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STRUCTURE, PHASE TRANSFORMATIONS, AND DIFFUSION

Mechanism of Competitive Grain Growth in a Curvilinear Channel of Crystal-Sorter during the Orientational Solidification of Nickel-Based Heat-Resistant Alloy

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Abstract—Using numerical simulation in the ProCAST program complex, the conditions of the solidification of heat-resistant nickel alloy in curvilinear channels of a ceramic mold have been investigated. It has been shown that, in practically important cases, the vector of the temperature gradient is oriented along the axis of the curvilinear channel. In a spiral crystal selector, a cyclic change in the preferred direction of growth occurs because of the cyclic change in the direction of the vector of the temperature gradient. The fact that the vector of the temperature gradient is almost always directed along the axis of the curvilinear channel makes it possible to govern the orientation of the vector of the temperature gradient in space and, therefore, to obtain a grain with the preferred crystallographic orientation. Based on the results of this investigation, a method of the grain selection with a desired azimuthal orientation is proposed.

Keywords: nickel heat-resistant alloy, directional solidification, competitive growth, grain selection, azimuthal orientation, simulation

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INTRODUCTION

Nucleation and selection of grains with a required crystallographic orientation are the initial stages upon the formation of a single-crystal casting. In industry, two technologies of grain selection are employed, i.e., using a spiral selector (the so-called helicoid) and using preliminarily prepared seed crystal.

A helicoid ensures the selection of one grain with a preferred crystallographic orientation from many nucleated grains. This orientation is characterized by the smallest angle between the direction [001] and vector of the temperature gradient; however, the azimuthal orientation of the prevailing grains can be arbitrary. According to the other technology, the nucleation occurs on a seed, which makes it possible to govern both the axial and azimuthal orientation of a single crystal to be grown. However, in this case, the helicoid is a means of improving the quality of the obtained single crystal.

The broad applications of crystal selectors make it urgent to study grain growth depending on the geometric characteristics of the spiral channel employed.

In 2011, Dai et al. [1] used a CAFÉ module of the program complex ProCAST to performed a systematic study of the influence of the geometric parameters of a spiral crystal selector on the efficiency of the grain selection via simulation. The efficiency of the crystal selector was evaluated based on the length of the path of the solid phase before obtaining a single crystal. As the geometric parameters, the authors considered the take-off angle of the spiral channel, the diameter of the channel, and the diameter of the spiral rotation. The authors came to the conclusion that the selection of grains in the crystal selector occurs for the geometric reasons, and the efficiency of the selection grows with a decrease in the take-off angle of the spiral [2].

In 2012, based on experiments, Gao et al. [3] came to the conclusion that, in the crystal selector, the grain that is located near the internal wall of the channel usually becomes winner. In [4], a similar conclusion drawn based on the results of a simulation in the CAFÉ module is explained by the combined action of several factors, i.e., by the direction of the vector of heat flux in the crystal selector; the direction of the preferred growth, and the geometric restriction of the spiral walls on the grain growth. In [4], it is indicated that the vector of the heat flux in the crystal selector is oriented along the axis of the spiral; however, the effect of this factor on the grain selection was not cleared up to the end.

In all of the above-mentioned studies, no noticeable effect of the geometry of the crystal selector on

Table 1. Chemical composition of alloy ZhS26, segregation coefficients, and slope of liquidus line for 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	–

the crystallographic orientation of grains was revealed. The crystal selector makes it possible to significantly decrease the number of grains, but is not capable of optimizing the axial orientation of the single crystal to be grown.

The temperature gradient plays an important role in the competitive growth of grains. The orientation of the vector of the temperature gradient determines which of the [001] directions will be the preferred direction of growth. According to the theory of Walton and Chalmers [5], the value of the temperature gradient determines how far the leading grain grows ahead of the adjacent grains-competitors. Based on these concepts, it is assumed that the direction of the temperature gradient is important for grain selection in the spiral grain selector. Nevertheless, relatively little attention has been paid to the temperature distribution in the spiral selectors and the deviation of the vector of the temperature gradient from the general direction of the motion of the mold.

In our previous work [6], we investigated the influence of the cyclic change in the direction of the preferred growth based on the example of the solidification of a toroidal casting and came to the conclusion that the cyclic change of the growth conditions in the toroidal channel in fact eliminates the advantages of one grain before others.

Based on these facts, we devoted the present article to a study of the relationship between the conditions of solidification, geometry of the crystal selector, direction of the vector of the temperature gradient, and the competitive character of grain growth. Based on this study, we have shown the opportunity of the selection of grains with an assigned azimuthal orientation.

COMPUTATIONAL EXPERIMENT

At the first stage of the work, we investigated the thermophysical features of the solidification of nickel heat-resistant alloy in a curvilinear channel. In this part of the work, the simulation of the process of the solidification of the casting was performed using the thermal module of the ProCAST system [7]. The result of the simulation using this module is the temperature distribution in the metal at different time moments up to the complete solidification of the casting. Based on these data, we calculated the temperature gradient G on the liquidus isotherm and the rate W of the displacement of this isotherm along the axis of the casting.

The chemical composition of the alloy and the thermophysical properties of the ceramic shell used in the calculations are given in Tables 1 and 2. The temperature of the solidus of the alloy is 1591 K (1318°C); the temperature of the liquidus is 1683K (1410°C). The thermophysical properties of the alloy were calculated for the conditions of equilibrium solidification based on its chemical composition in the COMPUTERM (ProCAST) thermodynamic database.

In this part of the work, we intended to simplify the model of the process of directional solidification by assigning the temperature distribution on the external surface of the mold that imitates the displacement of the mold from the heating zone into the zone of cooling of the setup. Using the UserFunction module of the ProCAST system, at each time step, we assigned the temperature on the external wall of the mold, which was calculated according to the following rule:

$$T = \begin{cases} T_{\min}, & T \le T_{\min} \\ u = T_L + G_{\text{env}}(z - V\tau), & T_{\min} \le u \le T_{\max}, \\ T_{\max}, & T \ge T_{\max} \end{cases} \quad (1)$$

where τ is the time, T_L is the liquidus temperature, $T_{\min}$ = 1200°C, and $T_{\max}$ = 1450°C.

The temperature field on the surface of the mold was characterized by a linear law of variations in temperature along the z axis and by a constant temperature gradient G_{env} = 5000 K/m in the region of $T_{\min} \le T \le T_{\max}$; the mold was moved along the Z axis at a velocity of V = 83.3 μm/s. The initial temperature of the metal and the mold was equal to $T_{\max}$ = 1450°C. The temperature of the lower end of the casting, which had contact with the conditional crystallizer, changed in accordance with (1) from $T_{\max}$ to $T_{\min}$.

A series of computational experiments was carried out that were characterized by the different assigned thermal conductivity coefficient λ_m of the alloy, the coefficient of heat transfer at the metal–mold bound-

Table 2. Thermophysical properties of the material of the mold

Property	Dimensionality	Value
Coefficient of thermal conductivity	W/(m K)	2.2
Heat capacity	J/(kg K)	1200
Density	kg/m^3	2700

Table 3. Parameters that describe nucleation and growth kinetics of dendrites in ZhS26 alloy

Parameter	Dimensionalty	Value
Gibbs–Thomson coefficient, Γ	K m	2×10^{-7}
Coefficient of diffusion in the melt, D_L	$m^2 s^{-1}$	1×10^{-9}
a_2	$m s^{-1} K^{-2}$	0
a_3	$m s^{-1} K^{-3}$	3.44×10^{-6}
ΔT_N	K	0.5
ΔT_σ	K	0.1
n_{max}	m^{-2}	1×10^8

ary, and distance H from the lower end of the mold, i.e., the crystallizer, to the bend. The coefficient of the thermal conductivity λ_m of the alloy changed in the range of 2–40 W/(m K). The coefficient of heat transfer at the metal–mold boundary took the values α_m = 2000 and 10000 W/(m K). The distance H was taken to be equal to 20, 50, and 100 mm.

In the second part of the work, we examined the process of the formation of the macrostructure of the casting block, which consists of the starter block, crystal selector, and three cylindrical samples (using the vertical directional solidification in the setup for crystal growth by the Bridgman method).

We simulated the following technological process. At the initial time moment, an empty mold mounted on the crystallizer was placed into the furnace for preheating of the mold at an initial temperature equal to 293 K (20°C). After the furnace reached the necessary temperature (at a time of ~1 h) and a short holding at a temperature, the crystallizer with the melt poured into the mold moved downward at a constant velocity of 5 mm/min (83.3 μm/s). The temperature of the upper heater in the process of directional solidification was 1813 K (1540°C), while that of the lower heater was 1873 K (1600°C) and the initial temperature of the ZhS26 alloy was 1873 K (1600°C).

To simulate the grain growth, the module CAFÉ of the ProCAST program complex for the computer simulation of foundry processes was used.

It was assumed that, in the starter block, only the surface nucleation of grains occurred on the surface that was in contact with the crystallizer. The opportunity of the nucleation of grains on the surface of the mold or the nucleation of grains in the bulk of the melt before the growth front has not been considered.

The dependence of the number of grains on the degree of the supercooling of the melt in the CAFÉ module is determined by the normal distribution

$$\frac{dn}{d(\Delta T)} = \frac{n_{\max}}{\Delta T_\sigma \sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\Delta T - \Delta T_N}{\Delta T_\sigma}\right)^2\right], \quad (2)$$

where ΔT is the supercooling; ΔT_N and ΔT_σ are the parameters of a Gaussian distribution, and n_{max} is the maximum density of the nucleation centers. The parameters of the surface nucleation used in the calculations are given in Table 3.

The coefficients of the kinetic equation $v = a_2\Delta T^2 + a_3\Delta T^3$, which connects the growth rate v of the dendrite tip with supercooling ΔT, were calculated using the CAFÉ module. The necessary data, i.e., the slope of the liquidus line m_i and the segregation coefficients k_i for the main alloying elements present in the ZhS26 alloy, were estimated using the binary phase diagrams of the systems of Ni with the alloying elements. The chemical composition of the ZhS26 alloy and other data that were used to calculate coefficients a_2 and a_3 are given in Tables 1 and 3. The details of the calculation of these coefficients are given in [8].

ANALYSIS OF THE RESULTS OF THE COMPUTATIONAL EXPERIMENT

Direction of the Vector of the Temperature Gradient

In order to establish the relationship between the direction of the vector of the heat flux and the thermophysical properties of the metal and the mold, a series of computational experiments on the directional solidification of a casting in the form of a bent cylinder with a diameter of 8 mm was carried out.

Figure 1 displays the results of calculations in which the heat-transfer coefficient at the metal–mold boundary was α_m = 2000 W/(m K) and the coefficient of the thermal conductivity of the alloy was assigned in the form of the function $\lambda(T)$ calculated based on the chemical composition of alloy using the COMPUTERM (ProCAST) thermodynamic database. The process of solidification was considered for the case of a ceramic mold with a flat massive wall (Fig. 1a) and for the case of a thin-walled ceramic mold with a wall thickness of 6 mm (Fig. 1b).

The 3D model of the flat mold represented a parallelepiped with a base $L = 50 \times 50$ mm. On the side surfaces of the parallelepiped formed by the planes $x = 0$ and $x = L$, adiabatic conditions were assigned. Thus, the mold represented a wall that was infinite on the coordinate x. On all other surfaces of the mold in contact with the external medium, the temperature distribution given by Eq. (1), which imitated the process of directional solidification, was specified using the UserFunction module. Figures 1c–1f display the typ-

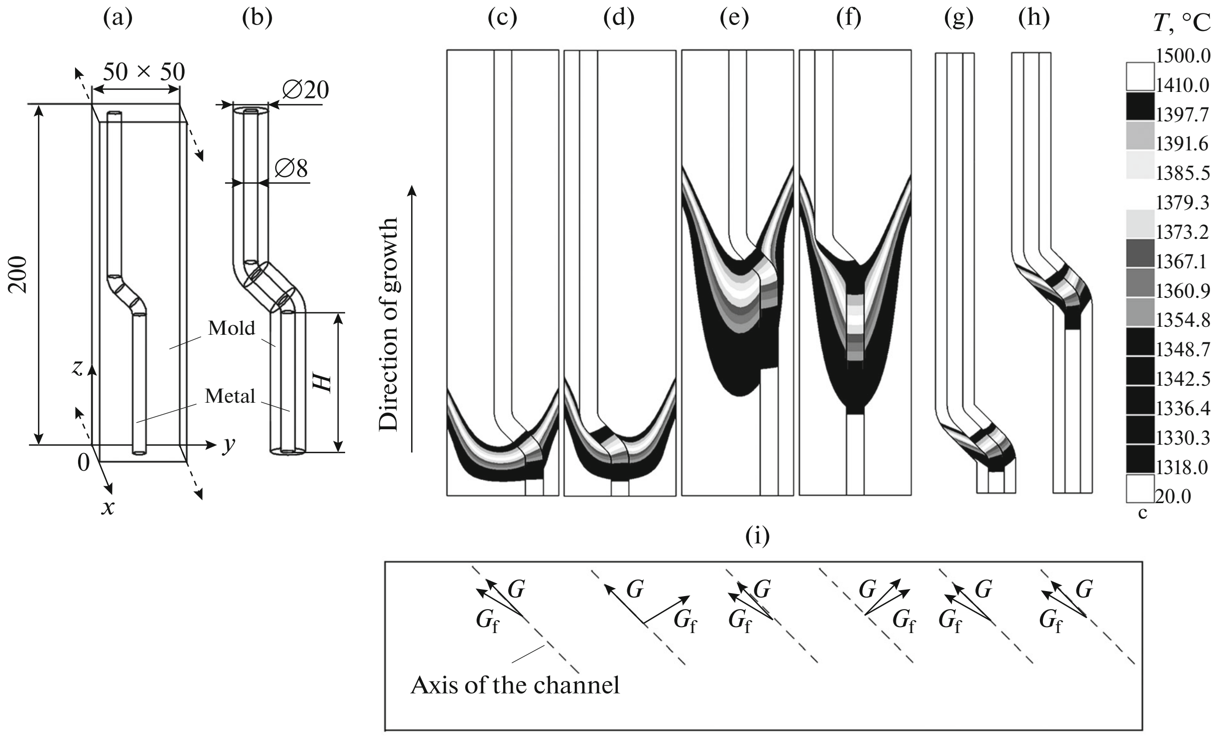

Fig. 1. Temperature distribution in the ceramic mold and in the casting: (a, c–f) thick-walled mold; (b, g, h) thin-walled mold; and (i) orientation of the vector of the temperature gradient in the metal (G) and in the mold (G_f) relative to the axis of the inclined portion of the channel. Axis is shown by the dashed line.

ical results of the simulation that relate to the case of directional solidification in the mold in the form of a flat massive wall.

The computational experiments were performed for the case of a massive mold with different arrangement of the casting relative to the central plane $y = 25$ mm (Fig. 1a). In one series of the experiments, the axis of the lower part of the casting (to the point of the bend) was located in the plane $y = 25$ mm, as is shown in Figs. 1a, 1d, and 1f. In another series of experiments, the axis of the upper part of the casting (after bend) was located in the plane $y = 25$ mm, as is shown in Figs. 1c and 1e.

The simulation showed that the orientation of the vector of the temperature gradient G at the isotherm T_L in the metal depends on the angle between the axis of the casting and the vector of the temperature gradient G_f in the ceramic mold at the same isotherm, and also on the distance to the lower base of the casting, i.e., to the crystallizer. At a sufficient distance from the crystallizer (Fig. 1e, 1f), the temperature distribution in the casting depends only on the temperature distribution in the mold. Therefore, regardless of the value of the coefficient of the thermal conductivity of the metal and of the heat-transfer coefficient at the metal–mold boundary, the direction of the vector G is close to the direction of the vector G_f. If the vector G_f is oriented along the axis of the casting, then the temperature gradient in the metal will also be oriented along the axis of the casting (Fig. 1e). If the vector G_f deviates significantly from the axis of the casting, then the temperature gradient in the metal will also exhibit a strong deviation from the axis of the casting (Fig. 1f). The vectors G and G_f are shown in Fig. 1i by arrows, while the direction of the axis of the channel is shown by dashed lines.

If the distance H to the crystallizer is small, the larger part of thermal energy is transferred from the two-phase zone to the crystallizer through the casting, rather than through the shortest path via the ceramics. In this case, the temperature field in the metal is formed under the effect of the crystallizer. The isotherms in the metal remain perpendicular to the axis of the curved casting at a distance of several diameters d_w from the crystallizer.

The thermal resistance at the metal–mold boundary plays an important role in the orientation of the temperature gradient in the metal. Even at identical values of the coefficients of the thermal conductivity of the metal and ceramics, the existence of even a small thermal resistance at the metal–mold boundary is sufficient for vector G be directed along the axis of the channel.

In the case of a thin-walled mold, the vector G_f changes its direction, along with a change in the orientation of the ceramic shell (Figs. 1g, 1h). Therefore, in

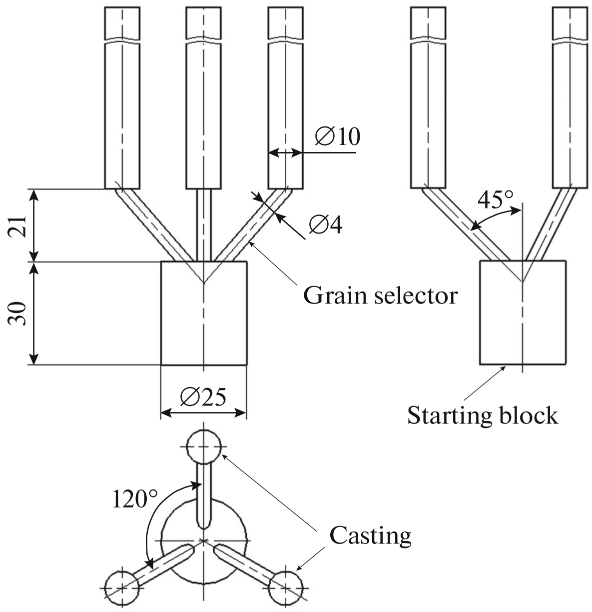

Fig. 2. Procedure of casting for obtaining single crystals with an assigned azimuthal orientation (schematic).

the thin-walled mold, the vector of the temperature gradient G and, therefore, the vector of the heat flux, are always oriented along the axis of the casting.

Based on the results of the performed calculations, the following conclusion can be made. Most probably, the vector of the temperature gradient G will be oriented along the axis of the channel of the grain selector (1) if the coefficient of the thermal conductivity of the metal is higher than that of the mold; (2) if there is thermal resistance at the metal–mold boundary; and (3) if the distance from the two-phase zone in the casting to the crystallizer does not exceed several diameters of the channel cross section.

Effect of the Curvature of the Crystal-Growth Channel on the Grain Selection

The crystallographic orientation of the columnar grains that grow in the casting remains almost constant relative to the laboratory coordinate system during the entire process of directional solidification. The orientation of the vector of the temperature gradient also remains unaltered (as well as of the rate of growth) upon the orientational solidification of simple cylindrical castings.

Upon solidification in a curvilinear channel, the temperature gradient G changes its direction following the turn of the channel, which can lead to a change in the preferred direction of growth. During solidification in a helicoid, the temperature gradient changes its direction cyclically, which leads to a cyclic change in the preferred direction of growth. This circumstance principally distinguishes the competitive grain growth in the helicoid from the growth of castings with the rectilinear axis of symmetry.

It is known from the available experimental data and results of simulation that the misorientation of two grains by an angle less than 10° does not give an advantage to any of the competing grains, and it is impossible for one grain to be displaced by another. However, a cyclic variation in the preferred direction of growth and a turn in the channel create conditions under which the internal grain is capable of extruding the competitor and of forming a single crystal at an angle of misorientation of 5° [6].

The fact that the vector of the temperature gradient is almost always oriented along the axis of a curvilinear channel makes it possible to affect the direction of the vector of the temperature gradient and, therefore, to lead to a situation where the desired crystallographic orientation becomes the preferred direction of growth.

Controlling the Process of Grain Selection

The control of the selection of grains with the necessary azimuthal orientation is connected to the opportunity to govern the direction of the vector of the temperature gradient. Figure 2 displays the simplest variant of a grain selector for selecting three grains with identical axial orientation and the desired azimuthal turn. The grain selector consists of a starter block and three inclined channels rotated relative to the direction of directional solidification by 120°.

Figure 3 shows the results of simulating the process of directional solidification using the Bridgman method with a velocity of the displacement of the mold of $V = 83.3$ μm/s. The figure shows the macrostructure and the pole figures for the sections of the grain selector at different distances from the crystallizer. As a result of the competitive growth, grains with arbitrary azimuthal orientations and axial orientations close to [001] are retained at the outlet from the starter block (section d). Some of these grains turn out to be located near the entrance into the inclined channels C_i. As was shown above, in each of these channels, the vector of the temperature gradient G was oriented along the axis of the channel. Therefore, each of these channels has its own preferred direction of growth and, correspondingly, in each channel, a grain that has a preferred orientation relative to the vector G_i in a given channel becomes a winner.

Figure 4 displays the pole figures for single crystals that were formed in the grain selectors C_1, C_2, and C_3. On the whole, it can be recognized that the selection of grains on the azimuthal orientation does occur in the grain selectors. The azimuthal orientation of single crystals G_1, G_2, and G_3 corresponds to the orientation of the corresponding grain selectors, although the accuracy of the orientations is not too great.

It is important to note that the selection of grains with the required azimuthal orientation depends on

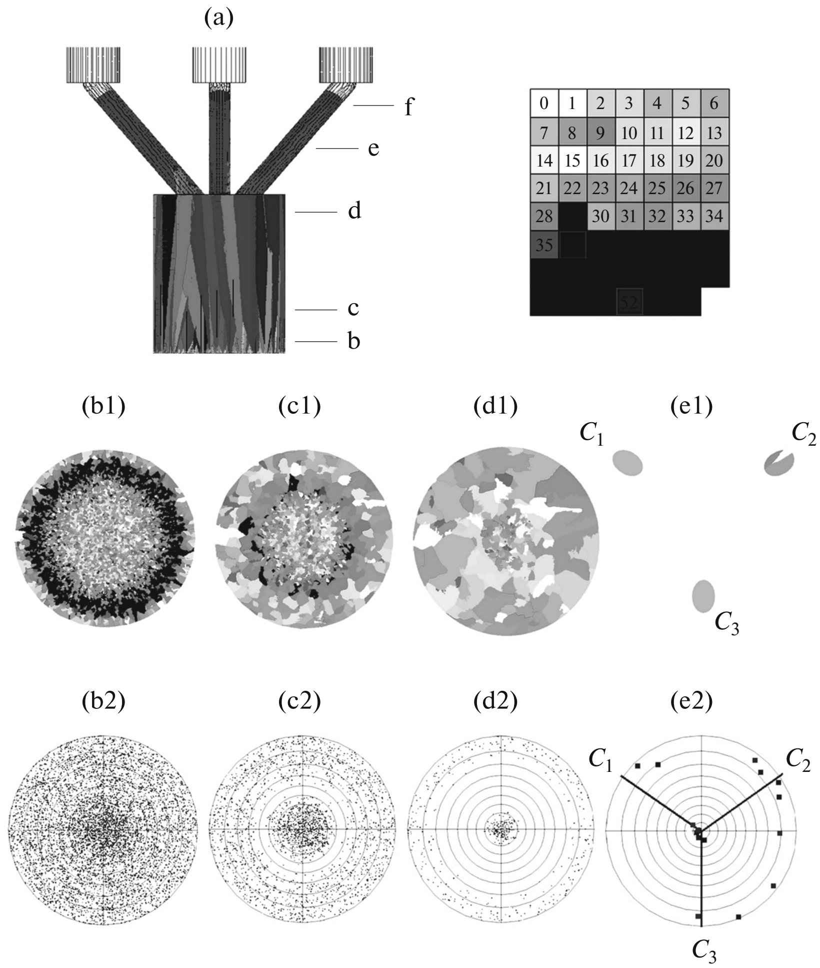

Fig. 3. Results of simulating the macrostructure in the starting block and in grain selectors C_1, C_2, and C_3: (a) appearance of grains on the external surface of casting; (b1–e1) macrostructure in sections b–d; (b2–e2) pole figures for directions $\langle 001 \rangle$ relative to the normal to the plane of cross sections b–e.

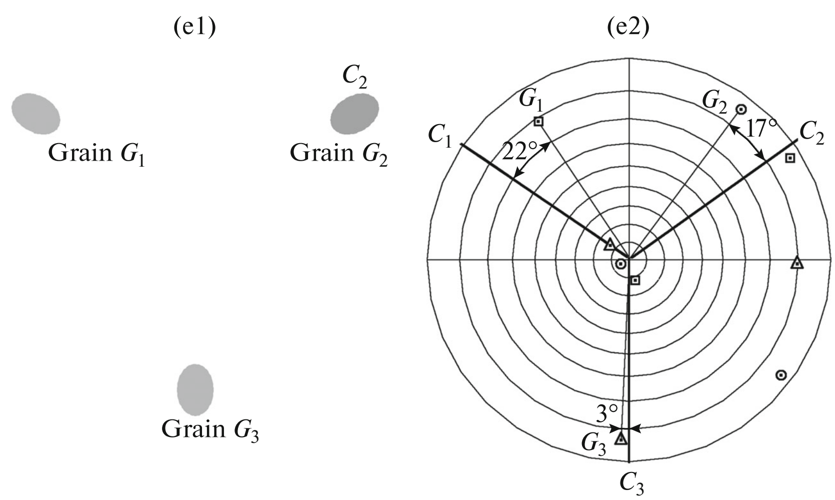

Fig. 4. Orientation of grains in grain-selection channels C_1, C_2, and C_3 in section f (see Fig. 3) at entrance to casting.

the number of grains at the inlet into the inclined grain selector. The greater the number of grains at the inlet to the channel, the greater the probability of the presence of a grain with the required azimuthal orientation in this ensemble of grains. Therefore, the greater the number of grains at its inlet, the higher the accuracy of the azimuthal orientation of grain at the outlet from of the inclined channel.

The conditions for the successful selection of grains with the required azimuthal orientation can be formulated as follows:

(1) The nucleation of the maximum number of grains at the bottom of the starter block is desirable.

(2) The length of the starter block should be sufficient to suppress grains with axial orientations far from the normal to the crystallizer.

(3) A large number of grains with the required axial orientation and different azimuthal orientations should take place near the inlet to the grain selector.

(4) The construction of the ceramic mold and geometric characteristics of the channel should ensure the orientation of the vector of the temperature gradient along the axis of the inclined channel of the grain selector.

CONCLUSIONS

The direction of the vector of the temperature gradient at the liquidus isotherm during the solidification of metal in the curvilinear channel depends on the conditions of the solidification and on the thickness of the mold walls.

Upon the solidification in a shell mold, when the external surface of the mold assigns the turns of the axis of the casting, as a rule, the direction of the vector of the temperature gradient is close to the direction of the tangent to the axis of the casting. This gives the opportunity to govern the orientation of the vector of the temperature gradient and, therefore, to influence the preferred direction of growth.

Based on the suggested method of controlling the preferred direction of growth, the construction of a grain selector for obtaining grains with a desired azimuthal orientation was proposed.

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