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PROPERTIES OF NICKEL-BASED SUPERALLOYS OF EQUIAXIAL CRYSTALLIZATION

Purpose. The aim of the work is to obtain predictive regression models, with the help of which, it is possible to adequately calculate the mechanical properties of nickel-based superalloys of equiaxial crystallization, without carrying out preliminary experiments.

Research methods. To find regularities and calculate the latest CALPHAD method was chosen, and modeling of thermodynamic processes of phase crystallization was performed.

Results. As a result of experimental data processing, the ratio of alloying elements $K\gamma'$ was proposed for the first time, which can be used to assess the mechanical properties, taking into account the complex effect of the main alloy components. The regularities of the influence of the composition on the properties of heat-resistant nickel alloys of equiaxial crystallization are established. The analysis of the received dependences in comparison with practical results is carried out. The relations well correlated with heat resistance, mismatch and strength of alloys are obtained.

Scientific novelty. It is shown that for multicomponent nickel systems it is possible with a high probability to predict a mismatch, which significantly affects the strength characteristics of alloys of this class. The regularities of the influence of the chemical composition on the structure and properties of alloys are established. A promising and effective direction in solving the problem of predicting the main characteristics of heat-resistant materials based on nickel is shown.

Practical value. On the basis of an integrated approach for multicomponent heat-resistant nickel-based alloys, new regression models have been obtained that make it possible to adequately predict the properties of the chemical composition of the alloy, which made it possible to solve the problem of computational prediction of properties from the chemical composition of the alloy. This allows not only to design new nickel-based alloys, but also to optimize the composition of existing brands.

Key words: nickel-based equiaxial crystallization superalloys, strength, mismatch (γ/γ' - mismatch), heat resistance.

Introduction

The development of new and optimization of existing alloys for cast parts, namely, the most heavily loaded, such as the working and nozzle blades of a gas turbine engine, is a material science, design and technological task that requires a comprehensive solution [1–4]. For modern thermally stressed gas turbine engines, the above-mentioned complex-profile parts are made from multicomponent heat-resistant alloys based on nickel, cobalt and iron by the methods of equiaxed, directional or monocrystalline casting [5–9].

Recent developments have focused on the study of blade materials with a low content of expensive elements for aircraft engine building. One of the problems of this type of materials is to increase their strength properties. To increase the high-temperature strength, the alloys are alloyed with a high chromium content. However, a high chromium content can cause the appearance of topologically close-packed phases of the μ , σ type in the casting structure during the development process, which will lead to phase-structural instability and embrittlement of parts [10–14].

Strengthening by the γ' -phase ensures long-term preservation of the high temperature performance of alloys of this class in a wide temperature range, up to 1150 °C. Consequently, the most important role in the

resistance to high-temperature creep superalloys nickel-based equiaxial crystallization belongs to such structural-phase characteristics as the period of the crystal lattices of the γ - and γ' - phases and their dimensional mismatch δ or γ/γ' - mismatch [15–20].

The aim of the work is to obtain predictive regression models, with the help of which, it is possible to adequately calculate the mechanical properties of the nickel-based superalloys, without carrying out preliminary experiments.

Material and research technique

For experimental and theoretical studies of temperature performance, a working sample of alloys was formed, consisting of well-known industrial nickel-based superalloys for equiaxed casting of domestic and foreign production, the following brands: ZhS6U, ZhS6K, VZhL12U, VZhL12E, B1900, IN 100, MAR M200, MAR M246, TRW NASA 6A, WAZ16, U500, U700, ZhS3DK, ZhS3LS, VH4L, ChS88U, ChS104, RENE77, IN939, IN738LC, CM681, RENE220, NFP1916, ChS70S, CM939WELDABLE. The selection of alloys was made from the standpoint of a variety of chemical compositions (alloying systems), which, in terms of the content of the main elements, cover a wide range of alloying.

The obtained values were processed in the Microsoft Office software package in the EXCEL package using the least squares method to obtain correlation dependences of the "parameter-property" type with obtaining mathematical equations of regression models that optimally describe these dependences and plotting trend lines. The dependences have a sufficiently high coefficient of determination $R^2 \geq 0.85$ and are suitable for determining the temperature characteristics of the nickel-based superalloys.

Research results and discussion

Considering that the role in the high-temperature creep resistance of heat-resistant nickel alloys belongs to such a structural parameter as the dimensional mismatch δ (γ/γ' - mismatch), which depends on the alloying system, the urgent task is to obtain an optimal regression model for calculating this characteristic for based on the chemical composition of alloys of the class nickel-based superalloys equiaxed crystallization.

All components used for alloying nickel-based superalloys can be conditionally divided into three groups: dissolving mainly in the γ -solid solution (Co, Cr, Mo, W, Re), dissolving mainly in the-phase (Al, Ti, Ta, Hf) and carbide-forming elements (Ti, Ta, Hf, Nb, V, W, Mo, Cr).

On the other hand, many elements can be included in the γ' -phase: Al, Ti, Nb, Cr, Co, Mo, W, V, etc. But their content in the γ' -phase and the effect on its amount in the structure are different. This effect is associated with the ability of the elements to form stable intermetallic phases of the Ni_3Me type with nickel. Hence, it follows that the misfit and mechanical properties of alloys are influenced not only by the elements that belong to the γ' - forming, but also those that are classified as γ - hard mortar hardeners [21–24].

As a result of processing the experimental data and the above reasoning, for the first time a relation was proposed $K_{\gamma'} = 5 \frac{\sum_{\gamma'} (Al + Ti + Nb + Ta + Hf)}{\sum_{\gamma} (Cr + W + Mo + Re + Co + Ru)}$ (ca-

libration factor 5 was determined empirically) for evaluating the mechanical properties, which takes into account the complex effect of the main components of the alloy. Since the dimensional mismatch of the lattice parameters is associated with the degree of concentration solid solution hardening of the γ - and γ' - phases, the efficiency of precipitation hardening of the alloy, the creep rate, and other properties, the $K_{\gamma'}$ ratio allows us to associate these properties with multicomponent systems [1–10].

It was found that the dimensional mismatch δ has parabolic dependences both at 20 and at 1000 (Fig. 1a, b) with the relations:

$$\delta^{20} = 0,1001(K_{\gamma'})^2 - 0,3257(K_{\gamma'}) + 0,4789;$$

$$\delta^{1000} = 0,0953(K_{\gamma'})^2 - 0,3427(K_{\gamma'}) + 0,0325.$$

An increase in the $K_{\gamma'}$ ratio leads to a decrease in the

misfit and the formation of an extremum at values of 1.5–2, this is associated with a reduction in the number of elements in the γ -solid solution, which most strongly increase the lattice period (Mo, W, Nb, Ta, etc.). At $K_{\gamma'}$ values greater than 1.5–2, an increase in misfit is observed, since the volume fraction of γ' - forming elements significantly increases and begins to prevail. The strength value with an increase in the ratio $K_{\gamma'}$ obeys a linear law ($\sigma_B = 146,34(K_{\gamma'}) + 713,73$ and has a tendency to a constant increase (Fig. 1c), since with an increase in the ratio, the number of elements forming the hardening phase increases.

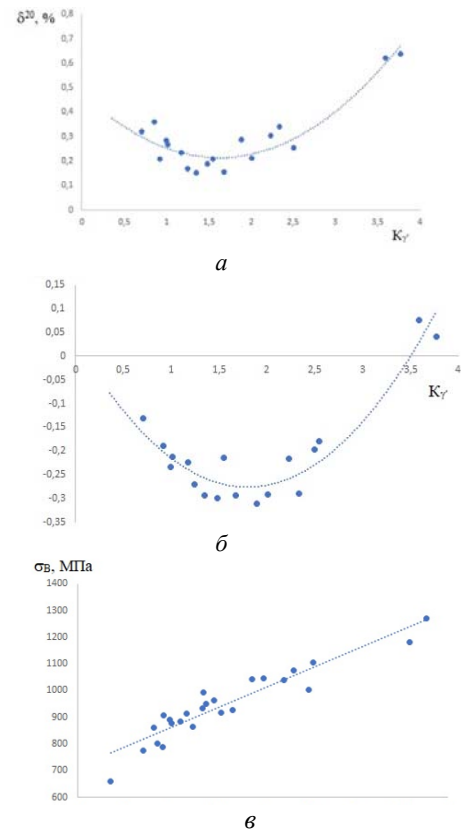


Fig. 1. Correlation dependences of the properties of equiaxed superalloy on the ratio $K_{\gamma'}$ in their composition: (a) – dependence of misfit (δ^{20}) on the value of the ratio $K_{\gamma'}$; (b) – dependence of misfit (δ^{1000}) on the value of the ratio $K_{\gamma'}$; (c) – dependence of the short-term strength limit (σ_B) on the value of the ratio $K_{\gamma'}$

It is shown that at a test temperature of 1000 °C, the dependence of the limits of 100- and 1000-hour long-term strength on the value of the misfit (Fig. 2a, b) is optimally described by the obtained models:

$$\sigma_{100}^{1000} = 65,185K_{\gamma'} + 56,683 \text{ (Fig. 3a);}$$

$$\sigma_{100}^{1000} = 57,689K_{\gamma'} - 26,58 \text{ (Fig. 2b).}$$

These dependences show that with an increase in the $K_{\gamma'}$ coefficient, the long-term strength of the alloys increases in direct proportion, since the number of γ' - forming elements increases, and, consequently, the volume of the-phase in the alloy increases.

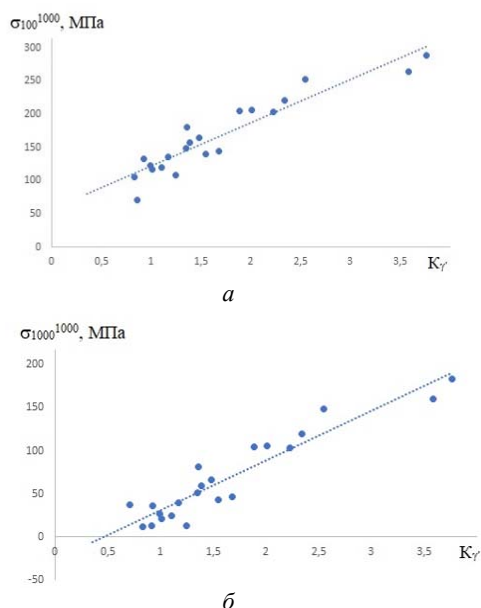


Fig. 2. Correlation dependences of the long-term strength of equiaxed superalloys on the ratio $K\gamma'$ in their composition: (a) – dependence of long-term strength (σ_{100}^{1000} , MPa) on the value of the ratio $K\gamma'$; (b) – dependence of long-term strength (σ_{1000}^{1000} , MPa) on the value of the ratio $K\gamma'$

It was found that the proposed ratio $K\gamma'$ has a close correlation with the volume fraction of the γ' - phase in equiaxed nickel-based superalloys (Fig. 3). All these dependences are linear with a positive slope and an error of no more than $\pm 3.8\%$. This behavior is explained by the fact that with an increase in $K\gamma'$, the volumetric amount of the main strengthening elements increases, which form the γ' - phase both at room temperature (Fig. 3a) and residual at elevated operating temperatures (Fig. 3a), and consequently the limits of short-term (Fig. 1c) and long-term strength (Fig. 3) of alloys increase.

To eliminate the influence of volumetric diffusion processes at high temperatures, expensive heavy metals such as tungsten, molybdenum, rhenium and ruthenium are introduced into the composition of the nickel-based superalloys, which significantly increased the density of alloys, and, consequently, the weight of the finished product. It is known that the density ρ is closely correlated with the average atomic mass of the alloy A_c ; therefore, the authors proposed a regression model obtained for multicomponent alloying systems of equiaxed nickel-based superalloys: $\rho = 0,1613A_c - 1,0026$ with an error not exceeding $\pm 1\%$ (Fig. 4).

In fig. 4 shows the dependence of the specific density on the average atomic mass of alloys, which has a linear character, since an increase in the number of elements with a high atomic mass (refractory) will inevitably increase the density of equiaxed alloys. This tendency manifests itself as a consequence of the fact that elements with a high atomic mass belong to elements with a high melting point, which strengthen the γ - solid solution and do not have a noticeable effect on the intermetallic hard-

ening of alloys. The obtained regression models make it possible to predict the specific gravity, short-term and long-term strength limit, misfit according to the obtained ratio of $K\gamma'$ of alloying elements in alloys and can be used both in the development of new equiaxed nickel-based superalloys and in the improvement of known industrial compositions within the graded composition.

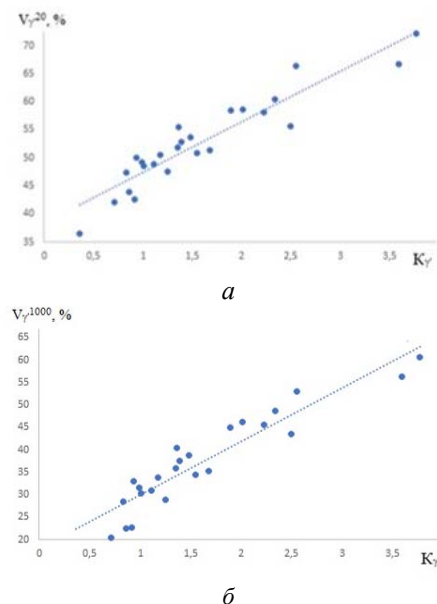


Fig. 3. Correlation dependences of the volume of the γ' – phase in equiaxed superalloys on the ratio of $K\gamma'$ in their composition (a) – dependence of the volume of the phase at room temperature ($V\gamma'_{20}$, %) on the value of the ratio $K\gamma'$; (b) – dependence of the volume of the γ' – phase at 1000 °C ($V\gamma'_{1000}$, %) on the value of the ratio $K\gamma'$ (• – calculated values; ♦ – experimental values)

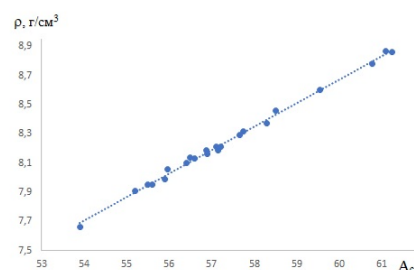


Fig. 4. Correlation dependence of the density of equiaxed superalloys on the atomic mass of the alloy. (• – calculated values; ♦ – experimental values)

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Глотка О. А., Ольшанецкий В. Ю. Власивості жароміцних сплавів на основі нікелю рівновісної кристалізації

Метою роботи є отримання прогнозних регресійних моделей, за допомогою яких можна адекватно розрахувати механічні властивості жароміцних сплавів на основі нікелю рівновісної кристалізації без проведення попередніх експериментів.

Методи дослідження. Для пошуку закономірностей було обрано найновіший метод CALPHAD та проведено моделювання термодинамічних процесів фазової кристалізації.

Отримані результати. В результаті експериментальної обробки даних вперше було запропоновано співвідношення легувальних елементів $K_{\gamma'}$, яке може бути використано для оцінки механічних властивостей з урахуванням комплексної дії основних компонентів сплаву. Встановлено закономірності впливу складу на властивості жароміцних нікелевих сплавів рівновісної кристалізації.

Наукова новизна. Показано, що для багатокомпонентних нікелевих систем можна з великою ймовірністю передбачити невідповідність кристалічних ґраток, що суттєво впливає на міцнісні характеристики сплавів цього класу. Показано перспективний та ефективний напрямок у вирішенні проблеми прогнозування основних характеристик жароміцних матеріалів на основі нікелю

Практичне значення. На основі інтегрованого підходу для багатокомпонентних жароміцних сплавів на основі нікелю отримані нові регресійні моделі, що дозволяють адекватно прогнозувати властивості за хімічним складом сплаву, що дало змогу вирішити проблему обчислювального прогнозування властивостей за хімічним складом сплаву.

Ключові слова: жароміцні сплави рівновісної кристалізації на основі нікелю, міцність, невідповідності (γ/γ' - невідповідність), термостійкість.

Глотка А. А., Ольшанецкий В. Ю. Свойства жаропрочных сплавов на основе никеля равноосной кристаллизации

Целью работы является получение прогнозных регрессионных моделей, с помощью которых можно адекватно рассчитать механические свойства жаропрочных сплавов на основе никеля равноосной кристаллизации без проведения предварительных экспериментов.

Методы исследования. Для поиска закономерностей был избран новейший метод CALPHAD и проведено моделирование термодинамических процессов фазовой кристаллизации.

Полученные результаты. В результате экспериментальной обработки данных впервые было предложено соотношение легирующих элементов $K_{\gamma'}$, которое может быть использовано для оценки механических свойств с учетом комплексного действия основных компонентов сплава. Установлены закономерности влияния состава на свойства жаропрочных никелевых сплавов равноосной кристаллизации.

Научная новизна. Показано, что для многокомпонентных никелевых систем можно с большой вероятностью предположить несоответствие кристаллических решеток существенно влияет на прочностные характеристики сплавов этого класса. Показано перспективный и эффективный направление в решении проблемы прогнозирования основных характеристик жаропрочных материалов на основе никеля.

Практическое значение. На основе интегрированного подхода для многокомпонентных жаропрочных сплавов на основе никеля получены новые регрессионные модели, позволяющие адекватно прогнозировать свойства по химическому составу сплава, что позволило решить проблему вычислительного прогнозирования свойств по химическому составу сплава.

Ключевые слова: жаропрочные сплавы равноосной кристаллизации на основе никеля, прочность, несоответствия (γ/γ' - несоответствие, термостойкость).