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PREDICTION CARBIDES COMPOSITION IN NICKEL-BASED SUPERALLOYS DIRECTIONAL CRYSTALLIZATION

Objective. To study the specifics of the distribution of alloying elements in the carbides of the multicomponent system Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C by directional crystallization, using the calculated method of CALPHAD prediction.

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

The obtained results. The results of thermodynamic calculations of the chemical composition of carbides are given in the form of mathematical dependences. The equation of the influence of alloying elements on the dissolution (release) temperature of carbides is obtained. It is shown that the obtained dependences are closely correlated with the thermodynamic processes occurring in the system.

Scientific novelty. It is shown that with increasing total concentration of carbide-forming elements, the chemical composition of carbides becomes more complicated. The titanium content of more than 2% leads to an increase in the temperature of the carbide liquidus, and at 4.5 % topologically densely packed phases is formed. When the concentration of molybdenum in the alloy is more than 4%, the probability of precipitating topologically close-packed phases in the structure increases markedly, which negatively affects the mechanical properties and heat resistance.

Practical value. Based on an integrated approach for multicomponent heat-resistant nickel-based alloys, new regression models were obtained that allow adequately predict the chemical composition of carbides by the chemical composition of the alloy, which allowed to solve the problem of calculated prediction of carbide composition by chemical composition of the alloy.

Key words: heat-resistant alloys based on nickel directional crystallization, alloying system, CALPHAD method, structure, composition of carbides.

Introduction

Numerous studies and statistical data on aircraft breakdowns due to engine failure have shown that the main reason for the destruction of the blades of gas turbine engines (the most loaded engine parts) is their rupture along grain boundaries oriented perpendicular to the main tensile stresses from centrifugal forces. This served as an impetus for the development of directional crystallization technology, which ensures the production of blades with a columnar structure, the grain boundaries of which are oriented parallel to the main axis of the blade. The blades with a columnar structure have a longer service life on the engine, in contrast to blades with an equiaxial structure. Nickel-based superalloys are used for the manufacture of directional solidification rotor blades. The main phases of such alloys are a solid solution based on nickel and a strengthening phase based on the Ni_3Al intermetallic compound with a superstructure of the $\text{L}1_2$ type (γ' -phase); in addition, there are carbides of the MeC , Me_{23}C_6 , and M_6C types, which are precipitated at the boundaries and within grains in the form of dispersed inclusions [1, 2].

The role of carbides is very complex in nickel-based superalloys. They affect mechanical properties depending

on their morphology and distribution. Fine blocky particles at the grain boundary can have a reinforcing effect, inhibiting the sliding of the boundaries, thereby improving creep and tensile strength. On the other hand, if they are present in the form of continuous films at the grain boundaries, they have a detrimental effect on the plasticity [3, 4]. The main methods for studying such fine structures is X-ray spectroscopy, which fully makes it possible to determine the main characteristics of [5].

The objective of this work is to study the specifics of the influence of alloying elements on the distribution of various types of carbides in the structure, their topology and morphology, as well as their composition for a multicomponent system such as Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C using the calculated prediction method CALPHAD (passive experiment) compared with data obtained by electron microscopy (active experiment).

Material and research technique

Modeling of thermodynamic processes occurring during crystallization (cooling) or heating in the structure of alloys was carried out by the CALPHAD method [6].

In the multicomponent alloying system (Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C), which corresponded

to the average composition of the ZhS-26VI alloy, the range of variation of the elements was chosen for reasons of maximum and the minimum amount of an element introduced into superalloys. Thus, for the study, carbide-forming elements were selected in the following alloying ranges: carbon (0.02–0.2) %, titanium (1–6) %, niobium (0.1–4) %, molybdenum (1–6) %; tungsten (1–16) % by weight.

Experimentally, the composition of carbides was determined using an REM-106I electron microscope with an energy-dispersive X-ray spectral microanalysis system. This method was used to study the morphology and chemical composition of precipitated carbides in the alloy structure. The conversion of qualitative values into quantitative analysis was carried out automatically according to the program of the device. The relative error of the method is ± 0.1 % (by weight). The calculation results of the type of carbides and their chemical composition were compared with the experimental data obtained using electron microscopy.

The obtained values were processed in the Microsoft Office software package in the EXCEL package by the least squares method with obtaining correlation dependences of the “parameter-property” type and obtaining trend lines with mathematical equations of regression models that optimally describe these dependences. The obtained dependences have sufficiently high coefficients of determination $R^2 \geq 0.85$ and can be used for predictive calculations of the indicated characteristics with a relative error of $\pm 3.9\%$.

Research results and their discussion

The study of phase precipitation during the crystallization of the investigated alloy in the temperature range (1600–20 °C) showed that the most probable for the ZhS-26VI alloy is the precipitation of the main phases in the following order: carbides of the MC type; γ - solid solution; eutectic $\gamma + \gamma'$; intermetallic compounds of the γ' -phase type based on (Ni_3Al) ; carbides of the M_6C type.

It is known [1, 7, 8] that MC carbides are formed in the process of crystallization (solidification) in the form of discrete particles in the intergrain and intragranular space, as well as in the interdendritic regions. Carbides of the MC type are formed in a liquid due to strong segregation of carbon, when its amount is higher than 0.05 %, as well as at temperatures slightly below the solidification temperature of the alloy. In carbide reactions in alloys, they serve as the main source of carbon. In order of decreasing stability in superalloys, carbides are arranged in the series HfC , TaC , NbC , TiC . Carbides of this type are very stable at low temperatures, but at higher temperatures tend to be converted (degraded) into different types of secondary carbides. Carbides of the M_6C type are formed at temperatures of 815...980 °C in alloys with a higher content of refractory elements of tungsten and molybdenum. Mostly they stand out along the grain boundaries. Compared with carbides of the M_{23}C_6 type, M_6C carbides

are more stable at high temperatures [9]. The formation of carbides M_6C and M_{23}C_6 occurs according to the well-known reaction:

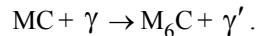


Figure 1 (a, b) shows that in the structure the volume fraction of both primary MC carbides and secondary M_6C carbides depends on the carbon content in the alloy composition and is optimally described by linear and parabolic functions (Table 1). It is shown that with an increase in the carbon content in the alloy, the volumetric amount of carbides of both types increases. However, upon reaching a concentration of 0.12 % C, the amount of secondary carbide decreases, which is explained by the lack of carbon for the simultaneous formation of two types of carbides. At the same time, it is shown in (Fig. 1c) that the effect of carbon on the temperature t_{L}^{MC} of dissolution (or precipitation) of MC carbides has a rather complex character and is optimally described by a quadratic polynomial (Table 1). The effect of carbon on the temperature of dissolution (or precipitation) of secondary carbide M_6C is described by a directly proportional relationship (Fig. 1, d).

It is known [2, 10, 11] that titanium is contained in the majority of superalloys. Titanium is present not only in the composition of the strengthening γ' -phase, but is also a strong carbide-forming element, on the basis of which MC carbides are formed. In the alloying system under study, the primary niobium-based carbide also contains elements such as titanium, tungsten, molybdenum, and chromium. It was found that titanium affects not only the temperature of dissolution (precipitation) of the primary carbide MC, but also the analogous temperature of formation of the secondary carbide M_6C (Fig. 2). It was found that the dependencies are complex and are optimally described by linear and cubic polynomials (Table 1).

It was found that with an increase in the titanium content in the alloy, its concentration in the MC carbide also increases to 48.53 by weight (Fig. 1, c), which is optimally described by a parabolic function (Table 1). At the same time, the tungsten content in carbide increases within (15.5–20)%, while molybdenum and chromium decreases within (1.45–0.5) % and (1.14–0.48) % by weight, respectively. The niobium content in carbide decreases with increasing titanium from a concentration of 49.6 wt% up to 17.4 wt%, which leads to the degeneration of the carbide MC. So, at a concentration of more than 2 % by weight Ti in the alloy, in MC carbide, the titanium content prevails over the niobium content, which is indirectly manifested at the temperature of dissolution (precipitation) of the secondary carbide by a minimum. In turn, at a titanium concentration of 4.5% wt. In the alloy, P - and μ -phases are formed, which belong to topologically close-packed (TCP) phases, which cause a decrease in the temperature of dissolution (precipitation) of the secondary carbide (Fig. 2, b).

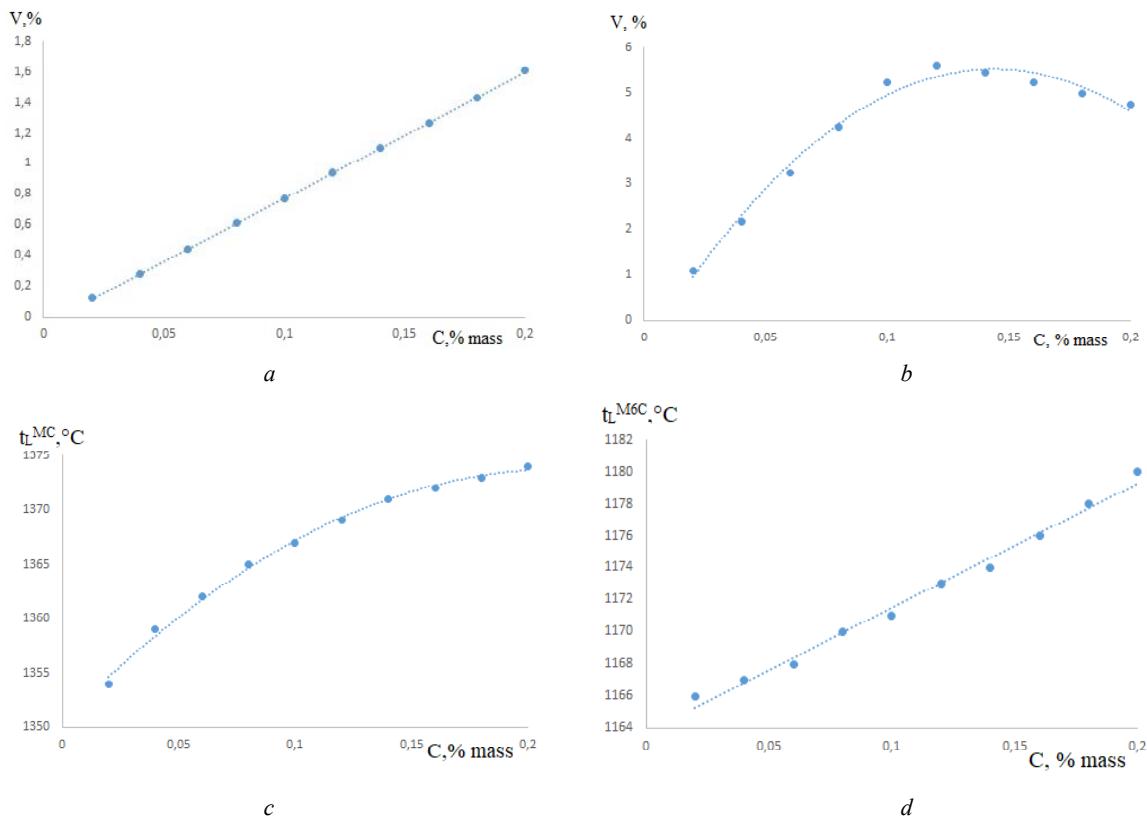


Fig. 1. Change in the amount of carbides of type MC (a), M₆C (b) and the temperature of dissolution of carbide MC (c), M₆C (d) as a function of carbon content in the alloy

Table 1 – Polynomial dependences of the temperature of dissolution (precipitation) of carbides and the content of alloying elements in carbides on the content of alloying elements in the alloy

| Alloying element | Dissolution (precipitation) temperatures of carbides, °C | Content of elements in carbide, wt% |
|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| C | $t_L^{MC}, ^\circ C = 8.2576(C) - 0.0513$ $t_L^{M6C}, ^\circ C = -300.28(C)^2 + 86.296(C) - 0.6652$ | $V_{MC} = -511.36(C)^2 + 217.95(C) + 1350.5$ $V_{M6C} = 77.879(C) + 1163.7$ |
| Ti | $t_L^{MC}, ^\circ C = 80.491 \cdot (C_{Ti}) + 1268.8;$ $t_L^{M6C}, ^\circ C = -8.7956(C_{Ti})^3 + 73.727(C_{Ti})^2 - 180.3(C_{Ti}) + 1294.6$ | carbides MC: $C_{Ti} = -1.0679(C_{Ti} \text{ in alloy})^2 + 12.85(C_{Ti} \text{ in alloy}) + 8.9873;$ $C_{Nb} = 2.1679(C_{Ti} \text{ in alloy})^2 - 21.36(C_{Ti} \text{ in alloy}) + 67.653;$ $C_W = -1.048(C_{Ti} \text{ in alloy})^2 + 8.2623(C_{Ti} \text{ in alloy}) + 8.6829$ |
| Nb | $t_L^{MC}, ^\circ C = 1.2382 \cdot (C_{Nb})^2 - 8.3294 \cdot (C_{Nb}) + 1381;$ $t_L^{M6C}, ^\circ C = -0.907(C_{Nb})^2 - 3.7649(C_{Nb}) + 1182.6$ | carbides MC: $C_{Nb} = -5.3041(C_{Nb} \text{ in alloy})^2 + 42.301(C_{Nb} \text{ in alloy}) + 6.8364;$ $C_{Ti} = 1.5703(C_{Nb} \text{ in alloy})^2 - 14.836(C_{Nb} \text{ in alloy}) + 40.095;$ $C_W = 3.9361(C_{Nb} \text{ in alloy})^2 - 27.475(C_{Nb} \text{ in alloy}) + 51.534$ |
| Mo | $t_L^{MC}, ^\circ C = -0.8252 \cdot (C_{Mo})^2 + 0.2308 \cdot (C_{Mo}) + 1371.5;$ $t_L^{M6C}, ^\circ C = -10.163(C_{Mo})^2 + 114.4(C_{Mo}) + 1052.3$ | carbides M₆C: $C_{Mo} = 4.7305(C_{Mo} \text{ in alloy}) + 3.7976;$ $C_W = -4.3064(C_{Mo} \text{ in alloy}) + 64.09$ |
| W | $t_L^{M6C}, ^\circ C = 49.214(C_W) + 595.07$ | carbides MC: $C_{Nb} = 0.2444(C_W \text{ in alloy})^2 - 4.2089(C_W \text{ in alloy}) + 65.006;$ $C_W = -0.1951(C_W \text{ in alloy})^2 + 3.9132(C_W \text{ in alloy}) - 3.1815;$ carbides M₆C: $C_{Mo} = -0.7443(C_W \text{ in alloy}) + 16.973;$ $C_W = 1.3639(C_W \text{ in alloy}) + 45.03$ |

A change in the titanium content in the alloy does not affect the chemical composition of the secondary carbide. The average content of alloying elements in M_6C carbide is at the level: 61.5W-15.6Ni-9Cr-7.7Mo-3.8Co-1.85C-0.55Nb.

Niobium, as a strong carbide-forming element, with titanium forms primary MC carbide on a mixed basis [3, 12, 13]. Niobium affects the temperatures of carbide formation (Fig. 3 a, b), lowering them according to parabolic dependences (Table 1), which is explained by changes in the interatomic bond forces in these precipitates.

It is shown in (Fig. 3, c) that with an increase in the niobium content in the alloy above 1 % by weight, its concentration in the primary carbide increases and exceeds the concentration of titanium and tungsten. Thus, the titanium content in MC carbide decreases from 36.7 wt% up to 6.25 wt%, and tungsten from 47 wt% up to 3.75 % by weight, which leads to the formation of niobium-based carbide.

A change in the niobium content in the alloy does not affect the chemical composition of the secondary carbide. The average content of alloying elements in M_6C is at the level: 61.8W-15.9Ni-7.9Cr-8.23Mo-3.8Co-1.85C-0.52Nb.

Molybdenum, one of the elements that participates in the formation of secondary carbides and on its basis can form carbides of the M_6C [14, 15] type, while molybdenum can be a part of the $M_{23}CS_6$ carbides. Since only M_6C carbides are formed in the investigated composition, the effect of molybdenum on them will be considered later. Figure 4 show that molybdenum has a complex effect on the temperature of dissolution (precipitation) of carbides. The temperature of dissolution (precipitation) of primary carbides decreases according to the parabolic dependence with an increase in the amount of molybdenum (Table 1), and for secondary carbides, an increase in temperature is observed according to the parabolic dependence. This behavior is explained by a change in the strength of interatomic bonds in the secondary carbide, due to an increase in alloying with refractory molybdenum.

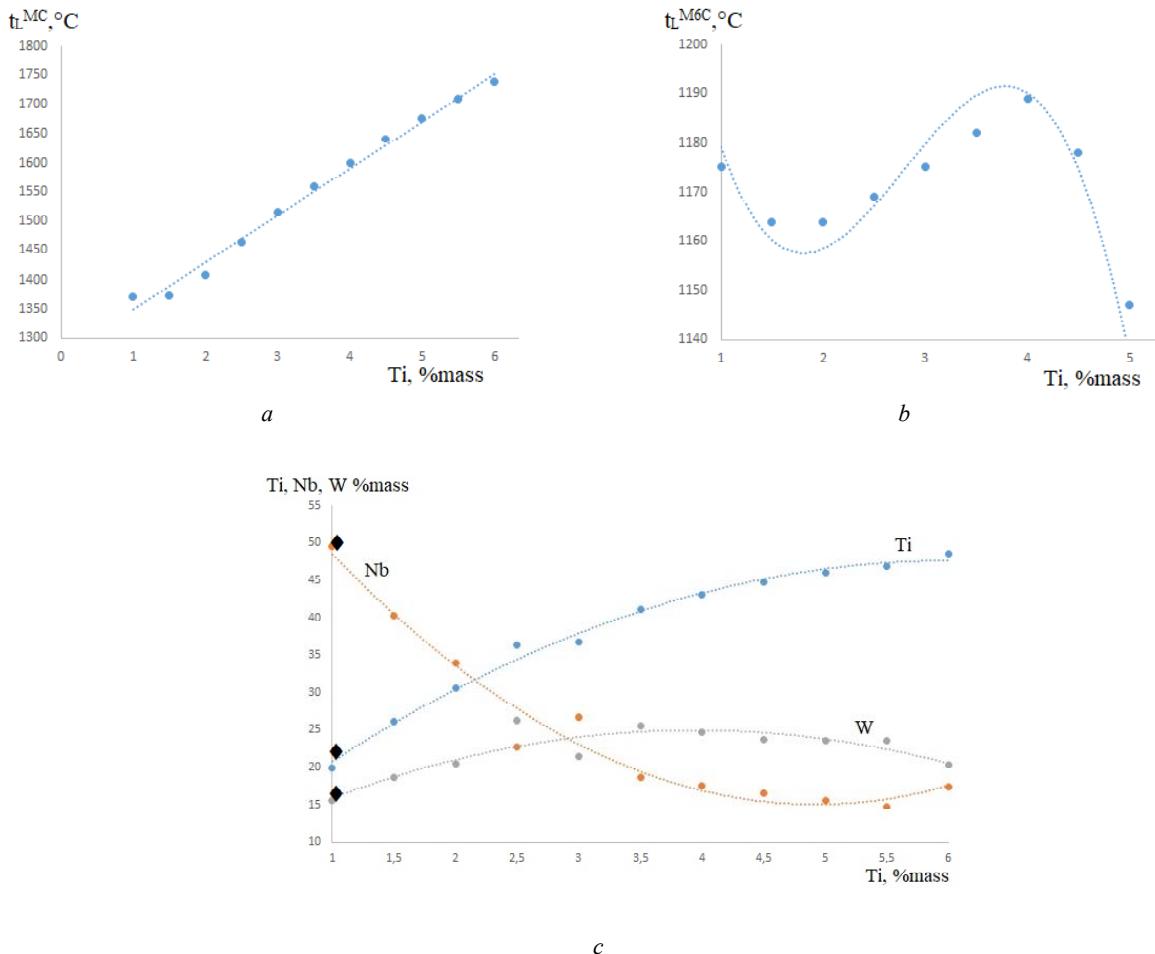


Fig. 2. The dependence of the temperature of dissolution (precipitation) of carbides of the type MC (a), M_6C (b) on the amount of titanium, tungsten and niobium in the primary carbide (c) on the content of titanium in the alloy

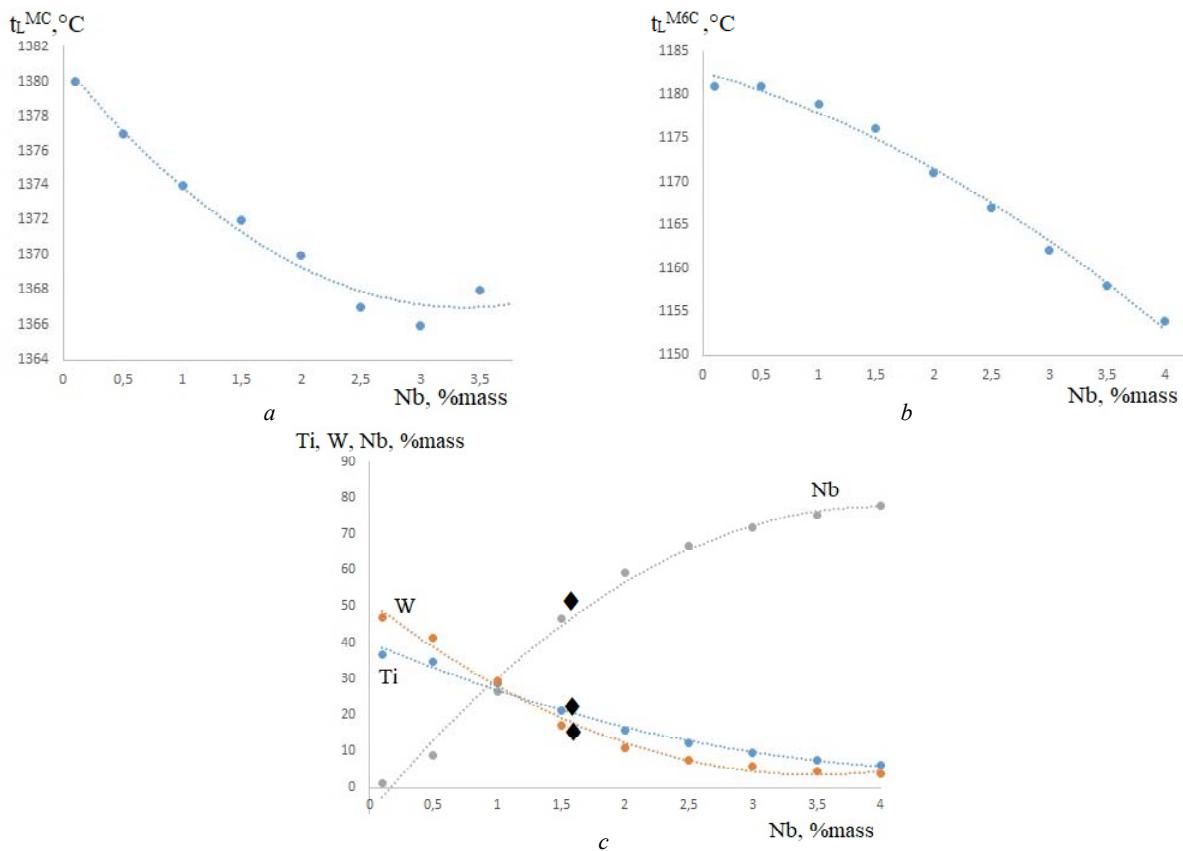


Fig. 3. The dependence of the temperature of dissolution of carbides MC (a), M_6C (b), the amount of titanium, tungsten and niobium in the primary carbide (c) of the niobium content in the alloy

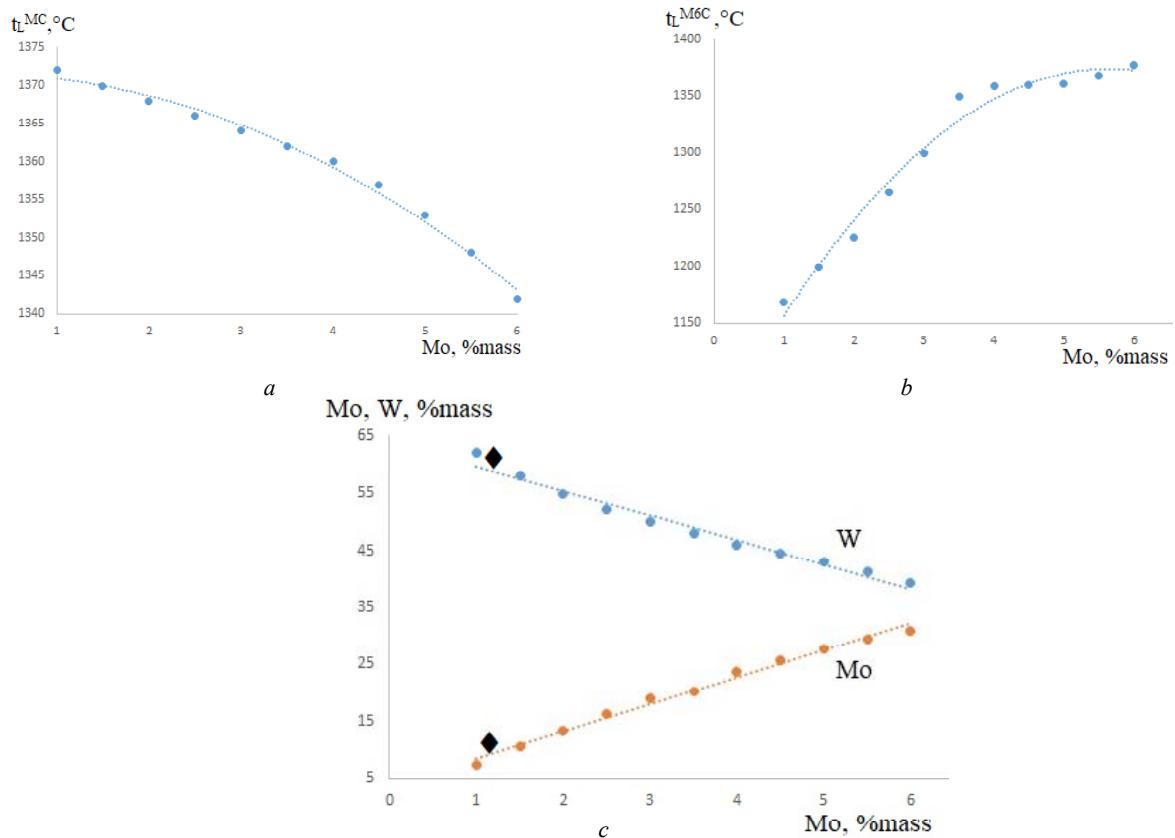


Fig. 4. The dependence of the temperature of dissolution of carbides MC (a), M_6C (b), the amount of tungsten and molybdenum in the secondary carbide (c) of the molybdenum content in the alloy

Molybdenum does not affect the chemical composition of the primary carbide, the average composition of which is at an average level of 46.7Nb-22.3Ti-15.3W-12.3C-2.6Mo-0.8Cr. However, when the content of molybdenum is more than 4%, the carbide degenerates. The composition of M_6C carbide changes significantly with an increase in the amount of molybdenum in the alloy. In addition to the fact that the content of molybdenum in the carbide increases and the tungsten content decreases (Fig. 4, c), the appearance of the m-phase is observed at a concentration of more than 4%, which reduces the strength characteristics of the alloy.

Tungsten is introduced into the composition of heat-resistant alloys in order to increase the temperature level of phase transformations, and, consequently, the heat resistance of the alloy [16]. The tungsten content in superalloys is within a fairly wide range of 1–16 % by weight. A further increase in the tungsten content significantly increases the probability of precipitation of phases in the TCP structure. Tungsten has practically no effect on the temperature of dissolution (formation) of MC carbide and has a linear effect on the temperature of dissolution (formation) of M_6C carbide (Fig. 5) (up to a concentration of 10 % tungsten, M_6C carbide is not formed).

An increase in the concentration of tungsten in the alloy leads to a decrease in the concentration of niobium in MC carbide and a simultaneous increase in tungsten, which obeys the parabolic law (Table 1). The extreme on the curves (Fig. 5, b) correspond to a concentration of 10 % W, which is associated with the appearance of M_6C carbides in the structure. Upon reaching 13 % W, the primary carbide degenerates.

The change in the concentration of alloying elements in the secondary carbide obeys a linear law (Table 1). In this case, the tungsten content increases by 10 %, for molybdenum, nickel and chromium it decreases by 5 %, 3 %, and 2 %, respectively. Thus, the secondary carbide approaches the tungsten-based monocarbide.

The results of calculating the phase composition obtained by the CALPHAD method were further compared with the experimental data obtained using electron microscopy in the microprobe mode on a scanning electron microscope REM-106I. Typical morphology of primary carbides, which is most often found in the structure of alloys of this class in the form of blocks and hieroglyphs (Fig. 6 a, b). Carbides of the M_6C type in this alloy are present in block form (Fig. 6 c, d). The most preferable is the block type of secondary carbide precipitation, since in this case we have a lower level of stress concentration with the matrix.

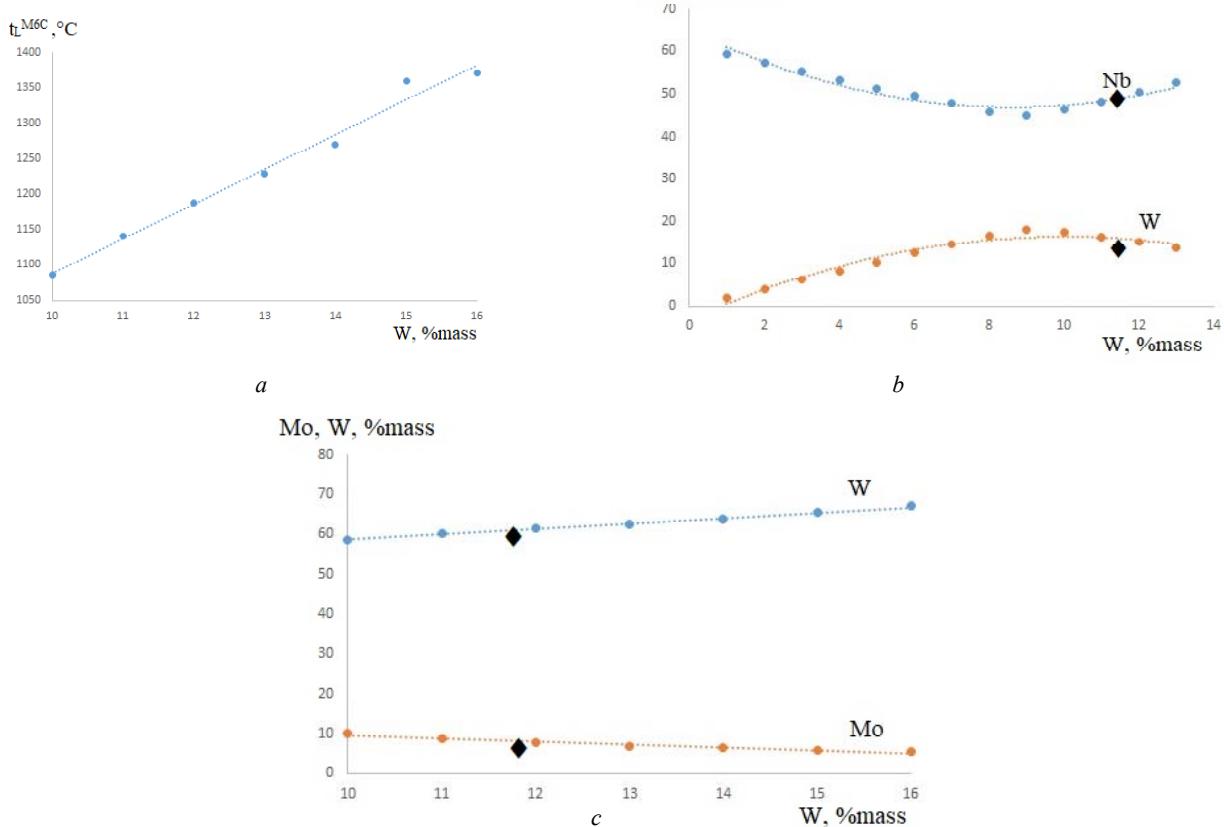


Fig. 5. The dependence of the temperature of dissolution of carbides M_6C (a), the amount of tungsten and niobium in the primary carbide (b), the amount of tungsten and molybdenum in the secondary carbide (c) of the tungsten content in the alloy

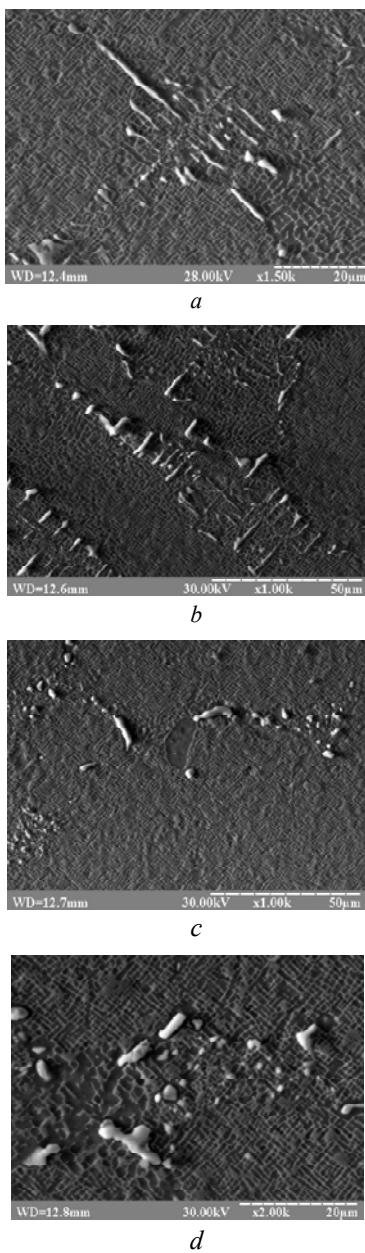


Fig. 6. Typical morphology carbides in the structure of superalloy ZhS 26

The composition of carbides was determined experimentally by X-ray diffraction analysis using an electron microprobe. The obtained experimental data agree with the results of thermodynamic calculations obtained by the CALPHAD method. It has been experimentally established that the composition of MC carbides includes niobium, titanium, tungsten, molybdenum, and cobalt; M_6C carbides include tungsten, molybdenum, cobalt, nickel, chromium, and niobium (Table 2). The X-ray spectra obtained from the characteristic points are shown in Figure 7. The errors in determining the elements by this method did not exceed $\pm 0.1\%$ by weight.

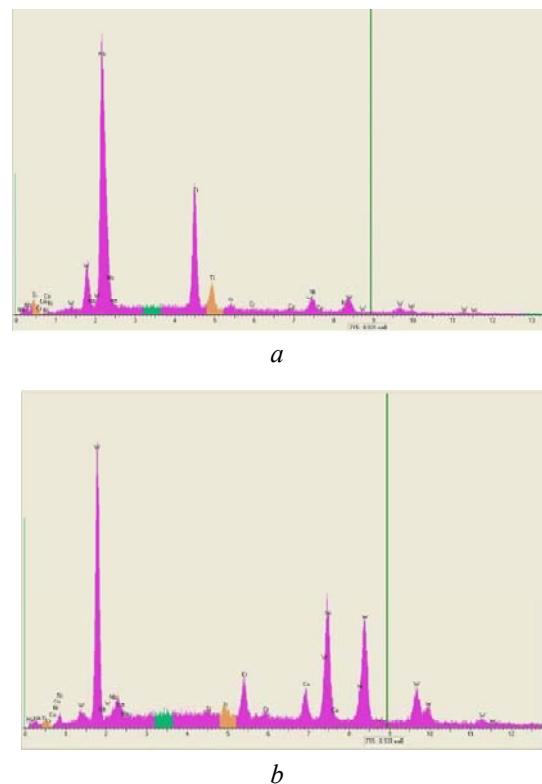


Fig. 7. X-ray spectra obtained from carbides MC (a) and M_6C (b) alloy ZhS 26

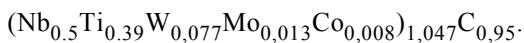
Table 2 – The chemical composition carbides, calculated according to the obtained dependences and the experimental X-ray microanalysis at 20 ° C for alloy ZhS 26

| Method of obtaining results | Element content,% wt. [at. %] | | | | | | | |
|-----------------------------|--------------------------------|------------------|------------------|----------------|----------------|-----------------|-----------------|-----------------|
| | Nb | Ti | W | Mo | Co | Ni | Cr | C |
| MC | | | | | | | | |
| Calculated | 49.6 [25.49] | 19.93 [19.88] | 15.54 [4.04] | 1.45 [0.72] | 1.14 [0.92] | - | - | 12.3 [48.9] |
| Experimental | 50.24 [25.8] | 20.42 [20.35] | 15.27 [3.96] | 1.3 [0.65] | 0.51 [0.41] | - | - | 12.3 [48.8] |
| M_6C | | | | | | | | |
| Calculated | 0.39 [0.38] | - | 61.26 [30.9] | 8.01 [7.74] | 3.78 [5.95] | 16.5 [26.05] | 8.22 [14.66] | 1.85 [14.28] |
| Experimental | 0.6 [0.58] | - | 59.62 [29.57] | 7.5 [7.12] | 4.92 [7.61] | 18.4 [28.6] | 7.1 [12.45] | 1.85 [14.05] |

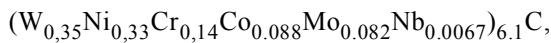
Note - the calculation of stoichiometric formulas for secondary carbides was carried out on the basis of the data shown in Table 2 in at. %

Table 2 shows that the calculated and experimental data are in good agreement with each other for almost all elements, the deviation between the calculated and experimental values does not exceed $\pm 2\%$ by weight.

Based on the obtained experimental values, the stoichiometric formula for carbides was calculated, which made it possible to establish the real type of carbides in the structure of the alloy under study. The stoichiometric formula of primary carbide with conversion from weight% to atomic% corresponds to the following ratio:



Based on the obtained formula for primary carbides, it follows that the total ratio of metallic elements and carbon does not fully comply with the rule of a rigid ratio of 1:1. There is a slight increase in the total concentration of metallic elements. The same feature is observed in carbides of the M_6C type; it corresponds to the following compound formula:



which also does not fully comply with the 6: 1 ratio rule in carbides of this type.

Thus, the calculated data obtained by the CALPHAD method for determining the type and chemical composition of carbides showed good convergence and agreement with the experimental data obtained by electron microscopy.

Conclusions

1. On the basis of an integrated approach, computational and experimental, for multicomponent superalloys, new regression models were obtained that allow to adequately predict the chemical composition of carbides by the chemical composition of the alloy, this made it possible to solve the problem of calculating the prediction of the composition of carbides by the chemical composition of the alloy, which was confirmed by the obtained experimental data.

2. Dependences of the influence of alloying elements on the temperature of dissolution (precipitation) of carbides in the alloy of the Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C system have been established. It is shown that changes in the course of the curves of the temperature dependence on the element content closely correlate with the thermodynamic processes occurring in the system, that is, the curves exhibit extrema accompanying the change in the stoichiometry of carbides or the precipitation of new phases.

3. It is shown that with an increase in the total concentration of carbide-forming elements, the chemical composition of carbides also becomes more complex. It was found that with an increase in the carbon content in the alloy, the volumetric amount of carbides increases. However, upon reaching a concentration of 0.12 % C, the amount of secondary carbide decreases, which is explained by the lack of carbon for the simultaneous formation of two types of carbides. At a concentration of more than 2 % wt. Ti

in the alloy, in MC carbide, the titanium content prevails over the niobium content, which is indirectly manifested at the temperature of dissolution (precipitation) of the secondary carbide by a minimum. In turn, at a titanium concentration of 4.5 % wt. In the alloy, P- and m-phases are formed, which belong to TCP - phases, which causes a decrease in the temperature of dissolution (precipitation) of the secondary carbide. With an increase in the niobium content in the alloy above 1 % by weight, its concentration in the primary carbide increases and exceeds the concentration of titanium and tungsten. An increase in the content of molybdenum over 4 % is accompanied by the appearance of the m-phase, which reduces the strength characteristics of the alloy. An increase in the concentration of tungsten in the alloy leads to a decrease in the concentration of niobium in the MC carbide and a simultaneous increase in tungsten. At 10 % W, M_6C carbide is formed, and at 13 % W, the primary carbide degenerates.

4. A comparative assessment of the calculated results obtained by the CALPHAD method and the experimental data obtained by the x-ray microanalysis was carried out. The results obtained for determining the type and chemical composition of secondary carbides are consistent with each other.

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Глотка О. А. Карбіди в жароміцних сплавах направленої кристалізації

Мета роботи. Вивчити специфіку розподілу легувальних елементів у карбідах багатокомпонентної системи Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C за направленої кристалізації, за допомогою розрахункового методу прогнозування CALPHAD.

Методи дослідження. Для пошуку закономірностей та розрахунку розподілу легувальних елементів в сплаві, було обрано новітній метод CALPHAD, та проведено моделювання термодинамічних процесів кристалізації фаз.

Отримані результати. Результати термодинамічних розрахунків хімічного складу карбідів наведені в вигляді математичних залежностей. Отримано рівняння впливу легувальних елементів на температуру розчинення (виділення) карбідів. Показано, що отримані залежності тісно корелують з термодинамічними процесами, що відбуваються в системі.

Наукова новизна. Показано, що при підвищенні сумарної концентрації карбідоутворюючих елементів, ускладняється і хімічний склад карбідів. Вміст титану більше 2 приводить до підвищення температури карбідного ліквідусу, а при 4,5 утворюються топологічнощільнопаковані фази. При концентрації молібдену в складі сплаву більше 4 помітно підвищується ймовірність виділення в структурі топологічнощільнопакованих фаз типу *t*, що чинить негативний вплив на механічні властивості і жароміцність.

Практична цінність. На основі комплексного підходу для багатокомпонентних жароміцних сплавів на основі нікелю отримані нові регресійні моделі, що дозволяють адекватно прогнозувати хімічний склад карбідів за хімічним складом сплаву, це дозволило реалізувати рішення задачі розрахункового прогнозування складу карбідів за хімічним складом сплаву.

Ключові слова: жароміцні сплави на основі нікеля спрямованої кристалізації, система легування, метод CALPHAD, структура, склад карбідів.

Глотка А. А. Карбиды в жаропрочных сплавах направленной кристаллизации

Цель. Изучить особенности распределения легирующих элементов в карбидах многокомпонентной системы Ni-5Cr-9Co-6Al-1Ti-11.7W-1.1Mo-1.6Nb-0.15C методом направленной кристаллизации с помощью расчетного метода CALPHAD.

Методы исследования. Для выявления закономерностей и расчета распределения легирующих элементов в сплаве был выбран новейший метод CALPHAD и выполнено моделирование термодинамических процессов кристаллизации.

Полученные результаты. Результаты термодинамических расчетов химического состава карбидов представлены в виде математических зависимостей. Получено уравнение влияния легирующих элементов на температуру растворения (выделения) карбидов. Показано, что полученные зависимости тесно коррелируют с термодинамическими процессами, происходящими в системе.

Научная новизна. Показано, что с увеличением общей концентрации карбидообразующих элементов химический состав карбидов усложняется. Содержание титана более 2% приводит к повышению температуры карбидного ликвидуса и при 4,5% образуются топологически плотно упакованные фазы. При концентрации молибдена в сплаве более 4% вероятность выделения в структуре топологически плотно упакованных фаз заметно возрастает, что отрицательно сказывается на механических свойствах и жаростойкости.

Практическая ценность. На основе комплексного подхода для многокомпонентных жаропрочных сплавов на основе никеля получены новые регрессионные модели, позволяющие адекватно прогнозировать химический состав карбидов по химическому составу сплава, что позволило решить задачу расчетного прогнозирования карбидного состава по химическому составу сплава.

Ключевые слова: жаропрочные сплавы на основе никеля направленной кристаллизации, система легирования, метод CALPHAD, структура, состав карбидов.