

UDC 669.245:621.74.045

<https://doi.org/10.17073/0021-3438-2025-2-55-65>

Research article

Научная статья



Grain structure simulation in a large-scale casting made of VZhL14N-VI nickel-base superalloy

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Abstract: The study addresses the problem of predicting the grain structure in large-scale castings made of the VZhL14N-VI nickel-base superalloy, which are bodies of revolution with very thin walls. To this end, the ProCast casting simulation software was used, including its CAFE module for grain structure prediction. Cooling rates in various areas of the casting were determined by computer simulation. Grain size measurements were then performed on real samples produced under industrial conditions at PJSC UEC Kuznetsov (Samara, Russia), and the correlation between grain size and cooling rate was established. It was found that grain size is affected not only by the cooling rate, but also by the geometric features of the casting, particularly its thermal modulus (according to Chvorinov’s rule). The results show that ProCast can be effectively used to predict casting defects in large-scale castings made of nickel-base superalloys. A comparison of the temperature-dependent density, specific heat capacity, and thermal conductivity of the VZhL14N-VI alloy – obtained through both direct measurements and ProCast thermodynamic database calculations – showed that the computed data are sufficiently accurate for use in casting process simulations. The CAFE module was found to be applicable for predicting grain structure in castings; however, accurate simulation requires the specification of key parameters, primarily the degree of undercooling during solidification and the number of grain nuclei in the alloy. Since these parameters cannot be measured directly, further research is required to determine them.

Keywords: nickel-base superalloys, VZhL14N-VI, investment casting, grain size, casting simulation, ProCast, CAFE module, thermal modulus.

Acknowledgments: This study was supported by the Ministry of Science and Higher Education of the Russian Federation under Government Decree No. 218, in accordance with Subsidy Agreement No. 075-11-2022-023 dated April 6, 2022, titled: “Development of a manufacturing technology for unique large-scale castings made of heat-resistant alloys for gas turbine engines, aimed at the use of domestically produced equipment and the establishment of a modern, resource-efficient, computer-aided casting production”.

For citation: Koltygin A.V., Nikitina A.A., Belova A.A., Bazhenov V.E., Belov V.D., Shchedrin E.Yu. Grain structure simulation in a large-scale casting made of VZhL14N-VI nickel-base superalloy. *Izvestiya. Non-Ferrous Metallurgy*. 2025;31(2):55–65.

<https://doi.org/10.17073/0021-3438-2025-2-55-65>

Моделирование макроструктуры крупногабаритной отливки из жаропрочного никелевого сплава ВЖЛ14Н-ВИ

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Аннотация: В работе рассмотрена проблема прогнозирования зеренной структуры в крупногабаритных отливках из никелевого жаропрочного сплава ВЖЛ14Н-ВИ, представляющих собой тела вращения с весьма тонкими литыми стенками. Для этого использовалась система компьютерного моделирования литейных процессов ProCast с модулем для расчета зеренной структуры CAFE. Путем компьютерного моделирования определена скорость охлаждения в различных частях отливки, после чего на реальных образцах, полученных в условиях промышленного производства в ПАО «ОДК-Кузнецов» (г. Самара, Россия), определены размеры зерен и построена их зависимость от скорости охлаждения отливки. Установлено влияние на размер зерна не только скорости охлаждения, но и геометрических особенностей отливки, в частности ее термический модуль (приведенная толщина). Показано, что система ProCast может быть эффективно использована для прогнозирования литейных дефектов в крупногабаритных отливках из жаропрочных никелевых сплавов. При этом путем сравнения температурных зависимостей плотности, теплоемкости и теплопроводности сплава ВЖЛ14Н-ВИ, полученных прямыми измерениями и расчетом с использованием термодинамической базы ProCast, выявлено, что расчетные данные достаточно точны для использования их в компьютерном моделировании литейных процессов. Установлено, что модуль CAFE может быть востребован для прогнозирования зеренной структуры в отливке, однако для его корректного применения необходимо установление параметров моделирования, прежде всего величины переохлаждения при затвердевании и количества зародышей зерен в сплаве. Поскольку эти параметры не поддаются прямому измерению, их определение потребует дополнительных исследований.

Ключевые слова: жаропрочные никелевые сплавы, ВЖЛ14Н-ВИ, литье по выплавляемым моделям, размер зерна, моделирование литейных процессов, ProCast, CAFE.

Благодарности: Работа выполнена при финансовой поддержке Министерства науки и высшего образования Российской Федерации в рамках Постановления Правительства № 218 по соглашению о предоставлении субсидии № 075-11-2022-023 от 06.04.2022 г. «Создание технологии изготовления уникальных крупногабаритных отливок из жаропрочных сплавов для газотурбинных двигателей, ориентированной на использование отечественного оборудования и организацию современного ресурсоэффективного, компьютероориентированного литейного производства».

Для цитирования: Колтыгин А.В., Никитина А.А., Белова А.А., Баженов В.Е., Белов В.Д., Щедрин Е.Ю. Моделирование макроструктуры крупногабаритной отливки из жаропрочного никелевого сплава ВЖЛ14Н-ВИ. *Известия вузов. Цветная металлургия*. 2025;31(2):55–65. <https://doi.org/10.17073/0021-3438-2025-2-55-65>

Introduction

Nickel-base superalloys are widely used as materials for manufacturing combustion chamber components of gas turbine engines (GTEs) [1; 2]. The composition of the VZhL14N-VI alloy (OST 1 90126-85) is given below (wt. %, max)¹:

Ni.....	Balance
C.....	0.08
Cr.....	20.0
Mo.....	5.0
Al.....	1.5
Ti.....	2.9
Nb.....	2.8
Fe.....	10.0

¹ Unless otherwise stated, all compositions are given in wt. %.

This alloy is used for large-scale cast GTE components and is characterized by a high content of the strengthening γ' phase ($\text{Ni}_3(\text{Al,Ti})$) [1–3]. In addition, the alloy is further strengthened by the precipitation of fine particles of δ (Ni_3Nb), η (Ni_3Ti), and σ (CrFeMoNi , CrMoNi , $(\text{Cr,Mo})_3\text{Ni}$) phases, as well as MC, M₂₃C₆, and M₆C carbides (where M is mainly Cr, but also Ti, Nb, and Mo) [4–8]. The high performance properties of VZhL14N-VI castings depend on their as-cast structure and its evolution during heat treatment [1; 4; 9], which are determined by a combination of grain size and the amount, size, and distribution of carbide and strengthening phases.

The grain size in a casting is affected by the cooling rate achieved during the solidification interval of the alloy. An increase in cooling rate leads to a higher ther-

mal gradient in the melt ahead of the solidification front, which results in the formation of a larger number of crystals in the two-phase region of the solidifying casting. As a result, competitive grain growth leads to grain refinement [10–12].

To simulate the grain structure in castings, the ProCast (ESI Group) casting simulation system is commonly used, which includes a dedicated CAFE module for grain structure prediction [13]. This module enables the simulation of grain size, shape, and growth direction in castings with equiaxed, columnar, or single-crystal structures [14]. The CAFE module has shown good performance in predicting grain structures in small-scale nickel-base superalloy castings, including turbine blades [15, 16]. However, its application to large-scale castings is limited by the extremely large number of elements in the computational mesh.

In this study, the effect of casting conditions in a shell ceramic mold on the macrostructure of a VZhL14N-VI alloy casting was investigated using computer simulation methods. An attempt was also made to use the CAFE module to predict grain size in large-scale castings. The simulation results were compared with experimental measurements of grain size on samples cut from the casting, with the aim of assessing the effect of cooling rate on grain size in large-scale castings with significant wall thickness variations.

Materials and methods

The test casting was produced using refractory shell molds by investment casting technology. Fused quartz of various fractions, manufactured by JSC DINUR (Pervouralsk, Russia), was used as the filler for both slurry and stucco coatings. Ultracast One+ and Ultracast Prime binders (Technopark LLC, Moscow, Russia) were selected for preparing the refractory slurry. The charge material was a ready-made batch of VZhL14N-VI alloy produced by the All-Russian Scientific Research Institute of Aviation Materials (VIAM, Moscow, Russia). Melting and pouring were performed using the VIAM-24 vacuum induction melting and casting unit (Russia) according to the process specifications of PJSC UEC-Kuznetsov (Samara, Russia).

To reveal the macrostructure, a metallographic template was cut from the casting (Fig. 1) after heat treatment, in a plane passing through the axis of rotation. The sectioned surface of the template was ground and polished using abrasive materials to obtain a mirror-like metallographic surface. The surface was then etched using Marble's reagent (20 g Cu_2SO_4 , 100 mL hyd-

rochloric acid, 100 mL ethanol) [17]. Macrostructure images were acquired using a Canon EOS 6D digital camera equipped with a Volna-9 macro lens and extension tubes.

The casting process simulation was carried out using the ProCast software (ESI Group), which has proven effective for simulating investment casting processes involving ceramic shell molds [18–20]. The CAD model included representations of the casting, ceramic mold, insulation, flask, and internal furnace space. The simulation was performed taking into account a 20-minute pre-cooling period of the mold prior to pouring (pouring temperature: 1490 °C), as well as radiative heat transfer. A more detailed description of the simulation procedure is available in [13]. The thermophysical properties of the refractory materials used in the simulation were found to be in good agreement with data reported by other researchers [21; 22]. The grain structure of the casting was simulated using the CAFE module of the ProCast software. The initial CAFE calculation parameters were adopted from [23].

To refine the thermophysical properties of the VZhL14N-VI alloy, measurements were conducted to determine the density (ρ), specific heat capacity (C_p), thermal conductivity (λ), and thermal diffusivity ($\lambda = \rho C_p$), as well as their temperature dependence.

Density at 25 °C was measured using the hydrostatic weighing method. The $\rho(t)$ dependence was calculated based on the thermal expansion coefficient measured with a DIL 402C dilatometer (NETZSCH, Germany). Thermal diffusivity was evaluated by the laser flash method using an LFA 447 instrument (NETZSCH). Specific heat capacity was measured using a DSC 204 F1 Phoenix differential scanning calorimeter (NETZSCH).

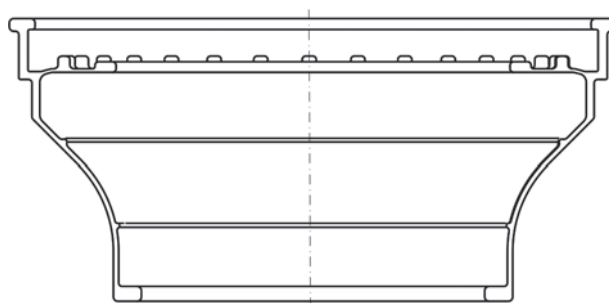


Fig. 1. Schematic cross-section of the test casting
Maximum overall dimension: 690 mm

Рис. 1. Эскиз тестовой отливки в разрезе
Максимальный габаритный размер 690 мм

Results and discussion

The test component, produced at PJSC UEC-Kuznetsov, is a large shell-type casting in the form of a body of revolution, with a maximum diameter of about 685 mm and a predominant wall thickness of 6 mm. Figure 2 shows its macrostructure in a longitudinal section through the axis of rotation.

It can be seen that grain size varies significantly across different areas of the casting. During the solidification of massive regions near the mold surface, a fine-grained structure forms, which rapidly transitions into a coarse-grained one. In the thin-walled sections, such transitions are not observed, and the structure remains relatively homogeneous and fine-grained. It is well known that such a structure is most desirable in polycrystalline castings, including those made from nickel-base superalloys, as it ensures optimal mechanical properties of the cast part in accordance with the Hall–Petch relationship [10].

Thus, the highest cooling rates during solidification were observed in the regions with the smallest

grain size, while the lowest cooling rates corresponded to coarser-grained areas. In practice, direct measurement of the cooling rate in a solidifying casting is difficult; therefore, the pouring and solidification processes of the VZhL14N-VI alloy were simulated to estimate the cooling rates in different regions of the casting.

Due to equipment limitations, direct measurements of the thermophysical properties of the VZhL14N-VI alloy were restricted to a relatively narrow temperature range (up to 300 °C). To extend the dataset, temperature-dependent properties were calculated using the ProCast thermodynamic database. These calculated values were validated by comparing them with experimental results. Fig. 3 shows both measured and simulated temperature dependencies of density, specific heat capacity, and thermal conductivity for the VZhL14N-VI alloy. The comparison confirms a good level of agreement. The calculated data were subsequently used in the simulation workflow.

The cooling rate in a ceramic shell mold is affected by numerous external factors, all of which were ac-



Fig. 2. Grain structure of the test casting wall (etched)

1–9 – grain size measurement areas

Рис. 2. Макроструктура стенки тестовой отливки (травлено)

1–9 – области определения размеров зерен

counted for in the simulation [13]. Fig. 4 presents the relationship between grain size and cooling rate within the solidification interval, based on simulation results at the locations where grain size measurements were performed, as shown in Fig. 2.

At constant wall thickness, higher cooling rates generally result in finer grain sizes. However, this trend is not observed in the relatively thick-walled areas corresponding to points 2 and 5 in Fig. 2: the grain sizes there are nearly identical despite differences in cooling rate. Fig. 5 presents the calculated thermal modulus (equivalent wall thickness) [12] and the temperature distribution across the cross-section of the casting at the moment of mold filling. It can be seen that the areas corresponding to points 2 and 5 had lower initial temperatures — close to the alloy's liquidus temperature — compared to neighboring areas. In addition, these areas exhibited a higher thermal modulus than the surrounding regions in the same cross-section.

These findings suggest that in castings with complex geometry, the relationship between grain size and wall thickness is not always clearly defined when comparing areas of different thicknesses. However, a consistent correlation between grain size and thermal modulus can be observed in areas with similar wall thickness. For example, in areas 1, 9, and 3 (see Fig. 2), the grain size increases progressively (see Fig. 4), which corresponds to an increase in the equivalent wall thickness (see Fig. 5). This correlation is logical, as the thermal modulus is defined as the ratio of the volume of a given casting region to its cooling surface area. A higher thermal modulus indicates slower heat removal and a more uniform temperature distribution in the solidifying casting. Therefore, grain size appears to depend not only on the cooling rate, but primarily on the degree of undercooling achieved in the molten alloy ahead of the solidification front [24; 25]. This principle underlies the grain size prediction model implemented in Pro-Cast [20; 23].

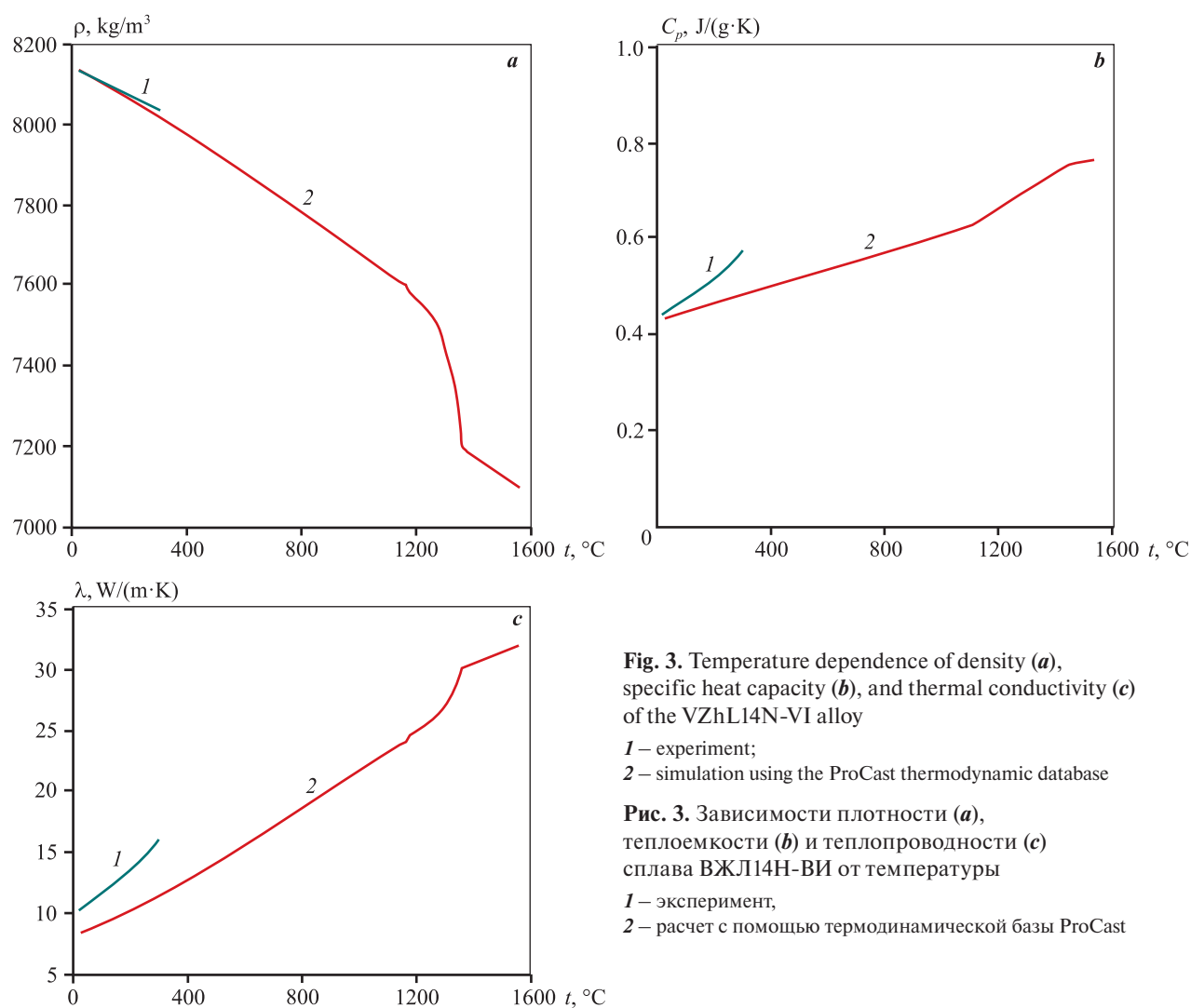


Fig. 3. Temperature dependence of density (a), specific heat capacity (b), and thermal conductivity (c) of the VZhL14N-VI alloy

1 — experiment;
2 — simulation using the ProCast thermodynamic database

Рис. 3. Зависимости плотности (a), теплоемкости (b) и теплопроводности (c) сплава ВЖЛ14Н-ВИ от температуры

1 — эксперимент,
2 — расчет с помощью термодинамической базы ProCast

Figure 6 shows the simulation results for the solid phase fraction in the casting at the beginning and just before the end of solidification. It can be seen that an

isolated thermal node forms at the Y-shaped junction of the walls (position 4), which leads to the formation of shrinkage porosity in this area, confirmed by metallographic examination. The presence of shrinkage defects does not affect the grain size in the corresponding areas (see Fig. 3). It should be noted that the revealed porosity zone was not identified during production using non-destructive testing methods and was discovered only after analyzing the simulation results. This demonstrates the great potential of computer-aided casting process simulation for improving the quality of castings.

The results of grain structure simulation using the CAFE module are shown in Fig. 7, with the input parameters listed in the accompanying table. The initial simulation (Fig. 7, *a*) was performed using parameter values proposed for the IN713C nickel-base superalloy [23]. However, since the VZhL14N-VI alloy has a different composition and was cast under conditions differing from those described in [23], the simulation parameters may vary significantly, and the simulation results may not correspond to the actual grain structure observed in the casting. Nevertheless, due to the lack of verified data for VZhL14N-VI, the parameters for IN713C superalloy were used as a starting point [23].

As shown in Fig. 7, *a*, the simulated grain sizes are significantly larger than those observed in the real casting. Nevertheless, the main trends are consistent with

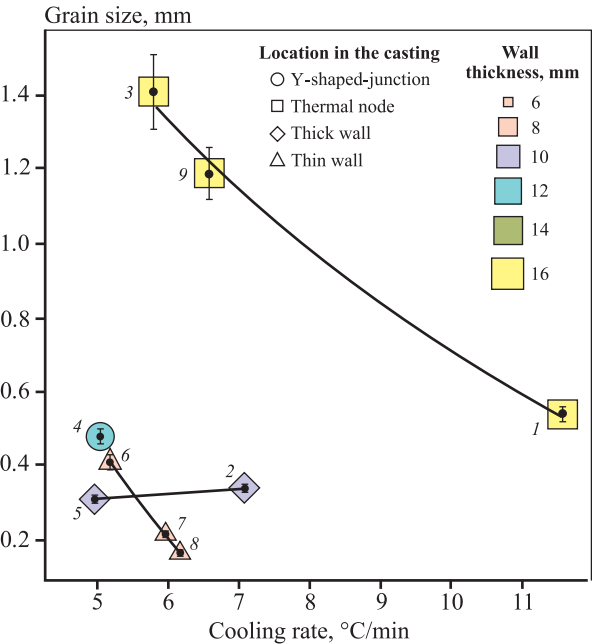


Fig. 4. Grain size vs. cooling rate in the solidification interval for the casing-shaped test component
Points 1–9 correspond to the locations shown in Fig. 2

Рис. 4. Зависимость размера зерна в отливке «корпус» от скорости охлаждения в интервале кристаллизации
Цифры 1–9 соответствуют точкам, обозначенным на рис. 2

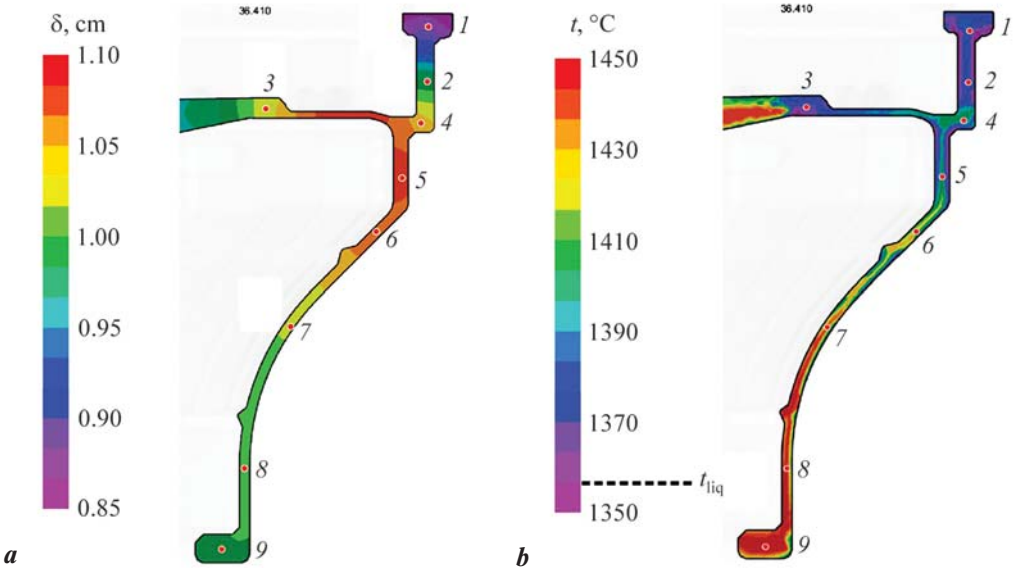


Fig. 5. Thermal modulus (δ) — equivalent wall thickness (*a*), and temperature at the moment of mold filling (*b*)

Рис. 5. Термический модуль отливки (δ) — приведенная толщина стенки (*a*) и температура в момент заполнения формы (*b*)

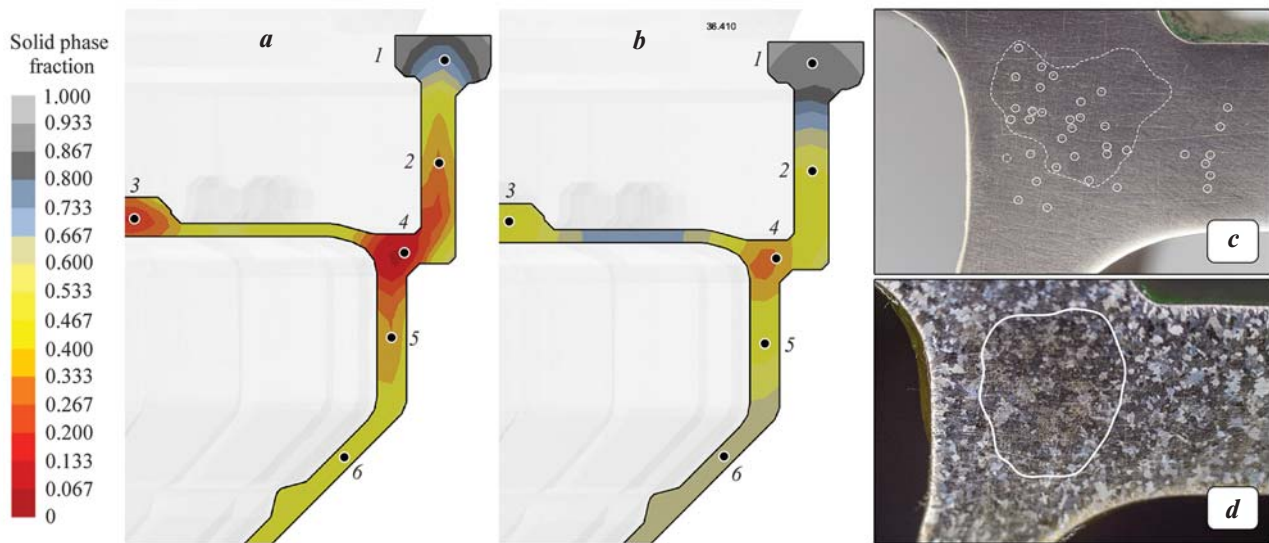


Fig. 6. Simulation results: solid phase fraction after 95 s (*a*) and 157 s (*b*) from the start of pouring; structure in area 4 on a polished sample (*c*) (dashed outline indicates the porous region; individual pores are marked with circles) and on an etched sample (*d*)

Рис. 6. Результаты моделирования: доля твердой фазы спустя 95 с (*a*) и 157 с (*b*) с начала заливки и структура в зоне 4 на полированном (пунктиром выделена область пористости, отдельными окружностями – визуально заметные поры) (*c*) и травленном (*d*) образцах

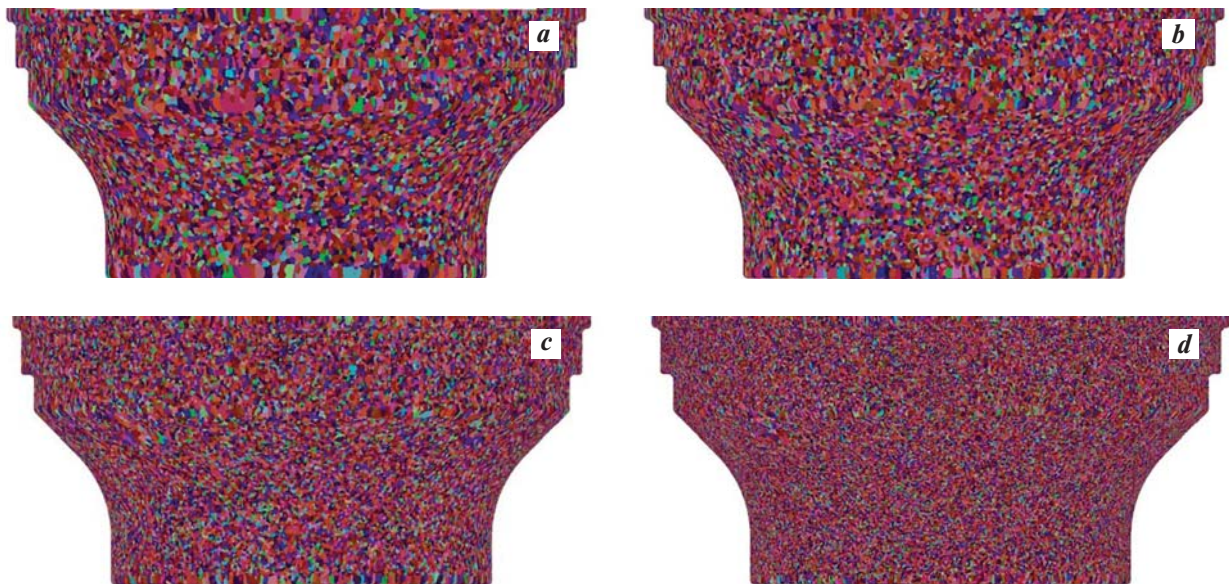


Fig. 7. Results of grain structure simulation using the CAFE module
Simulation cases: 1 (*a*), 2 (*b*), 3 (*c*), and 4 (*d*) (see table)

Рис. 7. Результаты моделирования зеренной структуры отливки с использованием модуля CAFE
Варианты моделирования 1 (*a*), 2 (*b*), 3 (*c*) и 4 (*d*) (см. таблицу)

the actual structure observed in the casting. The main parameters affecting the simulated grain size include the average undercooling (Δt_{avg}), its deviation (Δt_{dev}), and the number of grain nuclei in the melt (n_{max}), which

are defined separately for the casting volume and the mold-contacting surface layer [16].

Since the initial simulation produced grains larger than those found in the actual casting — while the overall

Key parameters in grain structure simulation with the CAFE module

Основные параметры моделирования зеренной структуры отливки с использованием модуля CAFE, применявшиеся в работе

Simulation case	Δt_{avg} , K		Δt_{dev} , K		n_{max} , m^{-3} , m^{-2}	
	Volume	Surface	Volume	Surface	Volume	Surface
1 [23]	6.5	5.5	0.7	0.2	$5 \cdot 10^7$	$1 \cdot 10^4$
2					$1 \cdot 10^7$	$5 \cdot 10^4$
3					$5 \cdot 10^7$	$1 \cdot 10^5$
4					$1 \cdot 10^8$	$5 \cdot 10^5$

distribution pattern remained comparable — subsequent iterations retained the same undercooling parameters but increased the number of grain nuclei. In practice, it is extremely difficult to determine the actual number of grain nuclei present in the alloy under industrial casting conditions. Therefore, this number must be adjusted by comparing simulation results with experimentally observed grain structures. This approach requires a separate, resource-intensive study.

The results of the follow-up simulations are shown in Fig. 7, *b–d*. It is evident that increasing the number of grain nuclei in the alloy leads to grain refinement in the casting.

Thus, it is possible to select a combination of initial parameters that yields results correlating with data obtained from actual castings. These parameter values can subsequently be used in simulations to predict grain structure in castings. However, selecting such parameters requires additional studies on a series of castings followed by corresponding simulations. It should also be noted that grain structure simulation in large-scale castings is a highly resource-intensive and time-consuming process that requires the use of high-performance computing systems.

Conclusions

1. Grain size in large-scale castings made of nickel-base superalloys depends on the thermal conditions during solidification — primarily the cooling rate, equivalent wall thickness, and thermal gradient developed in the casting during solidification.

2. Computer simulation using the ProCast software enables the determination of cooling rates in various areas of the casting and helps identify their effect on grain size in walls of similar thickness. In cases of significant variation in wall thickness, grain size is influenced by

multiple factors and does not always correlate directly with cooling rate.

3. The CAFE module can be used to simulate grain size in the walls of large-scale castings made of nickel-base superalloys; however, preliminary studies are required to determine key simulation parameters, especially the number of grain nuclei.

4. The ProCast simulation software can also be used to reliably predict shrinkage-related casting defects in large-scale castings made of nickel-base superalloys.

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The article was submitted 10.09.2024, revised 17.12.2024, accepted for publication 19.12.2024

Статья поступила в редакцию 10.09.2024, доработана 17.12.2024, подписана в печать 19.12.2024