Modeling Ultimate Tensile Strength and Phase Stability of Nickel-based Superalloys Different Generations

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Abstract: - Information about changes in the heat resistance and phase stability of Nickel-based superalloys is important for determining the service life of gas turbine engines. A model of the change in the ultimate tensile strength was obtained using machine learning and an analytical expression was proposed that allows determining the phase stability parameter of Nickel-based superalloys. Approximation and extrapolation of the ultimate tensile strength dependences were performed using the Larson-Miller temperature-time dependence. The adequacy of the obtained model is confirmed by satisfactory convergence of experimental and calculated results.

Key-Words: - Nickel-based superalloys, Simulation, Ultimate tensile strength, Larson-Miller parameter

1 Introduction

At present, several hundred Nickel-based superalloys of different composition have been developed and tested for the manufacture of gas turbine engine parts. Work on creating new compositions continues constantly. Main task is increasing the heat resistance and phase stability. One of the indicators of superalloys heat resistance is the ultimate tensile strength (UTS). It is a result of tensile tests after long isothermal exposures [1]. The result is represented as σ_T^τ (MPa). T is the pre - exposure temperature, (°C), and τ is the duration, hours.

To design the resource of products made of Nickel-based superalloys, information about their phase stability in wide temperature and time intervals is required. Therefore, the purpose of this work is to present a method for determining this parameter based on a model of changes by temperature – time test conditions.

2 Approach and experimental

Relevant are theories or models that comprehensively cover the relationship between the chemical composition and properties for different grades of alloys. More than 20 alloying elements (Cr, Co, Mo, W, Al, Ti, Nb, B, Fe, Y, Zr, Ta, Re, Ru, V, Ce, La, Si, Mn, Mg, Hf, Cu, Bi, Pb, Ir) that vary in concentration within some significantly different limits, which complicates the analysis and modeling of properties. In particular, these issues are solved using statistical analysis methods. However, this approach is only possible if there is a large amount of data describing the process. Statistically significant information about the composition and testing conditions of Nickel-based superalloys allows us to successfully use modern methods of mathematical statistics for modeling [2-4].

An available computational tool for solving these problems is the method of artificial neural networks (ANN). The method is based on the search for correlations between known input and output parameters [5], and refers to non-linear statistical methods that are widely used for solving problems with a large number of variable data.

Previously, this method has already been used for the analysis of Nickel-based superalloys [6–16]. The purpose of these works was as follows: synthesis of new chemical compositions of superalloys [6, 14, 15, 16, 17]; modeling of changes in the coefficient of thermal expansion [7–9]; modeling of energy hysteresis [8]; prediction of low-cycle fatigue energy [9]; modeling the development of fatigue cracks [10]; prediction of material defects [12]; simulation of time to destruction [13].

In this study, the input data are chemical compositions and known experimental values of UTS, and the output data are previously unknown UTS obtained as a result of modeling.

To obtain a statistically significant sample, we searched for information and formed a database that included melting compositions and values of the long-term strength limit of about 300 brands of Nickel-based superalloys.

The applied ANN is a direct propagation network, such as a multi-layer perceptron with 13 neurons in a single hidden layer, and a Bayesian regularization learning algorithm organized in the Matlab 2014a application package. [18, 19]

The temperature and time of isothermal exposure prior to the rupture test are converted to the Larson-Miller parameter (P_{LM}) [20, 21] (1)

$$P_{LM} = T \times (20 + lg\tau) \quad (1)$$

As a result of modeling using a database and an artificial neural network, the regularities of changes in heat resistance with changes in the chemical composition of the Nickel-basedsuperalloys were obtained. These correlations are multidimensional matrices. The chosen method of modeling allowed us to calculate previously unknown values of the long-term strength limit and present them as dependencies $\sigma=f(P_{LM})$ for all the studied chemical compositions of alloys.

To assess the accuracy of the model, chemical compositions belonging to different generations were selected separately (Table.1).

The division of Nickel-based superalloys on the generation is based on the principle of their alloying. The first generation includes alloys with classical alloying Al, Ti, Cr, Mo, W, Ta, Nb, Hf. In addition to the classic set, rhenium is added to the composition of alloys of the second and third generations in the amount of 2...4% and 5...6%, respectively. The fifth generation includes alloys with rhenium, additionally alloyed with ruthenium

3 Results and discussion

Figure 1 shows the dependences of the UTS on the temperature and time parameters of tests of heat-resistant Nickel superalloys of the validation group belonging to different generations. The dependence graphs $\sigma=f(P_{LM})$ have an s-shape characteristic of most heat-resistant Nickel alloys. The graphs show separately the values obtained as a result of tests [1] and as a result of simulation of ANN. With a relatively small spread of experimental and simulated values, the ANN gives a fairly accurate calculation result, with a standard deviation of 15% [18, 19]. Graphs of UTS dependencies on the Larson-Miller parameter (Fig.1), different generations of Nickel-based superalloys have the same type of change $\sigma=f(P_{LM})$, with the features inherent in each alloy composition. A generalized view of the dependencies is shown in Figure 2.

The ultimate tensile strength (Fig.1 and 2), which characterizes the heat resistance of the alloy, does not monotonously decrease with increasing Larson-

TABLE 1. CHEMICAL COMPOSITION OF THE VERIFICATION SUB-SAMPLE, WT%

Alloy/Elements	C	Cr	Co	Mo	W	Al	Ti	Nb	B	Zr	Ta	Re	Ru	Ce	Hf
First generation															
ZHS30M	0,01	7,0	7,5	0,6	11,7	5,1	1,8	1,1							0,10
ZHS6U	0,17	8,8	9,8	1,8	10,3	5,6	2,4	1,0	0,035	0,04				0,02	
ZHS26U	0,16	5,0	9,0	1,1	11,7	5,8	0,8	0,83	0,015						0,83
Second generation															
ZHS36		4,0	9,0	1,0	12,0	6,0	1,0					2,0			
CMSX4		6,5	9,0	0,6	6,0	5,6	1,0				6,5	3,0			0,10
ReneN5	0,03	7,0	7,5	1,5	3,5	6,1	0,8		0,027		5,8	4,5			0,15
Third generation															
CMSX10		2,0	3,0	0,4	5,0	5,7	0,2	0,1			8,0	6,0			0,15
ReneN6	0,05	4,2	12,5	1,4	6,0	5,8			0,004		7,2	5,4			0,03
TMS-75		3,0	12,0	2,0	6,0	6,0					6,0	5,0			0,10
Fourth generation															
EPM102	0,03	2,0	16,5	2,0	6,0	5,6					8,3	6,0	3,0		0,15
MC-NG		4,0		1,0	5,0	6,0					5,0	4,0	4,0		0,10
ВЖМ4		2,5	6,0	4,0	4,0	6,0					4,5	6,0	4,0		
Fifth generation															
TMS162		2,9	6,0	3,9	5,8	5,8					5,6	4,9	6,0		0,10
TMS196		4,6	5,6	2,4	5,0	5,6					5,6	6,4	5,0		0,10
MC645		5,0			6,0	6,0	0,5				5,0	4,0	5,0		0,10

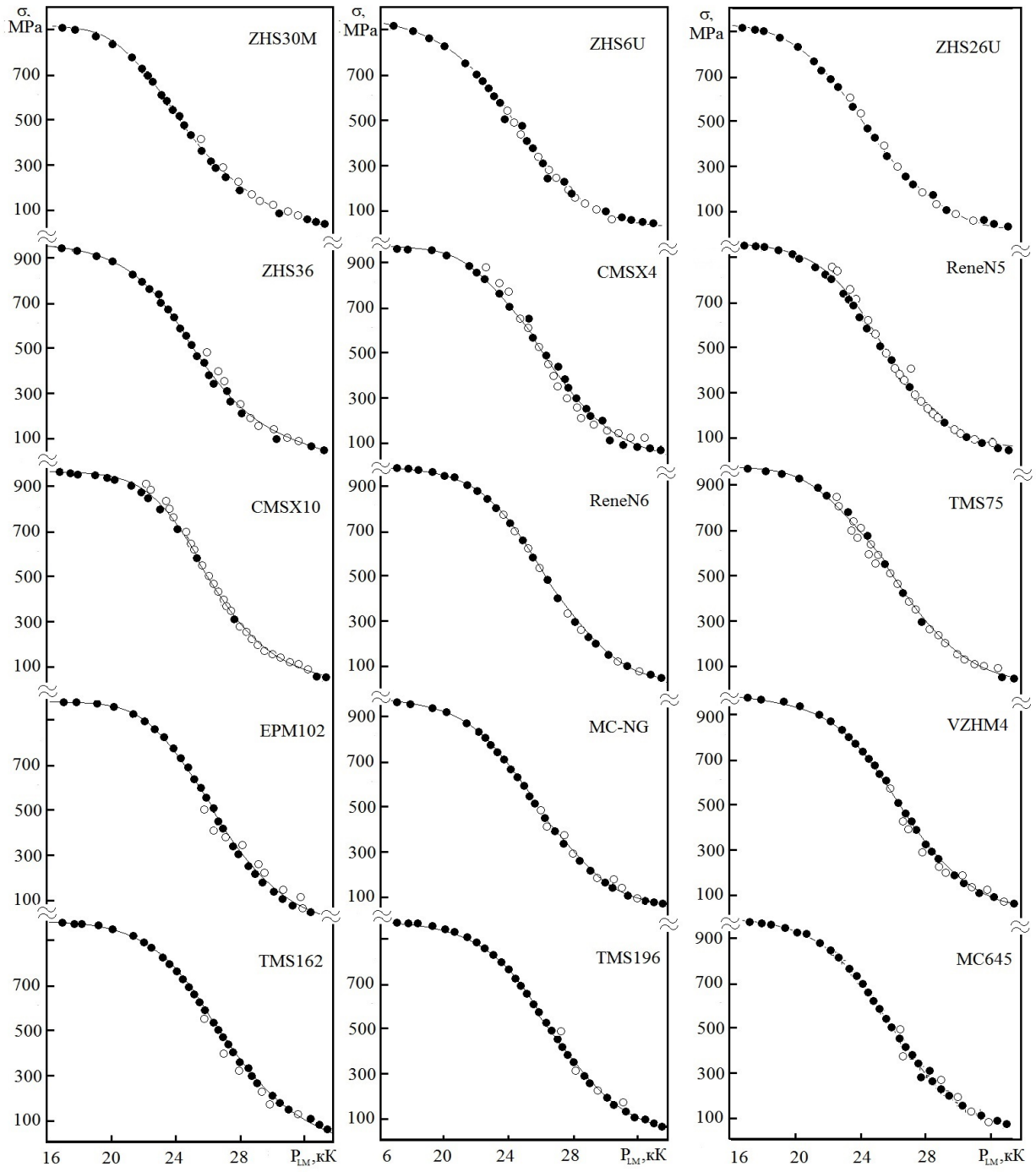
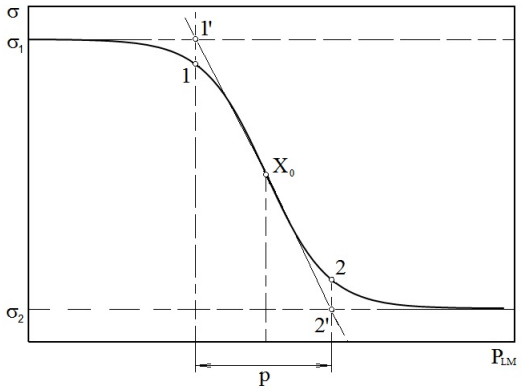


Fig.1. Dependences of the UTS on the Larson-Miller parameter of the validation group of heat-resistant Nickel alloys of different generations. ○ - experimental values ● – calculated values.

Miller parameter. On the curve, three sections are conditionally allocated, characterized by different rates of degradation of the structure before destruction, their boundaries are marked by points 1 and 2. Between these points there is a section with the maximum rate of decrease σ. The middle of this section, through which the tangent line is drawn, is marked as X_0. Obviously, the angle of the tangent reflects the structural stability of the alloy. The maximum and minimum heat resistance values are denoted as σ1 and σ2, respectively. The difference between the values of the Larson-Miller parameters at points 1 and 2 is indicated as ΔX. it Should also be noted that the value of ΔX indirectly characterizes the structural stability of heat-resistant alloys. The higher this value, the greater the fracture resistance of the alloy structure.

The adequacy of the obtained model of heat resistance changes is confirmed by the correlation of experimental and calculated values of the long-term strength limit.

The structure of heat-resistant Nickel alloys is heterophase, and its degradation process is multi-stage due to the different temperature stability of the structural components, which affects the intensity of the decrease in the tensile strength. Analysis of the literature data [34–37] and our research [38–40] allow us to form the most General picture of structural changes occurring in samples under long-term isothermal exposures that mimic operational ones. In a gamma-solid solution, a so-called raft structure is formed under the influence of temperature and applied load in a certain direction, and dislocations occur. Isolation of the main reinforcing γ'–secondary phase of the cubic morphology coagulates, individual particles coalesce with each other, the growth of blocks occurs.



Fig/2. The generalized dependence of the σ=f (P_{LM})

Coherence between the matrix and the main reinforcing intermetallic γ'-secondary phase is significantly reduced and completely disappears. At exposures above 1100°C, the amount of γ' phase is significantly reduced. Selection carboborite and eutectic carbonitride are reduced in size and replaced by colonies rounded, more dispersed particles. Carbides of eutectic origin of the MC type of typeface morphology break up into colonies of rounded particles and also dissolve in the matrix. Globular MC carbides are more stable, but with increasing operating time, carbide reactions occur along their boundaries, resulting in two new M_6C and $M_{23}C_6$ carbides belonging to topologically densely Packed phases (TSP). M_6C carbide of needle-like morphology destroys both the main reinforcing intermetallic phase and cuts its coherent bond with the matrix. The other $M_{23}C_6$ carbide is also not stable and is the basis for the occurrence of TSP phases, such as the μ-phase, σ-phase, *P*-phase and the laves phase. These structural changes lead to a multi-stage softening of the original structure, which is reflected in the course of the curve in Figures 1 and 2.

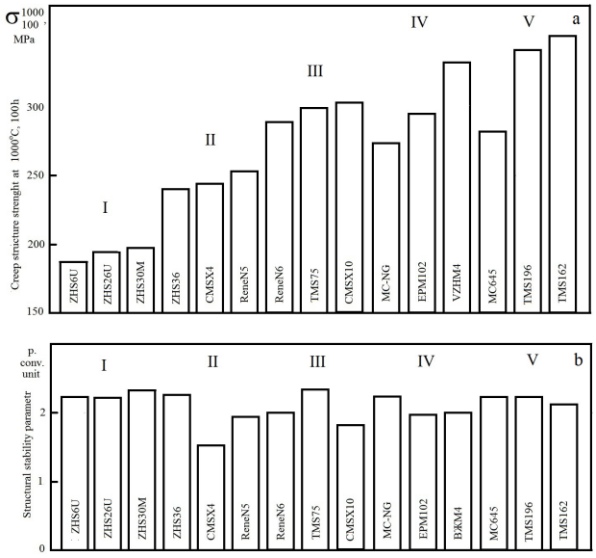
The dependence σ=f(P_{LM}) can be best described by the analytical function (2), which is a consequence of the Arrhenius equation. For convenience, x ≡ P_{LM}, p≡Δx.

Where σ1, σ2, x0, and p are the parameters set during the approximation of the dependence σ=f(P_{LM}) for a specific alloy composition. The value σ1 determines the invariance of σ at P_{LM} up to point 1, σ2 characterizes the asymptotic tendency of σ to zero, x_0 is the inflection point that geometrically corresponds to the middle of the range of linear reduction σ.

$$\sigma(x) = \sigma 2 + \frac{\sigma 1 - \sigma 2}{1 + \exp(\frac{x - x0}{p})} \quad (2)$$

Despite the fact that the dependence σ=f(P_{LM}) for all alloys has the same form, its parameters σ1, σ2, x_0 and p depend on the chemical composition of the alloy and, accordingly, the structural changes occurring in the alloys during long isothermal exposures preceding the rupture tests.

Fig. 3a shows nomograms of the long-term strength limit of the validation group alloys obtained by neural network modeling and corresponding to the isothermal exposure of discontinuous samples at a temperature of 1000°C for 100 hours. Nomograms illustrate a significant increase in heat resistance due to the alloying of rhenium and ruthenium alloys and correlate with previously known experimental results [22–34].



Fig/3. Nomograms a – ultimate tensile strength; b- parameter of structural stability of Nickel-based superalloys of the validation group, Roman numerals indicate the generation numbers.

Using the analytical function (3) the phase stability parameters were calculated for the alloys of the validation group.

$$y'(x) = \frac{\sigma_1 - \sigma_2}{[1 + \exp\left(\frac{x_1 - x_2}{p}\right)]^2} * \exp\left(\frac{x_1 - x_2}{p}\right) * \frac{1}{p}$$

$$y'(x_0) = \frac{\sigma_1 - \sigma_2}{4} * \frac{1}{p} \quad (3)$$

$$p = \frac{\sigma_1 - \sigma_2}{4y'(x_0)}$$

$$y'(x_0) = \frac{\sigma_1 - \sigma_2}{\Delta x}$$

$$\Delta x = 4p$$

$$p = \frac{\Delta x}{4}$$

The results are presented in the form of nomograms in Fig. 3b. First-generation alloys with low heat resistance are characterized by structural stability. Adding rhenium to the alloy significantly increases the heat resistance, but slightly reduces the phase stability. The fifth generation of Nickel-based superalloys is optimally alloyed with rhenium and ruthenium, and has a balanced chemical composition, where the previous level of phase stability was achieved at a high level of heat resistance. To clarify these facts, it is necessary to conduct additional research on the relationship between the structural stability parameter and the dissolution temperature of the main hardening phase for a larger sample of Nickel-based superalloys.

4 Conclusion

Using the machine learning method, we obtained a model for changing the heat resistance of Nickel-based alloys from the temperature-time parameters of the tests.

Comparison of experimental and calculated values of the limit of long-term strength of the validation group of heat-resistant Nickel alloys shows the accuracy of the obtained model.

Using the model, the graphs of the dependence σ=f(P_{LM}) are extrapolated. All dependencies have the same s-shaped form of lowering UTS with an increase in the Larson-Miller parameter, which is typical for most heat-resistant Nickel alloys and described by the analytical function (2). Each curve has features that are unique to a given alloy composition-the coordinates of points 1 and 2. This type of change in the Nickel-based superalloys is explained by the ongoing structural degradation.

A new method for determining the phase stability parameter of heat-resistant Nickel alloys (p) is proposed. By differentiating the analytical function σ(x), an expression is obtained for calculating the phase stability parameter (2). The variables for calculating (p) are determined by approximating the dependencies σ=f(P_{LM}). The increase in heat resistance from the first to the fifth generation of alloys is not accompanied by significant changes in the structural stability of Nickel-based superalloys.

References:

[1] ISO 204:2018(en) Metallic materials — Uniaxial creep testing in tension — Method of test https://www.iso.org/ru/standard/67737.html

[2] M. Morinaga, N. Yukawa, H. Adachi, and H. Ezaki. New phacomp and its application to alloy design. In Superalloys 1984. The Minerals, Metals & Materials Society, 1984. P.523-532.

[3] Saunders N., Fahrmann M., Small C.J. The Application of calphad Calculations to Ni-Based Superalloys // Superalloys 2000. — TMS. — 2000. — P. 803–811. 19. Saunders N. Phase Diagram Calculations for Ni-based Superalloys // Superalloys. — TMS. — 1996. — P. 101–110. 20.

[4] Saunders N. The application of Calphad techniques in the development of a New gas-turbine disk alloy // Mat. Research Soc. Bull. — April. — 1999. — P. 22. 21. Saunders N. Phase-Diagram Calculations for Ni-based Superalloys // Superalloys 1996 — TMS. — 1996. — P. 101–110

[5] Simon Heikin. Neural Networks: A Comprehensive Foundation. Moscou. Wiliams. 2017. 1104c

[6] Y.S.Yoo, I.S.Kim, D.H.Kim, C.Y.Jo, H.M.Kim, C.N.Jone. The application of neural network to the development of single crystal superalloys. Superalloys 2004. Edited by K.A. Green, T.M. Pollock, H. Harada, T.E. Howson, R.C. Reed, J.J. Schirra, and S, Walston TMS (The Minerals, Metals & Materials Society), 2004.

[7] N. Bano and M. Nganbe: Modeling of Thermal Expansion Coefficients of Ni based Superalloys using Artificial Neural Networks, Journal of Materials Engineering and Performance, Vol. 22, Issue 4, pp. 952-957, April 2013.

[8] N. Bano and M. Nganbe: Neural Network Approach for Modeling the Hysteresis Energy of Ni based Superalloys, Proceedings of the International Conference on Mechanical

Engineering and Mechatronics, Ottawa, Canada, August 2012.

[9] Bano, A. Fahim, and M. Nganbe: Neural Network Model to Predict Low Cycle Fatigue Failure Energy of Rene77, Proceedings of the AES-ATEMA'2010 Fifth International Conference, Montreal, Quebec, Canada, pp. 123-126, June 2010.

[10] N. Bano, A. Fahim, and M. Nganbe: Fatigue Crack Initiation Life Prediction of IN738LC using Artificial Neural Network, Proceedings of the AES-ATEMA'2010 Fifth International Conference, Montreal, Quebec, Canada, pp. 117-121, June 2010.

[11] N. Bano, A. Fahim, and M. Nganbe: Determination of Thermal Expansion Coefficient of IN738LC with Duplex Size Gamma Prime using Neural Network, Proceedings of the Conference of Metallurgists, Winnipeg, August 2008.

[12] Shuo Feng, Huiyu Zhou, Hongbiao Dong. Using deep neural network with small dataset to predict material defects. Materials & Design. doi.org/10.1016/j.matdes.2018.11.060

[13] Muhammad H Hasan, Muataz Al Hazza, Mubarak W. ALGrafi, Zubair Imam Syed. ANN Modeling of Nickel Base Super Alloys for Time Dependent Deformation. Journal of Automation and Control Engineering Vol. 2, No. 4, December 2014. C.353-356. doi: 10.12720/joace.2.4.353-356

[14] Nurgayanova O. S. Taneyev, A. A., Synthesis of cast Nickel heat-resistant alloys for castings with directed and monocrystalline structure. Bulletin of the Ufa state aviation technical University. 2007. Vol. 9. No. 1. Pp. 160-169. (in russian)

[15] Nurgayanova O. S., Ganeev A. A. Mathematical modeling of the effect of alloying elements on the heat resistance of Nickel alloys with a single-crystal structure. Bulletin of the Ufa state aviation technical University. 2006. Vol. 8. No. 4. Pp. 91-95. (in russian)

[16] Nurgayanova O. S., Ganeev A. A. Mathematical modeling of the effect of alloying elements on the heat resistance of Nickel alloys with a single-crystal structure. Bulletin of the Ufa state aviation technical University. 2006. Vol. 8. No. 4. Pp. 91-95. (in russian)

[17] Nurgayanova O. S., Ganeev A. A. computer-aided design System for casting Nickel heat-resistant alloys with a single-crystal structure. Polzunovskii almanac. 2006. No. 3. Pp. 22-26 (in Russian

[18] Sydikhov, A.S., Tyagunov, A.G., Milder, O.B., Ganeev, A.A. Application of artificial neural networks for the alloy features assessment based on the alloy compound. AIP Conference Proceedings, 2019, 2116, 20001

[19] Sydikhov, A.S., Tyagunov, A.G., Milder, O.B., Ganeev, A.A. ANN approach for Larson-Miller factor approximation in the space of alloy features AIP Conference Proceedings. 2019. 2116,2000

[20] Larson R.R., Miller J. Time-temperature relationship for rupture creep stress. Trans ASME. 1952.-74. №5. P.765-775.

[21] Sinayski B.N., Belyaev M.S., Zhukov N.D., Panteleev A.D. (1989) Temperature-time approach to approximation and extrapolation of characteristics of resistance of high-cycle nickel alloys to high-cycle fatigue. Strength problems. 3. 44–50. (in Russian)

[22] J.X. Zhang, T. Murakumo, H. Harada, Y. Koizumi, T. Kobayashi. Creep deformation mechanisms in some modern single crystal superalloys. Superalloys 2004. Edited by K.A.Green, T.M.Pollock, H.Harada, T.E.Howson, R.C.Reed, J.J.Schirra, S.Walston. TMS (The Minerals, Metals & Materials Society), 2004. P.189-195.

[23] Akihiro Sato, Hiroshi Harda, An-Chou YEH, Kyoko Kawagishi, Yutaka Koizumi, Toshiharu Kobayashi, Tadaharu Yokokawa, J-X.ZHANG. A 5th generation SC superalloy with balanced high temperature properties and processability. Superalloys 2008. Edited by Rodger C.Reed, Kenneth F.Green, Pierre Caron, Timothy P.Gabb, Michael G.Fachrmann, Eric S.Huron, Shiela A.Woodard. TMS (The Minerals, Metals & Materials Society), 2008. P.131-138.

[24] Yafang Han, Wenyou Ma, Ziqiang Dong, Shusuo Li, Shengkai Gong. Effect of ruthenium on microstructure and stress rupture properties of a single crystal nickel base superalloy. Superalloys 2008. Edited by Rodger C.Reed, Kenneth F.Green, Pierre Caron, Timothy P.Gabb, Michael G.Fachrmann, Eric S.Huron, Shiela A.Woodard. TMS (The Minerals, Metals & Materials Society), 2008. P.91-97

[25] Walston, A. Cetel, R. MacKay. Joint development of a fourth generation single crystal superalloys. Superalloys 2004, ed. K. A. Green, et al, (Warrendale, PA:TMS, 2004). P.15-24.

[26] G. L. Erickson, The development and application of CMSX-10, Superalloys 1996, ed. P. D. Kissinger, et al, (Warrendale, PA:TMS, 1996). P.35-44.

[27] Y. Murata, R. Hashizume, A Yoshinari. Alloying effects on surface stability and creep strength of nickel based single crystal superalloys containing 12mass%Cr. Superalloys 2000. ed.T.M. Pollock, et al. (Warrendale, PA:TMS, 2000). P.285-294.

[28] J.X. Zhang, T. Murakumo, H. Harada. Dependence of creep strength on the interfacial dislocations in a fourth generation SC superalloy TMS-138, Scripta Materialia. 48 (2003). P.287–293

[29] K .Yutaka, K .Toshiharu, Y.Tadaharu. Development of next –generation Ni-base single crystal superalloys. Superalloys 2004. ed. K. A. Green, et al, (Warrendale, PA:TMS, 2004). P.35-43

[30] D. Argence, C. Vernault, Y. Desvallees, D. Fournier. 4th MC-NG: A generation single-crystal superalloy for future aero-nautical turbine blades and vanes, Superalloys 2000, ed.T.M. Pollock, et al, (Warrendale, PA:TMS, 2000). P.829-837

[31] A.C. Yeh, S. Tin. Effects of Ru and Re additions on the high temperature flow stresses of Ni-base single crystal superalloys. Scripta Materialia. 52 .2005. P.519–524.

[32] J.X. Zhang, T. Murakumo, H. Harada. Dependence of creep strength on the interfacial dislocations in a fourth generation superalloy TMS-138. Scripta Materialia. 48. 2003. P.287–293

[33] A.C. Yeh, S. Tin. Effects of Ru and Re additions on the high temperature flow stresses of Ni-base single crystal superalloys. Scripta Materialia 52 (2005). P.519–524

[34] G. E. Fuchs. Solution heat treatment response of a third. generation single crystal Ni-base superalloy. Materials Science and Engineering A300(2001). P.52-60

[35] Davydov D. I., Vinogradova D. I., Kazantseva N. V., Stepanova N. N. Investigation of the structure of two Nickel alloys after high-temperature deformation. Metal physics and metal science. 2015. Vol. 116. No. 2. Pp. 210-218 (in russian)

[36] Kuznetsov V. P., Lesnikov V. P., Popov N. A. Structure and properties of heat-resistant Nickel alloys. Publishing house of the Ural University. 2016. 164c

[37] Kamaraj, M. Rafting in single crystal nickel-base superalloys – An overview / M. Kamaraj // Sadhana, – 2003. – P. 115-128.

[38] Tyagunov A.G., Baryshev E.E., Kostina T.K., Baum B.A., Lesnikov V.P., Semenova I.P. The effect of long-term high-temperature heat treatment at 950°C on the structure and mechanical properties of the zhs6u superalloy. The Physics of Metals and Metallography. 1998. T. 86. № 1. pp. 65-69.

[39] Tyagunov A.G., Baryshev E.E., Kostina T.K., Semenova I.P., Lesnikov V.P. Thermal stability of the structure of a high-temperature nickel alloy fabricated by two different technologies. Metal Science and Heat Treatment. 1999. T. 41. № 11-12. pp. 538-541

[40] Tyagunov.G., Kostina T. K., Lesnikov V. P., Baryshev E. E. Influence of high-temperature processing of the melt on the structure of Nickel heat-resistant alloy EP539L. Foundry. 1994. No. 1. Pp.13-14.