ, ϕ. We calculate angles between the normal direction and preferential directions by

$$\cos(\alpha_1) = \left|\frac{\boldsymbol{n}\cdot\boldsymbol{p}_1}{|\boldsymbol{n}|\cdot|\boldsymbol{p}_1|}\right|,\ \cos(\alpha_2) = \frac{\boldsymbol{n}\cdot\boldsymbol{p}_2}{|\boldsymbol{n}|\cdot|\boldsymbol{p}_2|},$$

$$\cos(\alpha_3) = \frac{\boldsymbol{n}\cdot\boldsymbol{p}_3}{|\boldsymbol{n}|\cdot|\boldsymbol{p}_3|} \quad (6)$$

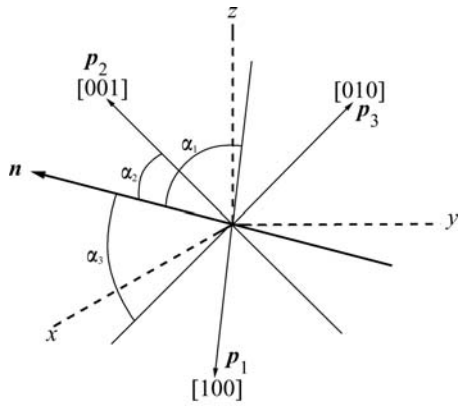

Fig.2 Angles between preferential and normal directions

Then the minimum angle among α_1, α_2, α_3, is selected, namely

$$\alpha = \min(\alpha_1, \alpha_2, \alpha_3) \quad (7)$$

An approximation method is used to calculate the interface area. Three reference surfaces for a cubic cell are defined as shown in Fig.3. The interface inside the 'envelope cell' is taken as paralleling to one of the reference surfaces approximately.

Growth rate of the dendrite envelope in the preferential orientation, $v_{tip}(\Delta T)$, is calculated with the fitted polynomial approximation based on the Kurz, Giovanola and Trivedi(KGT) growth kinetics model[17, 18]

$$v_{tip}(\Delta T) = a_2\Delta T^2 + a_3\Delta T^3 \quad (8)$$

where α_1 and α_2 are growth parameters that can be obtained from the fitted polynomial function or experiments.

The increment of dendrite volume fraction is calculated by

$$\Delta f_e = \frac{S\cdot v_{tip}(\Delta T)\cdot\Delta t}{a^3} f(\alpha) \quad (9)$$

where $f(\alpha)$ is the anisotropy factor to characterize the preferential growth of dendrite, which is a function of α, in this study, $f(\alpha)=\cos\alpha$. The different characters can be obtained by adjusting the expression of $f(\alpha)$[16].

When an "envelope cell" is occupied by the dendrite envelope completely, the dendrite volume fraction of 10^{-4} is distributed to its neighboring liquid cells as propagation "seeds", and the orientation of the "envelope cell" is also assigned to these cells. The "envelope cell" is changed to "solidifying cell", and each neighbor liquid cell is changed to "envelope cell".

However the strong anisotropy introduced by the initial cell arrangement leads to a grain shape always aligned with the axes of the grid but not the real preferential directions. It is a serious problem leading to a poor accuracy of structure simulation. A dynamic selecting neighbor cells method according to the normal direction of interface is proposed to eliminate the artificial anisotropy.

5 Results and discussion

Fig.4 shows 2D calculation with solute rejection at the dendrite envelope for the super alloy IN738LC (nickel-base) whose thermal properties and nucleation parameters are respectively shown in Tables 1 and 2. In the case of k_e=0.99, grains tends to grow parallel each

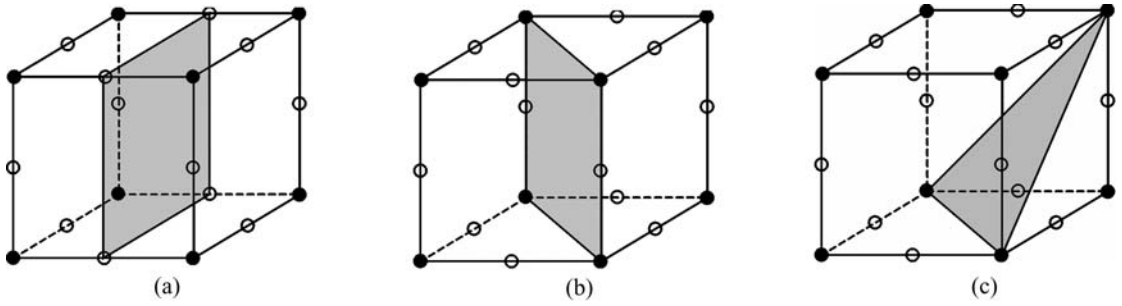

Fig.3 Three reference surfaces: (a) Orthogonal surface; (b) Diagonal surface; (c) Inclined surface

Table 1 Thermal properties for IN738LC super alloy[4]

Property	Value
Density	8 110 kg/m^3
Thermal conductivity	19.8 W/(m·℃)
Specific heat	558.3 J/(kg·℃)
Solidus temperature	1 212 ℃
Liquidus temperature	1 332 ℃
Latent heat	234 kJ/kg

other in the growth direction. The calculated results do not significantly differ from the results without consideration of the solute rejection (i.e. k_e= 1.0). On the other hand, the dendrite envelope becomes wavy due to the high solute rejection at the envelope in the case of k_e= 0.95. As a result, some grains with the favorite growth orientation tend to compete with other grains in the upper part. The calculated results indicate that the consideration of the solutal field is important in case the solute rejection from the mushy zone to the dendrite envelope cannot be negligible. In practice, it is still uncertainty to estimate of the effective partition coefficient, since the coefficient should depend on not only the physical properties but also solidification conditions such as convection, cooling rate and temperature gradient.

Fig.5 shows a turbine-blade-shape model with the emulating unidirectional cooling condition: a water-cooled chill is put under the bottom of the starter, the temperature of hot zone is 1 400 ℃ and the cool zone one is 100 ℃, the withdrawal rate is 50 mm/h, and the pouring temperature is 1 350 ℃. The alloy of casting is super alloy IN738LC. The calculation cell size is 500

Table 2 Nucleation and growth kinetics parameters used for grain structure simulation[4]

Item	ΔT_m/℃	ΔT_σ/℃	n_{max}	Growth parameter, α_2	Growth parameter, α_3
Surface nucleation	0.5	0.3	$1.0\times10^6\cdot m^{-2}$	6.577×10^{-7} m·s^{-10}·℃$^{-2}$	
Bulk nucleation	6.7	1.5	$2.5\times10^8\cdot m^{-3}$		7.842×10^{-7} m·s^{-10}·℃$^{-3}$

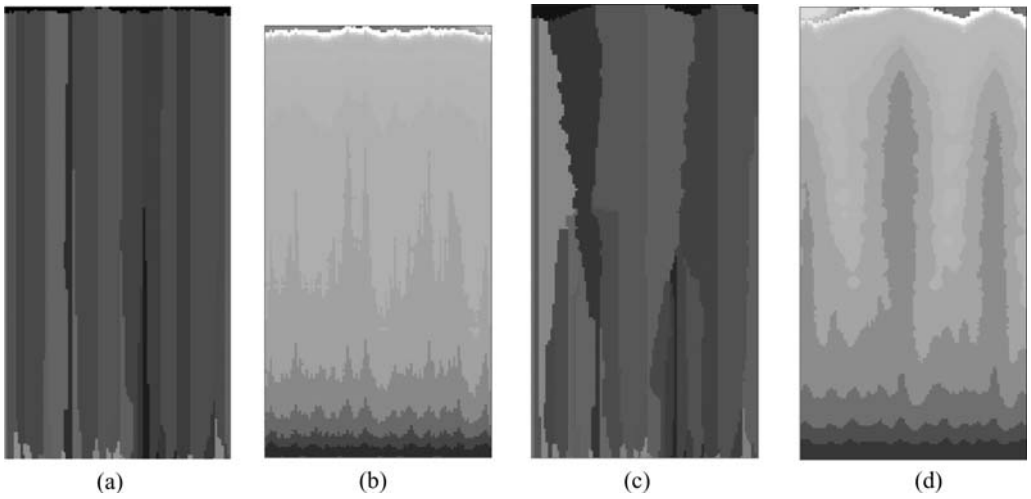

Fig.4 Predicted structure and concentration field during unidirectional solidification of IN738LC: (a) Structure, k_e=0.99; (b) Concentration, k_e=0.99; (c) Structure, k_e=0.95; (d) Concentration, k_e=0.95

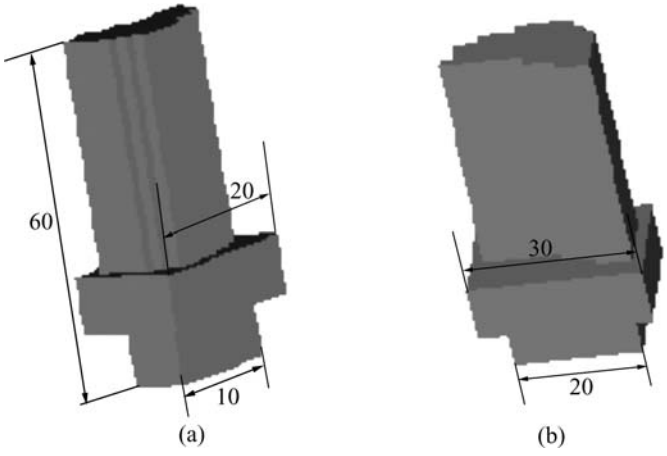

Fig.5 Turbine-blade-shape model(mm): (a) Front view; (b) Back view

μm. It should be mentioned that only the bottom surface contacting with the chill is taken as the "surface nucleation", and the other parts including the external surfaces are taken as "bulk nucleation". The simulated structure results for various solid fractions are shown in Fig.6 and those with different cross sections are shown in Fig.7. Several stray grains are found at the platform, and a few at the body of blade. The discontinuity of long columnar structure can be found at the blade part due to the competition of grain growth. The grains number decreases and the grains transverse size increases with increasing distance from the bottom surface, which is also due to the competitive grain growth. The results show that the present grain growth algorithm can reproduce the competitive growth of grains well.

Fig.8 shows a turbine-blade-shape model with a simple grain selector and water-cooled disk-chill for the same alloy. The calculation cell size is 500 μm. The simulated results with different solid fractions are shown in Fig.9 and those at various transverse sections are shown in Fig.10. It can be seen that many grains form in the bottom of the starter. The grain number decreases, and the grain size increases from section *A* to section *B* of the starter. Some of them start to enter the helix selector (pigtail). It can be noted that the grains number is reduced greatly from section *C* to *D*, *E* by the selector due to the grain selection mechanism. At last, two grains survive and pass through the pigtail. Of course, it will be

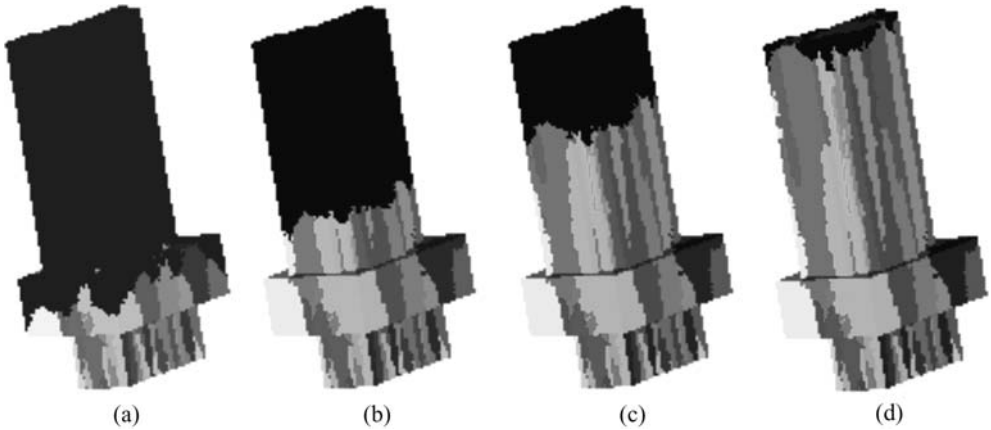

Fig.6 Simulated columnar structure of model in Fig.5: (a) f_s=0.2; (b) f_s=0.4; (c) f_s=0.6; (d) f_s=0.99

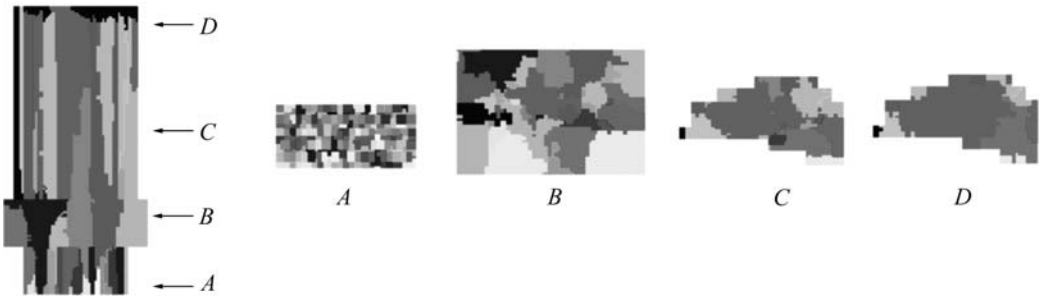

Fig.7 Simulated grain structure in different cross sections

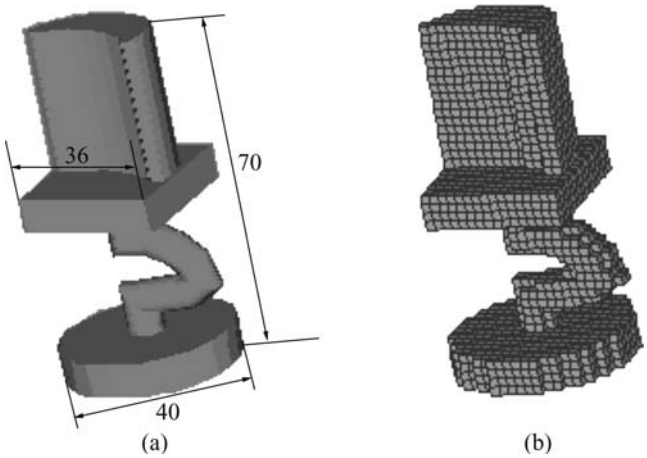

Fig.8 Turbine-blade-shape model with simple pit-tail(mm): (a) STL model; (b) Enmeshed model

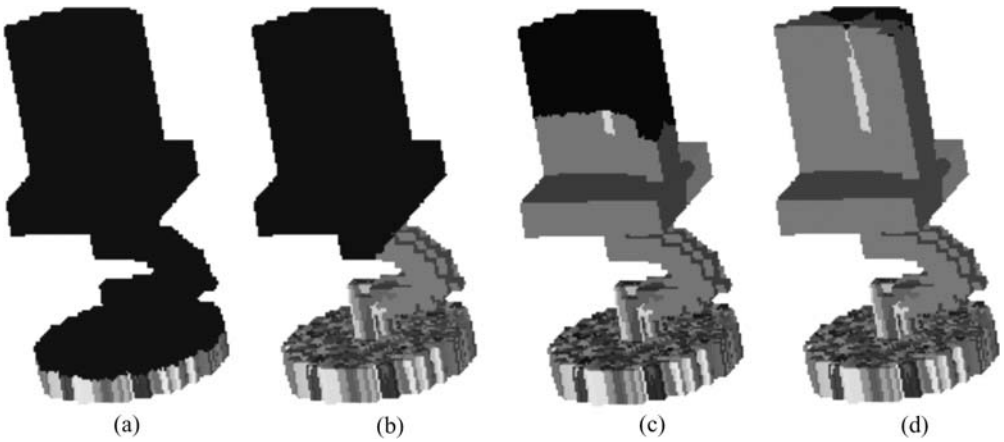

Fig.9 Simulated structure of model in Fig.8: (a) f_s=0.1; (b) f_s=0.2; (c) f_s=0.6; (d) f_s=0.99

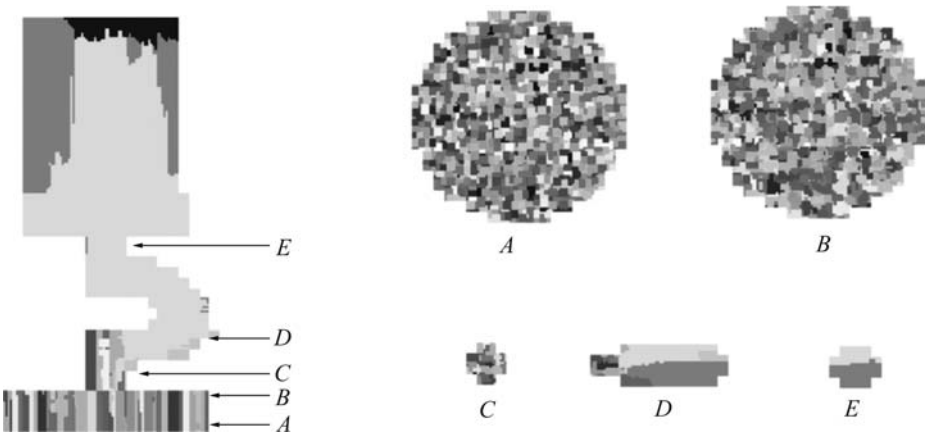

Fig.10 Simulated grain structure in different cross sections

a large defect if the case happens in practice. The interesting thing is, a sliver defect is found in the body of the blade. It is because that one survived grain grows into another one.

6 Conclusions

1) The solute reject at the dendrite envelope is introduced in the solidification structure prediction. Grain growth is significantly affected by the solute rejection when the solute rejection from the mushy region is not negligible. Even in practical cases, solute rejection is recognized when the growth rate is rather small or convection in the mushy region occurs. Therefore, development of the estimation of the effective partition coefficient at dendrite envelope leads to better prediction of the grain structure and defect.

2) The calculated results demonstrate the grain competition and selection in 3D configuration and reproduce the evolutions of columnar structure and single crystal.

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