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STRUCTURE, PHASE TRANSFORMATIONS, AND DIFFUSION

Simulation of Competitive Grain Growth upon the Directional Solidification of a Ni-Base Superalloy

A. N. Pozdniakov[a], V. P. Monastyrskiy[a], M. Yu. Ershov[a], and A. V. Monastyrskiy[b]

[a] *Moscow State University of Mechanical Engineering MAMI, ul. Semenovskaya 38, Moscow, 107023 Russia*

[b] *ZAO CSoft, ul. Molodogvardeiskaya 46, korp 2, Moscow, 121351 Russia*

e-mail: tzp@mami.ru; Http://www.csofi.ru

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Abstract—Using the numerical simulation in the CA-FE module of the ProCAST simulation program, a systematic investigation of competitive growth of grains in a thin plate has been performed over a wide range of values of the temperature gradient and solidification rate. It has been established that the result of the simulation in the case of converging grains depends on the only parameter, i.e., the ratio of the value of the overgrowth of the grain with the preferred orientation to the size of the cell of the computational grid. Thus, the size of the cell is an important adjusting parameter of the model and must be coordinated with the parameters of the dendritic structure under given growth conditions. The grain with the preferred orientation always displaces neighboring diverging grains. The converging grains are eliminated if their deviation from the vector of the temperature gradient exceeds 20°. At the smaller angles of deviation, the result of the competitive growth depends on the size of the computational cell and varies from their joint growth (at the cell size of 5 μm) to the displacement of grains with the preferred orientation (at the cell size of 20 μm). However, all of the results of the simulation agree with the experimental data available in the literature. For the efficient selection of grains with the preferred orientation, regimes with a low temperature gradient and high growth rate are favorable.

Keywords: nickel-base superalloys, competitive growth, simulation, method of cellular automation

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INTRODUCTION

When using the unseeded growth technology, at the initial stage of obtaining single-crystal casting, competitive growth in many nucleated grains occurs, which leads to the selection of one grain with a preferred crystallographic orientation.

It is known that, for the growth of a dendrite, which forms a grain, the supercooling of the melt is necessary, which is defined as the difference between the temperature of the equilibrium liquidus of the alloy and the temperature near the tip of the primary axis of the dendrite. It is also known that it is the grains with a crystallographic orientation [001], which exhibits a minimum deviation from the vector of the temperature gradient, that have an advantage in the competitive growth. According to the model proposed by Walton and Chalmers [1], the growth of a grain with a preferred crystallographic orientation requires the smallest supercooling of the melt. Therefore, this grain overgrows grains with other crystallographic orientations and gradually displaces them.

The model [1] was experimentally confirmed on bicrystal castings of nickel-based superalloys in the case of the growth of two diverging grains, one of which has orientation [001] [2–5]. The work [3] confirms the basic thesis of the Walton–Chalmers model that the grains with the orientation [001] overgrow other grains. It has been experimentally shown that grains with the crystallographic orientation [001] overgrow both the diverging and converging grains. At the same time, experimental data are known that indicate the absence of suppression by the grain with the orientation [001] of the grains that are converging with it [4, 5], or the displacement of the grain with the orientation [001] by grains that are converging with it [2, 3], which contradicts the model of Walton and Chalmers. In [6], it was assumed that the results that contradict the geometric model of Walton and Chalmers can be explained by the interaction of diffusion fields of the competing dendrites, which leads to the suppression of the growth of the secondary branches.

According to the model [1], the value of the lag of growth of the tip of a dendrite must depend on the solidification conditions, i.e., on the local values of the temperature gradient G and of the solidification rate W. In experimental studies, the researchers usually deal with technological parameters of the processes, with the withdrawal rate and an estimated value of the temperature gradient for a given directional casting furnace, which can substantially differ from the real conditions of the solidification in a given section of a casting [7]. Since the methods of estimating the tem-

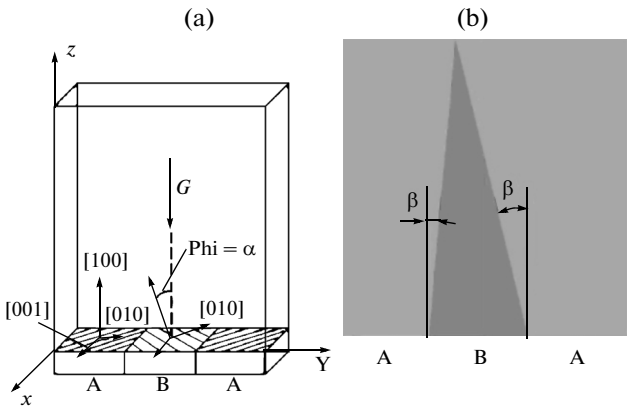

Fig. 1. (a) Scheme of the experiment and (b) a typical macrostructure of the casting obtained in a computational experiment.

perature gradient in different works can differ, this impedes the comparison of experimental data.

In connection with the complexity of determining the local conditions of solidification in experiments, to investigate the competitive growth, a computational experiment can be carried out with the use of a cellular-automation–finite-element (CAFÉ) module of the ProCAST simulation program [8]. In [9–11], the adequacy of the program module and of the CAFÉ model have been confirmed experimentally, and studies of a competitive grain-growth in spiral crystal selectors of different sizes have been carried out during directional solidification of nickel superalloys.

In this work, we used the method of numerical simulation in the CAFÉ module of the ProCAST software to carry out a systematic study of the influence of the solidification conditions on the competitive grain growth in a casting of the GS26 superalloy in the form of a plate over a wide range of values of the temperature gradients and solidification rates.

EXPERIMENTAL

To simulate grain growth, we used the CAFÉ module of the ProCAST simulation program. We simulated the process of directional solidification of a thin plate with the dimensions of 200 × 40 × 4 mm at a given temperature gradient G in the mushy zone and the velocity of the motion of the liquidus isotherm W, which remained constant during the entire process of solidification. It was assumed that on the lower end of the plate there were nucleated three grains (A, B and A, Fig. 1) of a certain crystallographic orientation. The opportunity of the formation of any other grains, for example, before the front of growth or on the lateral boundaries of the plate (stray grains) was not considered.

The azimuthal orientation of all the grains was such that the lateral faces of the plate were parallel to the crystal plane (001). In all the calculations, the grains of the type A were oriented in such a way that one of the crystallographic orientations [001] be coincident with the longitudinal axis of the plate. The deviation of the crystallographic orientation [001] of grain B from the casting axis varied in the limits of angles $\alpha = 5°–54°$. In the CAFÉ module, the orientation of grains is assigned by the Euler angles (Phi1, Phi, Phi2), where the angle Phi1 determines the azimuthal turn of the crystallographic lattice, and the angle Phi determines the deviation of the primary axes of dendrites from the vector of the temperature gradient. Thus, the crystallographic orientation of grains A was always specified by the angles Phi1 = 0, Phi = 0, and Phi2 = 0. The crystallographic orientation of grain B changed as follows: Phi1 = 0, Phi = α, Phi2 = 0.

The conditions of the grain growth upon directional solidification, i.e., the parameters G and W, change along the casting even if this is a casting of simple geometric shape and constant cross section [12]. Therefore, the microstructure in a given section of the casting depends not only on the current conditions of solidification, but also on the prehistory of the grain growth. In order to avoid its influence and to ensure a one-to-one correspondence of the results of the competitive growth to the current conditions of solidification, in the calculations, we used model temperature distributions that corresponded to the following requirements: the radial temperature gradient is equal to zero; the axial temperature gradient is constant throughout the entire mushy zone; and the velocity of the motion of the liquidus isotherm is constant. The following linear temperature distribution in the mushy zone satisfies these conditions: $T = G(x - x_S) + T_S, G = \text{const}, x_S = W\tau$. The temperature distributions were calculated in the thermal module of the ProCAST software using a UserFunction module; the data were used as the initial data for the simulation of grain growth in the CAFÉ module.

The calculations were performed for the values of the temperature gradient of 5, 10, 40, 70, 100, and 300 K/cm and the solidification rates of 1, 5, and 10 mm/min, thus covering almost the entire range of the temperature gradients and solidification rates observed upon the solidification of castings of the type of turbine blade.

Coefficients of the kinetic equation, which connect the rate of growth of the tip of the dendrite with the supercooling ΔT

$$V = a_2\Delta T^2 + a_3\Delta T^3 \quad (1)$$

were calculated with the aid of the CAFÉ module. The necessary data, i.e., the slope of the liquidus surface and the segregation coefficient, were estimated based on the binary phase diagrams of the systems of Ni with the basic alloying elements of the GS26 alloy. The chemical composition of the GS26 alloy and the data necessary for calculating the coefficients a_2 and a_3 are

Table 1. Chemical composition of the alloy GS26, the related segregation coefficients, and the slope of the liquidus line for the alloying elements

Element	C	Cr	Co	Mo	W	Nb	Al	Ti	V	Ni
Concentration, wt %	0.15	4.9	9.0	1.1	11.7	1.7	5.9	1.0	0.9	Base
m, 1/K	–	–1.4	–	–4	11.9	–2.3	–3.5	–11	–5.5	–
k	–	0.9	–	0.8	0.67	0.34	0.85	0.88	0.7	–

given in Table 1. The Gibbs–Thomson coefficient G, which characterizes the influence of the curvature of the interphase interface on the supercooling of the melt, and the coefficient of diffusion in the melt, which also are necessary to calculate a_2 and a_3, are given in Table 2.

According to the Walton–Chalmers theory [1], the grain with the preferred crystallographic orientation suppresses its neighbors, since it overgrows them. The scheme of competitive grain growth proposed in [13] is represented in Fig. 2 in a somewhat changed form. In the steady-state regime of solidification, the axial component of the growth rate of a dendrite is equal to the velocity of motion of the liquidus-curve isotherm, i.e., $V\cos\alpha = W$, where α is the angle of the deviation of the direction [001] from the vector of the temperature gradient. The lag of the dendrite tip from the surface of the equilibrium liquidus is determined by the expression $h = \Delta T/G$, where ΔT is the supercooling before the dendrite tip. Using expression (1), we can obtain an expression for the value of the lag of grain B from grain A (Fig. 1) in the following form:

$$\Delta h = (W/a_3)^{1/3}\left(\cos^{-1/3}\alpha - 1\right)/G. \qquad (2)$$

As follows from (2), the value of the step at the growth front between the grains A and B depends on the temperature gradient and, to a lesser extent, on the velocity of the advance of the solidification front. The

Table 2. Parameters that describe the kinetics of growth of a dendrite of the GS26 alloy

Gibbs–Thomson coefficient Γ	Km	2×10^{-7}
Coefficient of diffusion in the melt D_L [15]	$m^2\ s^{-1}$	1×10^{-9}
a_2	$m\ s^{-1}\ K^{-2}$	0
a_3	$m\ s^{-1}\ K^{-3}$	3.44×10^{-6}

curves of the variation of Δh depending on the orientation of grains and parameters of the solidification process are shown in Fig. 3.

In [14], the CAFÉ module using the method of cellular automation was employed to simulate growth of the solid phase on a regular three-dimensional grid with a cubic cell. The motion of the front of the solid phase occurs in directions [001] of the grains under consideration. The motion in the direction [001] can be represented as the sum of displacements in the directions of the normals to the faces of the mesh cells. If it is true that in the competitive growth an important role is played by the lag of grain B, then we can assume that the grid should be fairly fine in order to adequately describe the step at the front of growth of grains with different crystallographic orientations, i.e., the size of the cell should be less than Δh. In this case, the solid

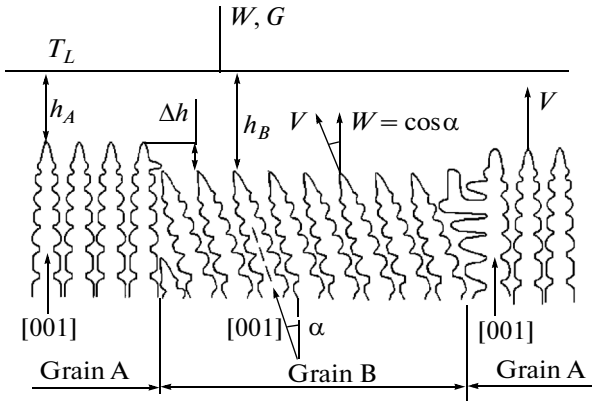

Fig. 2. Growth of grains with different crystallographic orientations according to [13] (schematic).

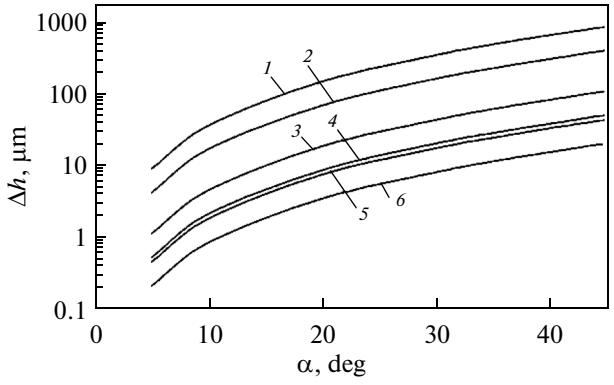

Fig. 3. Lag of grain B from the grain A depending on the angle α, temperature gradient G, and solidification rate W: (*1*) $G = 5$ K/cm, $W = 10$ mm/min; (*2*) $G = 5$ K/cm, $W = 1$ mm/min; (*3*) $G = 40$ K/cm, $W = 10$ mm/min; (*4*) $G = 40$ K/cm, $W = 1$ mm/min; (*5*) $G = 100$ K/cm, $W = 10$ mm/min; and (*6*) $G = 100$ K/cm, $W = 1$ mm/min.

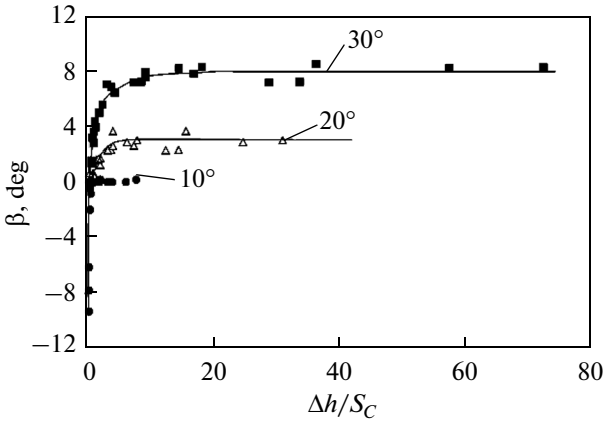

Fig. 4. Angle of deviation of the boundary between the converging grains A and B at α = 10°, 20°, and 30° depending on the parameter $\Delta h/S_C$.

phase obtains the opportunity of lateral growth, which leads to the suppression of the lagging grain.

A typical macrostructure of a casting obtained in the computational experiment is shown in Fig. 1. The boundary between the grains A and B is a plane, and the line of its intersection with the lateral boundaries of the casting is a straight line, which is explained by the constancy of the temperature gradient and of the velocity of the displacement of the isotherm of the liquidus. As a result of a joint growth of the grains, as a rule, the boundary between the grains shifts toward the grain B, i.e., a displacement of the grain B occurs, which has a nonzero angle of deviation of the growth direction [001] from the vector of the temperature gradient. The rate of the displacement of the grain B is characterized by the angle β of the inclination of the grain boundary.

The calculations carried out for different temperature gradients and solidification rates in the ranges of G = 5, 10, 40, and 100 K/cm and W = 1, 5, and 10 mm/min have shown that the angle of the deviation of the boundary between the converging grains at a fixed angle α is uniquely determined by the only parameter, i.e., the ratio $\Delta h/S_C$ (Fig. 4).

The calculations were performed at S_C = 5 and 20 μm. For G = 40 K/cm and W = 1 and 10 mm/min, additional calculations were carried out at S_C = 40, 50, and 80 μm.

At $\Delta h/S_C$ greater than a certain value $\Delta\tilde{h}_\alpha$, which depends on the angle α, the result of simulation depends neither on the choice of S_C nor on the solidification conditions. As can be seen from Fig. 4, at α = 30°, we have $\Delta\tilde{h}_\alpha \approx 20$, i.e., the size of the cell is many times less than the step at the growth front.

At $\Delta h/S_C < \Delta\tilde{h}_\alpha$, the result of simulation completely depends on this parameter. Even at a significant deviation of grain B from the preferred orientation (α = 30°), at the values $\Delta h/S_C < \Delta\tilde{h}_\alpha$, the angle of the deviation of the boundary β decreases sharply with the decrease in the parameter $\Delta h/S_C$.

The decrease in $\Delta h/S_C$ can be connected with the conditions of solidification: with a high temperature gradient G and/or low solidification rate W, at which $\Delta h \to 0$, or with the use of too coarse grid, i.e., when $S_C \geq \Delta h$. Thus, to obtain simulation results adequate for the real picture of competitive growth, the correct choice of S_C is of decisive importance.

The value of S_C should be selected based on the analogy between the propagation of the solid phase over the cells of a cubic grid and growth of dendrite branches, i.e., based on the parameters of the dendritic structure that is formed under the given conditions of solidification.

In the case of converging grains, one of the possible mechanisms of the suppression of the lagging grain is mechanical obstruction to its growth. The authors of [16] supposed that the efficient suppression of the lagging grain is possible if the leading grain overgrows its competitors by an amount equal to or greater than the distance between the secondary axes of dendrites λ_2. This permits the secondary branches of the leading grain to freely develop before the tips of the dendrites of the lagging grain and thereby to prevent its growth. Based on the experimental results obtained on transparent organic substances, the authors of [13] supposed that only some secondary branches of the dendrite, the distance between which is equal to several λ_2, were capable of lateral growth, and that the mesh size should be correlated with this distance.

In [3, 6], distances between the secondary axes of dendrites have been measured on castings quenched from the process of directional solidification. It was established that at the initial stage of development of secondary axes the distance λ_2 was 10–15 μm. Based on the results of these studies, we accepted that the size S_C of the unit cell of the computational grid must be selected in the range of 5–20 μm.

RESULTS AND DISCUSSION

Results of the Computational Experiment

Diverging grains, S_C = 5 μm. In the case of the diverging grains (Figs. 5a, 5b), the lag of grain B does not play a significant role, since the displacement of grain B occurs via the propagation of the secondary branches of the dendrite of grain A into the side gap between the grains [3, 5].

The displacement of grain B is observed in the entire investigated range of angles α from 5° to 45°. The change in the angle β in this range is very well described by the dependence β = 0.5α, which completely agrees with the results of work [5].

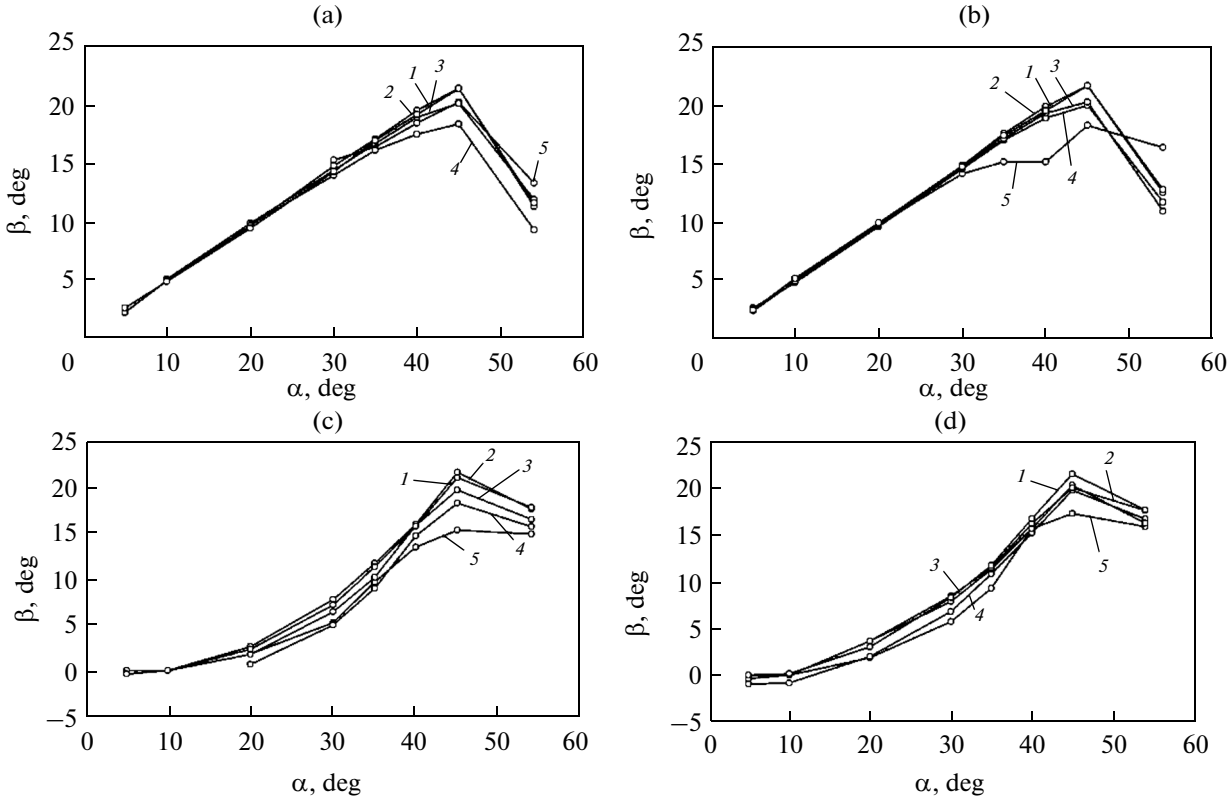

Fig. 5. Angle β of the boundary between the grains depending on the orientation of grain B: (a) diverging grains, $W = 1$ mm/min; (b) diverging grains, $W = 10$ mm/min; (c) converging grains, $W = 1$ mm/min; (d) converging grains, $W = 10$ mm/min. Calculation: (*1*) $G = 5$ K/cm; (*2*) $G = 10$ K/cm; (*3*) $G = 40$ K/cm; (*4*) $G = 100$ K/cm; and (*5*) $G = 300$ K/cm.

The decrease in the angle β at the angles $\alpha > 45°$ is connected with a change in the status of grain B. From the diverging grain, it becomes converging, since the smallest angle of deviation from the vector of the temperature gradient will have the direction [001] oriented toward grain A, rather than from grain A. Therefore, the values of the angle β at $\alpha = 45° + x$ for the diverging grains are approximately equal at $\alpha = 45° - x$ for the converging grains.

Converging grains, $S_C = 5$ μm. The results presented in Figs. 5c and 5d show that, in the case of the converging grains at the angles $\alpha < 20°$, the displacement of grain B hardly occurs. This result also agrees with the experimental data given in [2, 5, 6, 10]. According to the theory, in the case of the converging grains, grain B is blocked by the secondary branches of the dendrite of grain A. To implement this mechanism of competitive growth, it is necessary for grain A to overgrow grain B by a distance exceeding S_C. At $\alpha < 20°$, the value of the overgrowth Δh is close to the size of the unit cell S_C (Fig. 3), which impedes the lateral propagation of the front of the solid phase.

At large angles α, the lag of grain B from the grain A is substantially greater than the size of the unit cell, which permits grain A to freely propagate perpendicularly to the temperature gradient and to block the neighbor. As in the case of the diverging grains, at $\alpha > 20°$ the angle β of the inclination of the boundary of the converging grains can be approximated by the linear dependence $\beta = 0.5(\alpha - 20°)$.

Influence of the mesh size. The results presented in Fig. 6 were obtained upon the simulation of the competitive growth on a computational grid with the size of cells $S_C = 20$ μm.

In the case of the diverging grains (Figs. 6a, 6b), at the temperature gradient of more than 100 K/cm and angles $\alpha < 10°$, the joint growth of grains A and B occurs without the displacement of the latter, which is apparently connected with the fact that, under these conditions, the gap between the grains is substantially less than S_C and, therefore, is undistinguished at the given mesh size. These results can be confirmed by the experimental data of [6] given in Table 3.

At a low temperature gradient, i.e., under the conditions where the gap between the grains A and B is comparable with or more than S_C, the results presented in Figs. 6a and 6b (curves *1*–*3*) are generally similar to those shown in Figs. 5a and 5b.

In the case of the converging grains at the temperature gradient of more than 40 K/cm and angles $\alpha < 20°$, the grain B displaces grain A. On the whole,

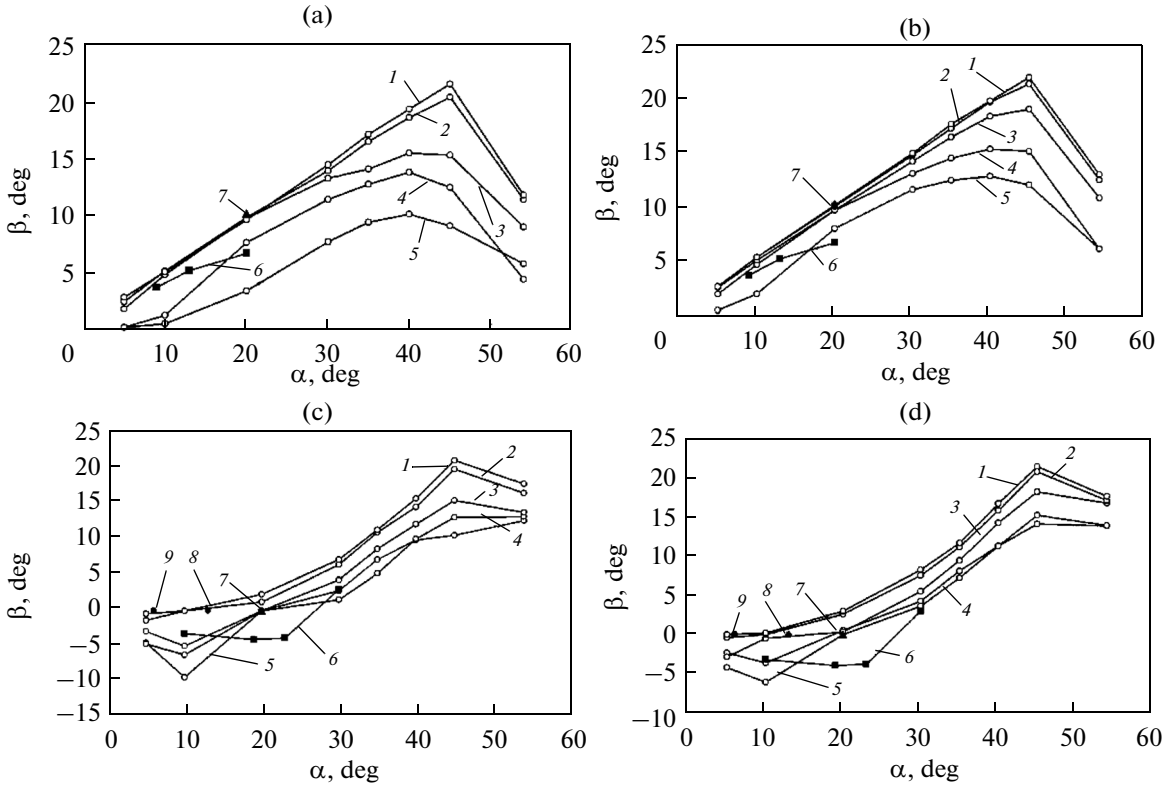

Fig. 6. Angle β of the boundary between grains A and B depending on the orientation of grain B: (a) diverging grains, W = 1 mm/min; (b) diverging grains, W = 10 mm/min; (c) converging grains, W = 1 mm/min; and (d) converging grains, W = 10 mm/min. Calculation: (*1*) G = 5 K/cm; (*2*) G = 10 K/cm; (*3*) G = 40 K/cm; (*4*) G = 100 K/cm; and (*5*) G = 300 K/cm. Experiment: (*6*) [3]; (*7*) [5]; (*8*) [6]; and (*9*) [2].

this is confirmed by experimental studies [3]. However, at present, the explanation of this result within the framework of the geometric model of interaction of grains is absent.

A comparison of Figs. 5 and 6 shows that the choice of the mesh size can substantially change the results of simulation. On the fine grid, the results of the simulation for the diverging grains show that the grain A reliably suppresses grains with other crystallographic orientations. The suppression of the converging grains also occurs under the solidification conditions for which Δh is substantially greater than S_C.

An increase in S_C leads to results that predict difficulties with the suppression of the converging and diverging grains B with the angle of deviation $\alpha < 20°$ at the low solidification rate and high temperature gradient. In essence, S_C is an adjusting parameter for the CAFÉ model, which should be coordinated with the physical picture of the competitive growth on the basis of the analogy between the propagation of the solid

Table 3. Experimental data for diverging grains

G, K/cm	W, mm/min	α_A, deg	α_B, deg	$\alpha = \alpha_A - \alpha_B$, deg	β, deg	Refs
90	10	0	15–25	15–25	$\beta = 0.5\alpha$	[5]
20	3.5	0	15–25	15–25	$\beta = 0.5\alpha$	[5]
128	1	0	10–30	10–30	$\beta = 0.25(\alpha - 8) + 3.5$	[3]
30	3–4.7	7	20	13	0	[6]
70	1.5–2.5	7	20	13	0	[6]

Table 4. Experimental data for converging grains

G, K/cm	W, mm/min	α_A, deg	α_B, deg	$\alpha_A - \alpha_B$, deg	β, deg	Δh, μm	$\Delta h/\lambda_2$*	Refs
30	1.62	0	7	7	0	5.0	0.2	[2]
70	1.62	0	7	7	0	2.0	0.1	[2]
90	10	0	25	25	0	42	2.1	[5]
20	3.5	0	25	25	0	132	6.6	[5]
90	10	0	15	15	0	14	0.71	[5]
128	1	0	10	10	−3.2	2.0	0.1	[3]
128	1	0	18	18	−4	6.8	0.34	[3]
128	1	0	23	23	−3.8	11.4	0.57	[3]
128	1	0	30	30	−3.2	20.5	1.0	[3]
30	3–4.7	7	20	13	0	20	1.0	[6]
70	1.5–2.5	7	20	13	0	8	0.4	[6]

*Upon the calculation of $\Delta h/\lambda_2$ it was assumed that $\lambda_2 = 20$ μm.

phase over the cells of the uniform grid and lateral growth of the secondary axes of dendrites.

Comparison with the Experiment

Tables 3 and 4 present experimental data for bicrystal castings of nickel superalloys. The difficulty of their comparison with the results of simulation lies in the fact that for the identification of the regimes, in which the castings were obtained, in some works the temperature gradient and the velocity of the displacement of the mold are indicated, whereas in others the temperature gradient and the distance between the primary axes of dendrites λ_1 or the velocity of the displacement of the mold and λ_1 are given. For comparison with the results presented in Figs. 6 and 7, the missing values of G and W were calculated using the expression $\lambda_1 = 620(GW)^{-0.333}$ [5, 17]. It was assumed that the values of the velocity of the displacement of the mold indicated in the literature can be accepted as the solidification rate. The thus-prepared data were superimposed onto the results of simulation. As can be seen from Fig. 6, there is a qualitative agreement between the computational and natural experiment.

For the diverging grains, the authors of [5] suggested expressions for calculating the angle β of the inclination of the boundary depending on the angle α. The angles calculated via these expressions agree well with the computational experiment. The results for the diverging grains obtained in [3] relate to the directional solidification at the temperature gradient of 128 K/cm. Taking into account the possible error in the determination of the gradient by thermocouples, it is possible to say that these data agree satisfactorily with the results of the computational experiment at $G = 100$ K/cm and $W = 1$ mm/min on the grid with $S_C = 20$ μm (Fig. 6a).

The experimental data for the converging grains indicate the absence of the displacement of grains B [2, 5, 6] or the suppression of grain A by grain B [3]. The computational experiment qualitatively coincides with these results. On the grid with a cell size of 5 μm, β is less than 1°–2° at the angles $\alpha < 15°$, which agrees with the data of [2, 5, 6]. On the grid with the cell size of 20 μm, grain B displaces grain A in the range of orientations $\alpha < 20°$ at the temperature gradient of more than 100 K/cm, which agrees with the data of [3]. These results again demonstrate the dependence of the results of simulation on the tuning parameter S_C. On the other hand, the results of [2, 5, 6] relate to the regimes of solidification in which the advance of grain A over grain B calculated via Eq. (2) lies in a narrow interval $\Delta h/\lambda_2 < 2$ (Table. 4). Thus, the castings that were used in studies were obtained under the conditions that are close from the viewpoint of the competitive growth, which explains the similarity of the results obtained in [2, 5, 6]. According to Fig. 5, under these conditions of growth, the angle of the inclination of the boundary is small; i.e., there does not occur a displacement of the grain B, which is confirmed by the experimental data.

Practical Recommendations

The temperature gradient and the solidification rate are technological parameters, which should be controlled in the process of solidification.

Above, we presented results that indicate that the angle β of the inclination of the boundary between the competing grains is uniquely determined by the ratio of Δh to the dispersity of the dendritic structure. In real process, the dispersity of structure is characterized by the distance between the secondary axes of dendrites λ_2, whereas in the CAFÉ model, by the parameter S_C. With the aid of expression (2), the $\beta = f(\Delta h/S_C)$

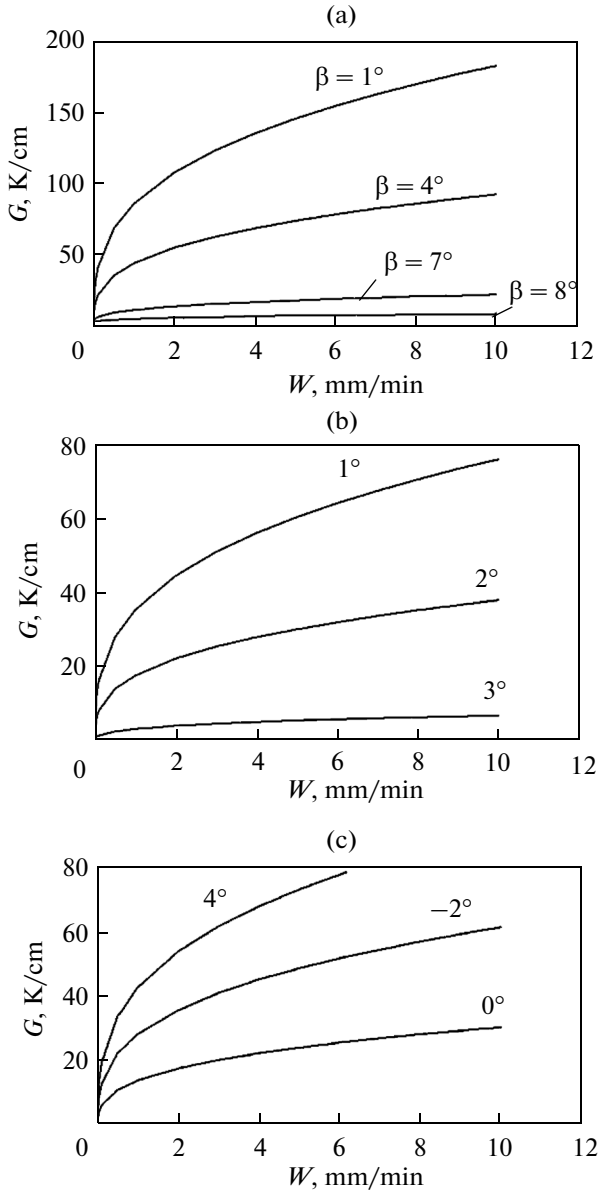

Fig. 7. Temperature gradient and the rate of growth that ensure the required conditions for a competitive growth of converging grains. Lines, β = const. Numbers, values of the angle β: (a) α = 30°; (b) α = 20°; and (c) α = 10°.

dependence constructed based on the results of computational experiments can be converted into the form $\beta = f(G,W)$, which makes it possible to make practical recommendations regarding the choice of the parameters of the technological process.

In Fig. 7, the lines of a constant angle β limit the regions of the regimes of growth in the G–W coordinates. The suppression of grains with the orientation $\alpha \geq 20°$ (Figs. 7a, 7b) occurs in a temperature-gradient range, the width of which depends on the rate of growth and angle α. With a decrease in the temperature gradient, the angle β of the inclination of the boundary increases, i.e., the rate of the displacement of grain B increases. With a decrease in the angle of the misorientation of grains (with a decrease in the angle α), the maximum temperature gradient at which the growth of grain B can be suppressed decreases. At angles of misorientation $\alpha \leq 10°$ (Fig. 7c), at low temperature gradients, the joint growth of grains A and B occurs (β = 0); on the contrary, at high gradients, grain B suppresses grain A. The suppression of grain A was observed experimentally in [3] (Table 4) at angles $\alpha \geq 10°$.

In the case of converging grains, the elimination of grains B occurs at any temperature gradient and solidification rate.

Thus, for the efficient selection of grains with the preferred orientation (of type A), the favorable regimes are those with a low temperature gradient and high growth rate. However, the suppression of grains with a misorientation less than 10° is problematic; the competitive growth results in either a bicrystal or in a single crystal with the orientation of the grain B, i.e., with a deviation from the direction [001]. Thus, to suppress the strongly misoriented grains, a low temperature gradient is preferable; whereas, to obtain a single crystal, it is necessary to increase the temperature gradient.

CONCLUSIONS

(1) The result of the simulation of the competitive growth of converging grains with an axial misorientation can depend on the only parameter, i.e., the ratio $\Delta h/S_C$. The sensitivity of the result to this parameter depends on the angle α of the misorientation of the grains.

(2) Based on the analogy between the propagation of the solid phase on a uniform grid in the method of cellular automation with the growth of a dendrite in directions [001], it can be assumed that the result of the competitive growth depends not only on the outgrowth of the grain with the preferred orientation, i.e., on the magnitude of Δh, but also on the distance between the secondary axes of dendrites.

(3) The results of the simulation in the CAFÉ module of the ProCAST software agree well with the available experimental data, which makes it possible to use this model for studying grain growth under conditions that meet difficulties from the experimental point of view.

(4) Using a computational experiment, we obtained laws governing the change in the angle β of the inclination of the boundary between the grains depending on the angle α of their misorientation, on the temperature gradient G in the isotherm of the liquidus curve, and on the velocity W of the isotherm propagation in the range of values characteristic of the technological process of the production of single-crystal castings of a nickel superalloy.

(5) For the selection of grains with a preferred orientation, regimes with a low temperature gradient and high growth rate are favorable. The efficiency of the selection falls with a decrease in the angle of the misorientation of the grains.

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