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Influence of alloying systems on the lattice parameters of nickel-based superalloys

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ABSTRACT

Purpose: The work aims to establish the relationship between the chemical composition, mechanical properties and dimensional mismatch of crystal lattices of heat-resistant nickel alloys.

Design/methodology/approach: The results of experimental and calculated data formed based on experimental and taken from open sources results are presented. The XRD method used Bragg-Brentano determined the phase composition, focusing on a RIGAKU MINIFLEX 600 diffractometer (CoKα-radiation). After heat treatment, strength characteristics were determined on cylindrical samples with a working part (diameter 5 mm, length 25 mm). Testing of the alloy for short-term strength was carried out on samples at a temperature of 20°C on UME-10TM and GCM-20 tensile machines. Alloy tests for long-term strength were carried out on similar samples at a temperature of 1000°C on AIMA-5-2 and ZTZ 3/3 machines by uniaxial stretching under a constant load based on 100 hours.

Findings: It has been established that with an increase in the value of the mismatch of crystal lattices, the strength of the alloys decreases due to significant internal stresses. It was revealed that for alloys of equiaxed and directional crystallisation, an extremum is observed at a value of 1.5 ... 1.6 K; this is associated with a decrease in the number of elements in the ϒ-solid solution.

Research limitations/implications: An essential problem is predicting the structure and properties of heat-resistant alloys without or with a minimum number of experiments. The results of comparative tests of the XDR method and calculated data are analysed.

Practical implications: The obtained dependences can be used both for designing new heat-resistant alloys and for improving the compositions of industrial alloys.

Originality/value: The value of this work lies in the fact that the dependences of the influence of alloying elements on the mechanical properties and the dimensional mismatch of crystal lattices were obtained, which made it possible to determine the properties without conducting experiments. It has been established that changes in the course of the relationship closely correlate with the processes taking place in the structure of alloys.

Keywords: Nickel-based superalloys, Lattice mismatch (ϒ/ϒ'-mismatch), A ratio of alloying elements, Heat resistance

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MATERIALS

1. Introduction

Details of modern thermally stressed gas turbine engines are made from multicomponent heat-resistant alloys based on nickel, cobalt and iron using equiaxial, directional or single-crystal casting methods. The gas turbine blades are the most critical parts of gas turbine engines, which determine the maximum temperature of the working gas at the turbine inlet. One of the ways to solve the problem of increasing the working temperature of the gas before the turbine is to increase the ratio of the parameters of the crystal lattice of the matrix and γ′-phases [1-7].

The microstructure of high-temperature nickel alloys is represented by γ′-phase particles scattered in a matrix of a complexly alloyed nickel-based γ-solid solution and, in some cases, carbides. Hardening with the γ'-phase provides long-term preservation of the high-temperature performance of such alloys in a wide temperature range, up to 1150°C. Therefore, the most important role in the resistance to high-temperature creep of nickel-based superalloys belongs to such structural-phase characteristics as the period of crystal lattices of γ- and γ'-phases and their size mismatch δ or γ/γ'-mismatch [8-12].

The purpose of this work is to establish the relationship between the chemical composition of nickel-based superalloys and the size mismatch between the crystal lattices of the γ- and γ'-phases, which can be used to adequately calculate the mechanical properties of nickel-based superalloys without conducting preliminary experiments.

2. Materials and test methods

A working sample of industrial superalloys was formed for experimental and theoretical studies of temperature performance. The selection of alloys was made from the standpoint of a variety of chemical compositions (alloying systems) (Tab. 1). According to the content of chemical elements, they have a wide doping range. The value of the properties of alloys was taken from open sources in articles, books and Internet resources. On their basis, correlation dependences of the "parameter-property" type were established in the form of mathematical models. The resulting equations have sufficiently high coefficients of the correlation criterion R^2>0.85 and can be used for predictive calculations of these characteristics with a relative error of about 4%.

The XRD method used Bragg-Brentano determined the phase composition, focusing on a RIGAKU MINIFLEX 600 diffractometer (CoKα-radiation). The samples were examined in the range of angles 20°... 120° according to the modes: U=30 kV, I=15 mA, scanning step 0.1°.

Dimensional discrepancy δ or γ/γ'-misfit was calculated using the formula from expression 1:

$$\delta=2\frac{a_{\gamma'}-a_{\gamma}}{a_{\gamma}+a_{\gamma'}}\times100\% \quad (1)$$

where a_γ and $a_{\gamma'}$ are the lattice periods of the γ- and γ'-phases, respectively.

The results obtained were compared with the calculated ones, while the error did not exceed 5…10%.

Spectral chemical analysis was carried out on an optical emission device ARL-4460 (quantometer of simultaneous multi-channel analysis) in the 170-800 nm wavelength range.

For a comparative evaluation of the strength characteristics of the studied alloys, mechanical tests of the metal were carried out on standard cylindrical samples with a working part (diameter 5 mm, length 25 mm) after heat treatment. At each temperature and stress level, at least 3...5 samples were tested.

Testing of the alloy for short-term strength was carried out on samples at a temperature of 20°C on UME-10TM and GCM-20 tensile machines (GOST 1497-61, GOST 9651-73, GOST 1497-84).

Alloy tests for long-term strength were carried out on similar samples at a temperature of 1000°C on AIMA-5-2 and ZTZ 3/3 machines (GOST 10145-81) by uniaxial stretching under a constant load based on 100 hours.

The MATLAB program was used to obtain mathematical dependencies.

3. Establishment of a relationship between the chemical composition, mechanical properties and dimensional discrepancy of crystal lattices

An important parameter that affects the high-temperature creep resistance of nickel-based superalloys belongs to such a structural parameter as the dimensional mismatch δ (γ/γ'-misfit). Since misfit depends on the doping system. The task is to obtain a regression relationship to evaluate this characteristic based on the chemical composition by calculation.

All components used in alloying heat-resistant nickel alloys can be divided into three groups: those that dissolve mainly in the γ-solid solution (Co, Cr, Mo, W, Re), those that dissolve mainly in the γ′-phase (Al, Ti, Ta, Hf) and carbide-forming elements (Ti, Ta, Hf, Nb, V, W, Mo, Cr) [13-16]. Since the carbon content is minimised in single-crystal alloys, the carbide-forming elements are distributed between the γ and γ′-phases. Thus, the division of alloying elements is reduced to two groups.

Table 1.
Chemical composition of the studied foundry nickel-based superalloys

Alloys	Element content, % mass													
	C	Cr	Co	Al	Ti	Mo	W	Nb	Ta	Hf	V	Re	Zr	B
Single-crystal alloys														
ZhS30M	0.05	7	7.5	5	1.8	0.6	12	1	-	-		-		
PWA1422	0.14	9.0	10.0	5.0	2.0	-	12	1.0	-	1.5	-	-	0.050	0.015
PWA1480	-	10	5.0	5.0	1.5	-	4.0	-	12.0	-	-	-	-	-
Rene N4	-	9	8	3.7	4.2	-	6	0.5	4	0.15				0.004
MC2	0.05	8	5	5	1.5	2	8	-	6	-		-		
NASAIR100	0.05	9	-	5.8	-	1	10.5	-	3.3	-		-		
DS16	0.06	16	5	3.5	3.5	3	-	-	3.5	1	-	-	0.015	0.015
Alloys of directional crystallisation														
GTD-111	0.10	14.0	9.5	3.0	5.0	1.5	4.0	-	3.0	0.15	-	-	0.030	0.010
Rene 80H	0.17	14.0	9.5	3.0	5.0	4.0	4.0	-	-	-	-	-	0.030	0.015
MAR-M246	-	9	10	5.5	1.5	2.5	10	-	1.5	-	-		0.05	0.01
MAR-M247	0.15	8.3	10	5.5	1	0.7	10	-	3	1.5	-	-	0.05	0.02
MAR-M002	0.15	8	10	5.5	1.5	-	10	-	2.6	1.5			0.03	0.02
Rene 150	0.05	5	12	5.5	-	1	5	-	6	1.5	2.2	3	-	-
MAR-M200	0.02	13	10	6	4	2.5	12	2	-	-	-	-	0.015	0.015
CM249LC	0.07	8.1	9.2	5.6	0.7	0.5	9.5	-	3.2	1.4	-	-	0.015	0.015
Rene 125	0.1	9	10	5	2.5	2	7	-	4	1.5	-	-	0.05	0.015
Alloys of equiaxed crystallisation														
ZMI-3U	0.12	13.3	5.0	3.4	4.8	0.9	7.3	-	-	-	-	-	-	0.015
ZhS 6K	0.18	10.6	4.5	5.7	2.8	4.0	5.1						0.04	0.015
ChS70	0.09	15.8	10.7	2.8	4.6	2.0	5.5	0.2	-	-	-	-	0.050	0.020
ZhS 3LC	0.09	16.0	5.0	2.7	2.7	4.0	4.0	-	-	-	-	-	0.015	0.015
IN-738	0.10	16.0	8.5	3.4	3.4	1.75	2.6	0.9	1.75	-	-	-	0.050	0.010
U-500	0.07	18.0	19.0	3.0	3.0	4.2	-	-	-	-	-	-	0.05	0.007
Rene220	0.03	20	12	-	1	3	-	5	3	-	-	-	-	-
IN100	0.18	10	15	5.5	4.7	3	-	-	-	-	1	-	0.06	0.014
NFP1916	0.07	13	4	3.7	5	-	1.9	-	5.1	-	-	-	0.015	0.015
CM939W	0.12	22.3	18.7	1.6	3.4	-	2.1	0.8	-	-	-	-	0.007	-
ZMI-M8	0.08	23	8.5	1.3	1.3	1.9	3.5	1.3	1.3	0.15	-	-	0.03	-
ChS104	0.1	20.5	11	2.5	3.5	0.7	3.5	0.25	-	-	-	-	-	0.015

On the other hand, the γ-phase composition includes many elements: 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 differ. This effect is associated with the ability of these elements to form stable intermetallic phases of the Ni_3Me type with nickel. Hence, it follows that elements related to - and -generators affect misfit and mechanical properties of alloys.

As a result of the analysis and processing of experimental data, the ratio of alloying elements:

$$K_{\gamma'} = 5\frac{\sum_{\gamma'}(Al+Ti+Nb+Ta+Hf)}{\sum_{\gamma}(Cr+W+Mo+Re+Co+Ru)} \quad (2)$$

which is used to assess the mechanical properties and considers the complex effect of the main components of the alloy [17-24]. The calibration factor (which is used) has been specially selected to provide the best ratio of elements according to the following considerations. γ′-forming elements make a much larger contribution (about 5 times greater) to the strengthening of the alloy due to an increase in the amount of the hardening phase and an increase in the lattice mismatch γ/γ′ (δ) compared with γ-hardening elements. The dimensional discrepancy between the lattice parameters is associated with the degree of concentration solid solution strengthening of the γ- and γ'-phases, the efficiency of the dispersion strengthening of the alloy, the creep rate and other properties. This makes it possible to relate the Kγ′ ratio with the properties of multicomponent systems.

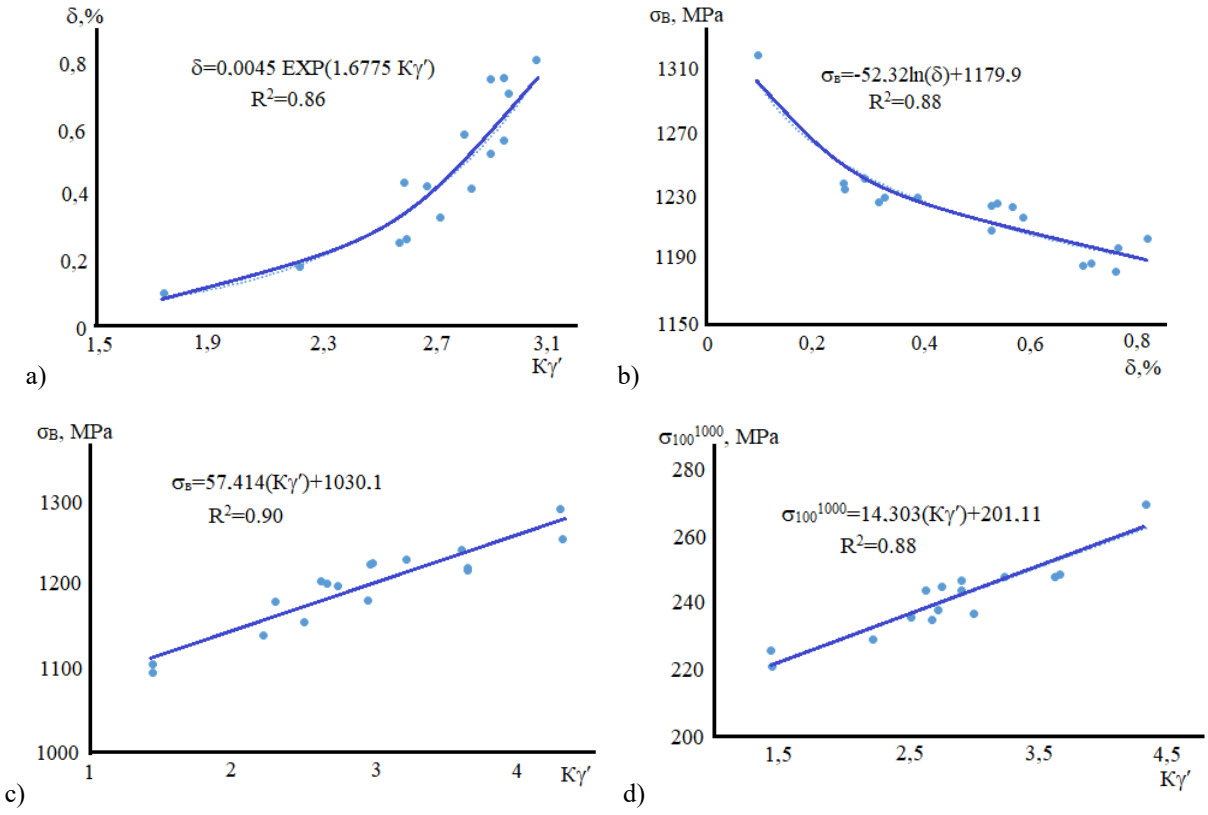

Fig. 1. Dependence of the mismatch value (a), short-term strength limit (b), 100-hour long-term strength limit (c) on the Kγ′ ratio and short-term strength limit (d) on the misfit value for single-crystal alloys

It has been established that the size discrepancy δ (for single-crystal alloys) has an exponential dependence (Fig. 1a). An increase in the Kγ′ ratio leads to an increase in δ. It's connected with a decrease in the number of γ-solution hardeners and an increase in γ′-forming elements that affect the parameters of the crystal lattices of the phases and maximizes their mismatch.

The short-term strength limit (σB) dependence on the misfit value (Fig. 1b) is optimally described by a logarithmic dependence. For single-crystal nickel-based superalloys, an increase in the misfit value is accompanied by a decrease in the short-term strength limit. Significant stresses form between the crystal lattices of the γ- and γ′-phases, which contribute to the processes of structural and phase instability. This leads to premature destruction of the material.

Also, a close correlation between the limit of short-term strength and the limit of 100-hour long-term strength has the ratio Kγ′ (Fig. 1c,d). These correlations are linear with a positive slope. This behaviour is explained by the fact that with an increase in Kγ′, the volume of the main strengthening γ′-phase at room temperature and the residual one at elevated operating temperatures increases. Consequently, the limits of short-term and long-term strength of single-crystal alloys increase.

For directional crystallisation alloys, it has been established that an increase in the Kγ′ ratio leads to a decrease in misfit (Fig. 2) and the formation of an extremum at values of 1.5...1.6 Kγ′. This is associated with a decrease in the number of elements in γ- solid solution, which most strongly increase the lattice period (Mo, W, Nb, Ta, etc.). At Kγ′ values more than 1.5…1.6, misfit increases, since the volume fraction of γ′-forming elements increases significantly and begins to prevail. This behaviour of the dependence is observed both at room temperature and at 1000°C (Fig. 2). The strength value with an increase in the Kγ′ ratio obeys a linear law and tends to increase constantly.

It has been established that the dependence of the 100-hour long-term strength boundary with an increase in the Kγ′ coefficient increases in direct proportion since the number of γ′-forming elements increases, and, consequently, the volume of the γ′-phase in the alloy rises.

Nickel-based superalloys of equiaxed crystallisation have a similar nature of mismatch depending on the Kγ′ ratio (Fig. 3).

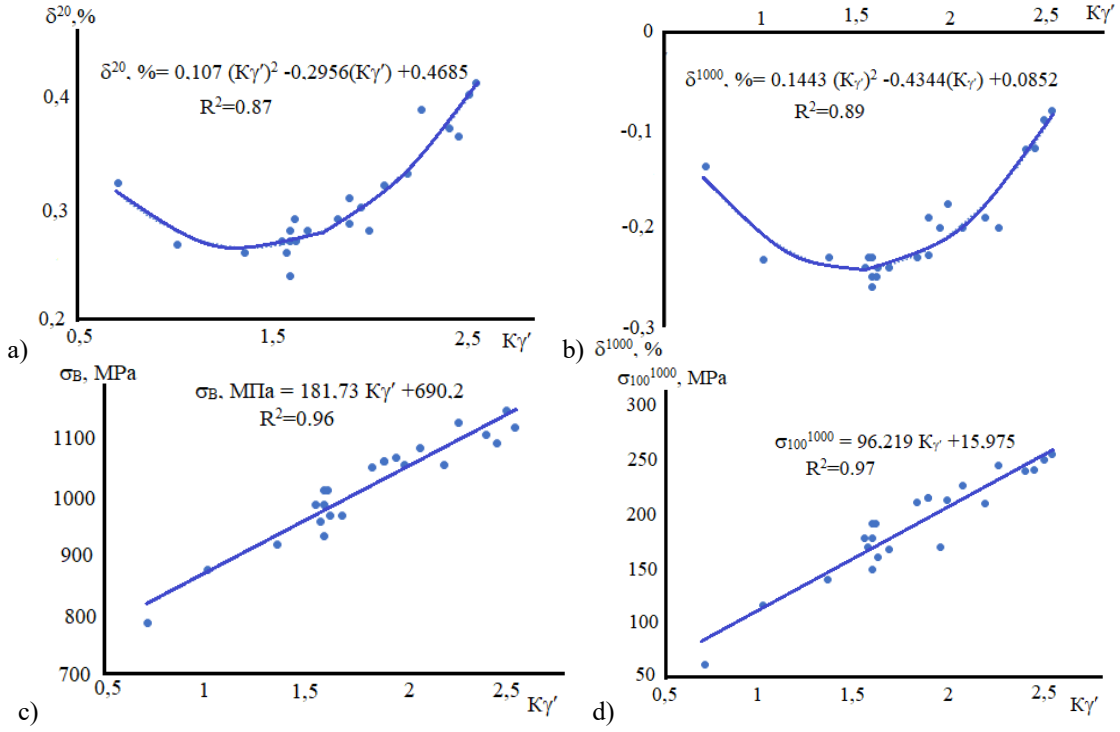

Fig. 2. Dependence of the value of mismatch at 20°C (a), a mismatch at 1000°C (b) short-term strength limit (c), 100-hour long-term strength limit (d) on the Kγ′ ratio for nickel-based superalloys of directional crystallisation

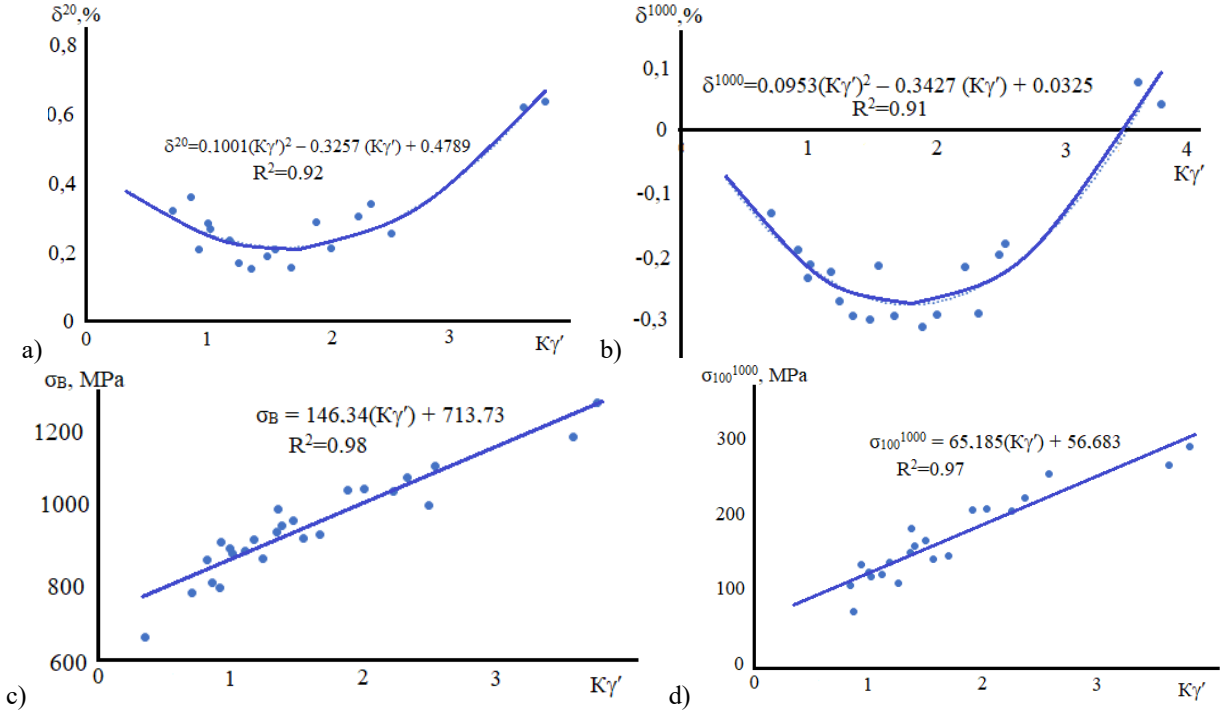

Fig. 3 Dependence of the value of mismatch at 20°C (a), v at 1000°C (b) short-term strength limit (c), 100-hour long-term strength limit (d) on the Kγ′ ratio for nickel-based superalloys of equiaxed crystallisation

The formation of an extremum at values of 1.5…2 Kγ′ is associated with a decrease in the number of elements in γ-solid solution and an increase in a mismatch at Kγ′>1.5…2, since the volume fraction of γ′-forming elements increases significantly. The strength of nickel-based superalloys increases with an increase in the Kγ′ ratio since, with an increase in the number of alloying elements, the volume content of the strengthening phase increases. The limit of 100-hour long-term strength depends on the Kγ′ ratio in direct proportion since the number of γ′-forming elements increases with an increase in the Kγ′ ratio, and consequently, the volume of the γ′-phase in the alloy increases.

4. Comparison of calculations and experimental data

Experimental verification of the obtained dependences was carried out on industrial nickel-based superalloys ZMI-3U [25,26], Udimed-500 [27] and ZMI-M8 [28] (different production technologies) for which the properties

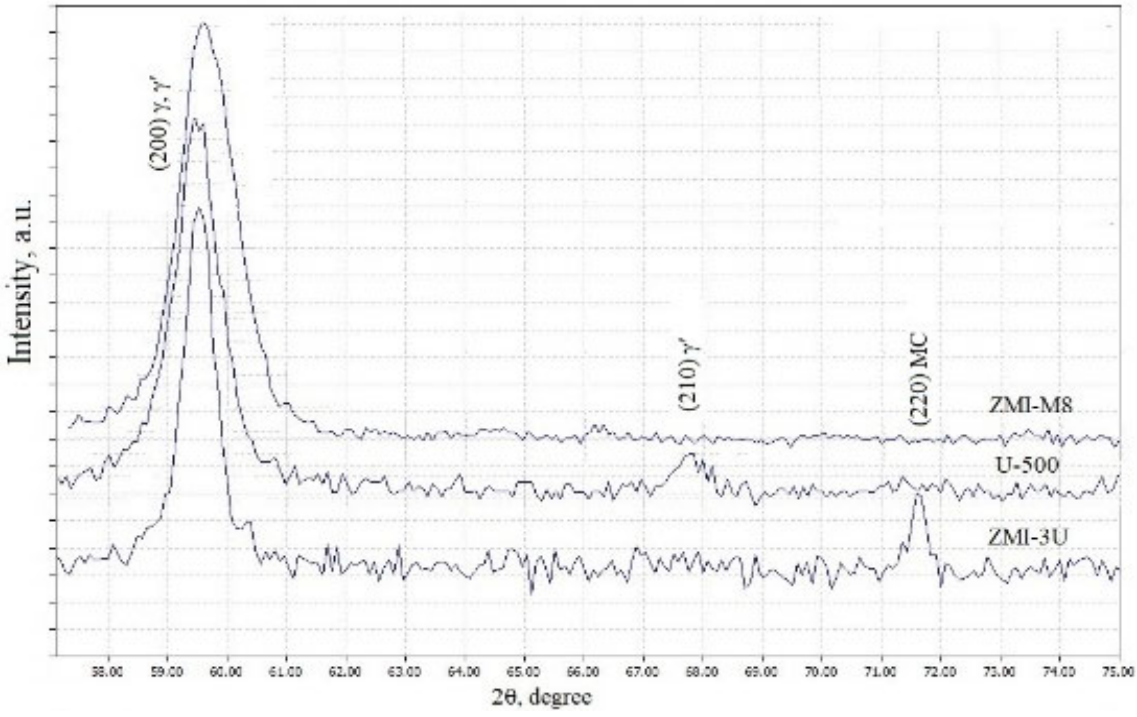

Fig. 4. XRD pattern of alloys ZMI-3U, Udimed-500 and ZMI-M8 (Co Kα radiation), λ = 1.79 Å

Table 2.
The measured and calculated values of lattice parameters, misfit, and mechanical properties of ZMI-3U, Udimed-500 and ZMI-M8 alloys

Method of obtaining results	aγ, Å FCC Fm3m	aγ', Å FCC ordered L12	δ^{20}, %	σ_B, MPa	σ_{100}^{1000}, MPa
ZMI-3U					
Calculated	3.578	3.585	0.207	920	155
Experimental	3.580	3.588	0.220	980	175
Udimed-500					
Calculated	3.569	3.580	0.322	810	100
Experimental	3.569	3.581	0.330	850	130
ZMI-M8					
Calculated	3.575	3.599	0.676	700	-
Experimental	3.575	3.600	0.697	670	-

obtained by calculation and empirical were compared. The results of calculations of the parameters of crystal lattices obtained from the diffraction pattern (Fig. 4), Table 2 shows the data obtained by calculation (according to the obtained dependencies) and experimental data (obtained by the methods described in the second section).

Table 2 shows that the calculated and experimental data agree with each other in almost all parameters. There is a slight discrepancy due to possible measurement and calculation errors. Thus, the dependencies obtained can be used to predict the properties of nickel-based superalloys when developing new compositions or improving existing ones.

5. Conclusions

An experimental and theoretical study of the structural and mechanical characteristics of nickel-based superalloys was carried out in this work. The established relationships between the chemical composition and properties of alloys are of practical interest for creating scientific methods for the development of new-generation alloys. The main results obtained in the work are as follows:

1. It has been established that with an increase in the value of the mismatch of crystal lattices (mismatch), the strength of single-crystal nickel-based superalloys decreases due to significant internal stresses that contribute to the processes of structural and phase instability.
2. It is shown that at values of 1.5…1.6 Kγ′, in alloys of equiaxed and directional crystallisation, there is a minimum for mismatch. This behaviour is associated with reducing the number of elements in the γ-solid solution, which increase the lattice period the most.
3. An increase in the ratio of alloying elements Kγ′ leads to an increase in the strength and heat resistance of nickel-based cast superalloys as a result of an increase in the amount of strengthening γ′ and alloying γ - matrix.
4. With the XDR, the established correlations between the properties of the alloys and the chemical composition were verified. Experimental and calculated data have a small divergence of values not exceeding 5-10%.

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