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FORECASTING THE PROPERTIES OF HEAT-RESISTANT NICKEL ALLOYS EQUALAXIAL CRYSTALLIZATION

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. 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. A promising and effective direction in solving the problem of predicting the main characteristics of heat-resistant materials based on nickel is shown.

Keywords: heat-resistant nickel alloys; mismatch (γ/γ'-mismatch) strength; heat resistance

1. 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 [1-6]. 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 [7-15].

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 [16-24].

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 heat-resistant nickel alloys (HRNA) 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 [25-29].

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 HRNA, without carrying out preliminary experiments.

2. Material and research technique

For experimental and theoretical studies of temperature performance, a working sample of alloys was formed, consisting of well-known industrial HRNA 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 re-

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gression 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 HRNA.

3. 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 HRNA equiaxed crystallization.

All components used for alloying HRNA 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 [30-33].

In the middle of the last century, the composition of superalloys did not contain many γ'-forming elements such as Al, Ti, Ta, Hf (Fig. 1). Since the end of the 1980s, rhenium has been introduced into alloys in an amount of 2-4%. Over the years, the amount of Re and Al increased with a simultaneous decrease in Ti and Mo. This is due to the fact that the gamma-strike-phase enriched in aluminum has an increased resistance to creep, and rhenium increases the heat resistance of the gamma solid solution. In the early 2000s, ruthenium began to be added to alloys, which leads to an increase in the heat resistance of the alloys [34].

As a result of processing the experimental data and the above reasoning, for the first time a relation was proposed $K_{\gamma'} = 5\frac{\sum_{\gamma'}(\mathrm{Al}+\mathrm{Ti}+\mathrm{Nb}+\mathrm{Ta}+\mathrm{Hf})}{\sum_{\gamma}(\mathrm{Cr}+\mathrm{W}+\mathrm{Mo}+\mathrm{Re}+\mathrm{Co}+\mathrm{Ru})}$ (calibration 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. 2a, 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 g-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 (σ_B = 146,34($K_{\gamma'}$) + 713,73) and has a tendency to a constant increase (Fig. 2c), since with an increase in the ratio, the number of elements forming the hardening phase increases.

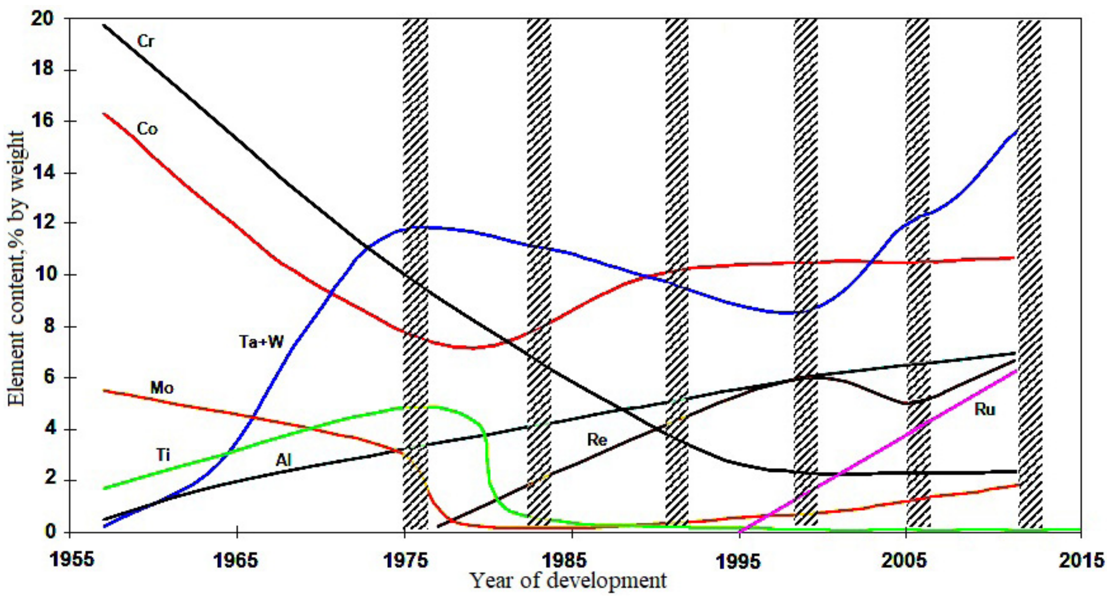

Fig. 1. Dependence of changes in the chemical composition of superalloys on the year of development

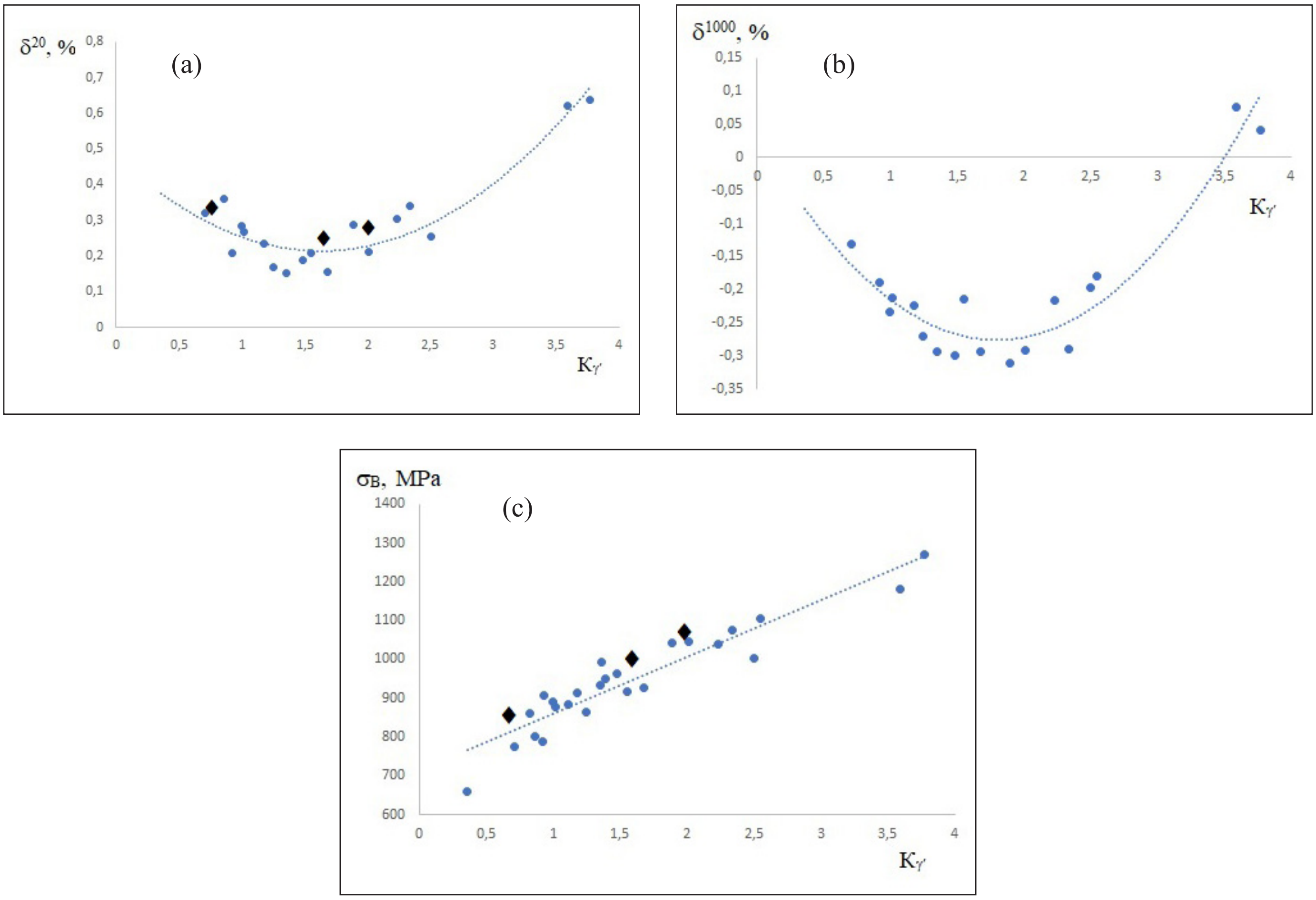

Fig. 2. Correlation dependences of the properties of equiaxed superalloy on the ratio $K\gamma'$ in their composition: (a) – dependence of misfit (δ^{20}) on the value of the ratio $K\gamma'$; (b) – dependence of misfit (δ^{1000}) on the value of the ratio $K\gamma'$; (c) – dependence of the short-term strength limit (σ_B) on the value of the ratio $K\gamma'$. (● – calculated values; ♦ – experimental values)

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. 3a, b) is optimally described by the obtained models: $\sigma_{100}{}^{1000} = 65{,}185K_{\gamma'} + 56{,}683$ (Fig. 3a); $\sigma_{1000}{}^{1000} = 57{,}689K_{\gamma'} - 26{,}58$ (Fig. 3b). 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.

It was found that the proposed ratio $K\gamma'$ has a close correlation with the volume fraction of the γ'-phase in equiaxed HRNA (Fig. 4). All these dependences are linear with a positive slope

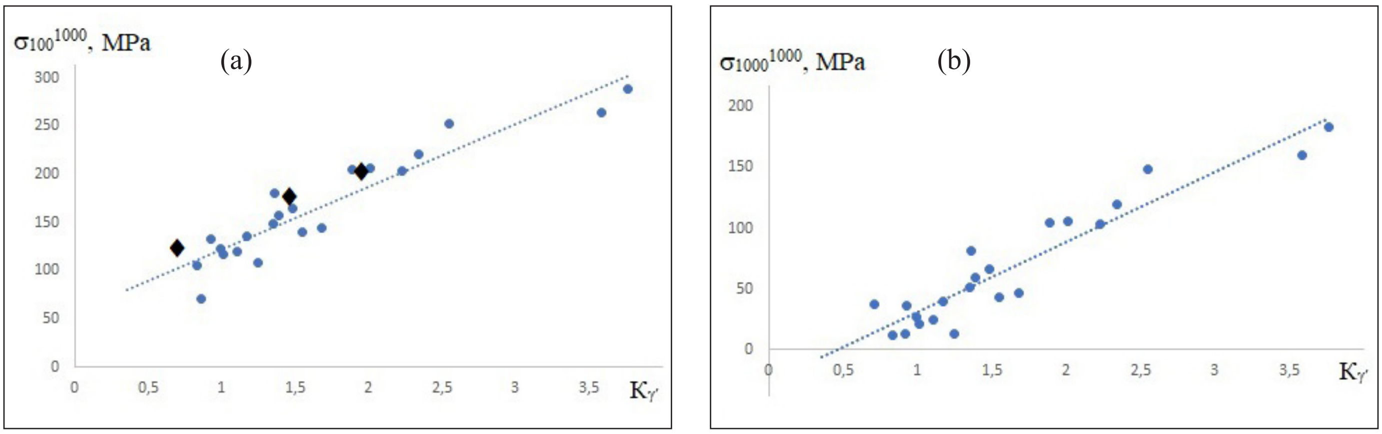

Fig. 3. Correlation dependences of the long-term strength of equiaxed superalloys on the ratio $K\gamma'$ in their composition: (a) – dependence of long-term strength ($\sigma_{100}{}^{1000}$, MPa) on the value of the ratio $K\gamma'$; (b) –dependence of long-term strength ($\sigma_{1000}{}^{1000}$, MPa) on the value of the ratio $K\gamma'$.(● – calculated values; ♦ – experimental values)

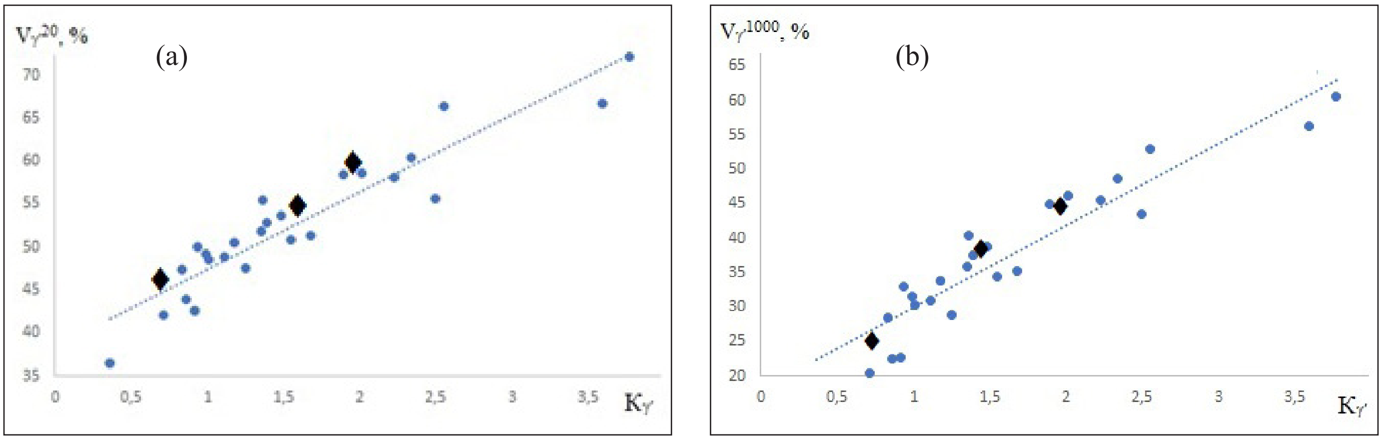

Fig. 4. Correlation dependences of the volume of the γ'-phase in equiaxed superalloys on the ratio of $K\gamma'$ in their composition (a) – dependence of the volume of the фазы-phase at room temperature ($V\gamma'$20, %) on the value of the ratio $K\gamma'$; (b) – dependence of the volume of the γ'-phase at 1000°C ($V\gamma'$1000, %) on the value of the ratio $K\gamma'\gamma'$(● – calculated values; ♦ – experimental values)

and an error of no more than ±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. 4a) and residual at elevated operating temperatures (Fig. 4a), and consequently the limits of short-term (Fig. 2c) 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 HRNA, 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 HRNA: $\rho = 0{,}1613 \cdot A_c - 1{,}0026$ with an error not exceeding ±1% (Fig. 5).

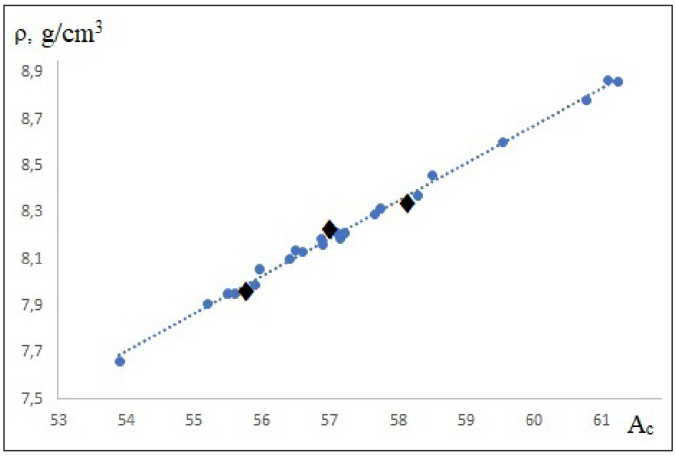

Fig. 5. Correlation dependence of the density of equiaxed superalloys on the atomic mass of the alloy. (● – calculated values; ♦ – experimental values)

In figure 5 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 hardening 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 HRNA and in the improvement of known industrial compositions within the graded composition.

The results of calculating the characteristics of the HRNA of equiaxed crystallization were further compared with the experimental data. To confirm the calculated values, the industrial heat-resistant nickel alloys Udimed520, DSMGA1400 and ZMI-3U were chosen. Based on the analysis of the experimentally obtained data on the mechanical properties of the studied alloys, Table 1 shows the values of the calculated parameters obtained using an active experiment.

TABLE 1

Computational and experimental properties
of heat-resistant nickel alloys

Result method	Properties of heat-resistant alloys					
	σ_B, MPa	δ^{20}, %	σ_{100}^{1000}, MPa	$V_{\gamma'}^{20}$, %	$V_{\gamma'}^{1000}$, %	ρ, g/cm^3
Udimed520						
Estimated	810	0,3	100	43	26	7,9
Experimental	850	0,33	130	45	25	7,85
ZMI-3U						
Estimated	920	0,21	155	53	35	8,15
Experimental	980	0,22	175	55	37	8,2
DSMGA1400						
Estimated	1060	0,22	180	56	42	8,35
Experimental	1090	0,27	198	59	45	8,3

Table 12 shows that the calculated and experimental data are in good agreement with each other in almost all parameters. Based on the calculated and experimental values obtained, the error does not exceed ±3%, thus, the obtained mathematical dependences make it possible to predict the characteristics that depend on the alloying system of alloys, both in the development of new compositions of HRNA for equiaxial crystallization, and in the improvement of known industrial compositions in within the brand composition.

4. Conclusions

1. This paper presents the studies carried out by modeling the thermodynamic processes of phase separation and their relationship with the strength characteristics for nickel alloys with different alloying systems of equiaxial crystallization.

2. On the basis of an empirical approach, a new $K\gamma'$ ratio was obtained by the value of which one can adequately predict the dimensional mismatch (γ/γ'-mismatch), short-term strength limit, volumetric amount γ'-phase in the structure, as well as the limits of 100- and 1000 hour long-term strength for multicomponent compositions HRNA.

3. Revealed the formation of an extremum at the values of $K\gamma'$ = 1.5-2, which is due to the reduction in the number of elements in the g-solid solution, which most strongly increase the lattice period. 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.

4. Shown is a promising and effective direction in solving the problem of predicting the main characteristics that affect the complex of service properties of alloys both in the development of new HRNA and in the improvement of the compositions of well-known industrial brands of this class.

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