Application of Artificial Neural Networks for Prediction of Nickel-based Superalloys Service Properties Based on the Chemical Composition

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Abstract: - Nickel-based superalloys are utilized in various fronts of industry; however, they are especially important in turbine building. To date, a large amount of data on the chemical compositions and performance of the alloys has been accumulated; however, usually, there is only data on a rather narrow range of temperatures and test exposures. The lack of information on the properties of alloys outside the studied ranges is a significant limitation on their possible applications. The available approaches are based mainly on practical experiments and, therefore, are expensive and time consuming. Moreover, the alloys development has a significant environmental impact since the chemical composition compound is conjugated with emissions and disposals of toxic and radioactive heavy metals. Up to date, it is possible to substantiate a new approach to analyzing the service properties of metallic materials based on the use of artificial neural networks. The previously obtained real test data formed the basis for estimation the missing values. In this work, we have studied the database of 210 nickel-based superalloys with regard to their tensile strengths in various conditions. The chemical composition and test conditions of the alloys were the input parameters of the ANN. Based on the ANN forecast, the dependences of tensile strength on temperature and time conditions were obtained, which were presented in the form of Larson-Miller parameter. The analysis of dependences allows one to select the parameters of the initial heat resistance (tensile strength) and thermal stability of the alloys. In addition, the dependence of tensile strength and thermal stability on the content of the main reinforcing elements was obtained using ANN modeling. The calculation results coincide with the experimental data.

Key-Words: - nickel-based superalloys, artificial neural network, tensile strength, heat resistance, thermal stability

1 Introduction

Heat resistant nickel-based alloys are extensively employed in the production of engines. In particular, they are the only material for manufacture the turbine blades. In this case, the single crystal casting is principally applied. The outstanding characteristics of these alloys provide the products operation under heavy loads and high temperatures for a long period of time. Due to such properties, they are called “superalloys”.

Nickel-based alloys are multiphase doped systems. The composition of modern alloys most often includes up to 30 chemical elements, in addition to Nickel (Cr, Co, Mo, W, Al, Ti, Nb, Ta, Re, Ru, Hf and some other elements). The purpose of adjunction additional elements in the alloy is to create a new set of service properties. Each of these additions is chosen to serve a particular purpose in optimizing the properties for high temperature application. The alloys creation and industrial cast have a significant environmental impact since the chemical composition compound leads to the emission and further disposal of toxic and radioactive heavy metals from the composition.

The major properties of the alloys and the casts are a tensile strength (or heat resistance) and a thermal stability. The heat resistance is the ability of a material to withstand stress at high temperatures without permanent deformation and destruction. The thermal stability is the ability of the structure to remain unchanged during the entire design period of use. Heat resistance and thermal stability of alloys are not related to each other [1, 2].

High temperature operating modes lead to increase in the diffusion processes. Due to the diffusion, initial reinforcing structural phases dissolve in the Nickel matrix. Excessive alloying elements create new phases, including destructive ones. The alloy's feedback aimed at slowing these processes might be defined as thermal stability.

Tensile tests are carried out to assess the heat resistance of the samples. The sample is kept at a certain temperature (t, °C) for a certain time (τ, hours) in advance, then the tensile strength (σ, MPa) is measured by breaking the specimens and determining the breaking strength. Test temperatures belong to the range from 50°C to 1150°C. The test time varies from 50 to 5000 hours.

Several isothermal exposures having a certain temperature and time are assigned to each alloy. However, each alloy composition does not have the full set of experimental test results, since the alloy is usually tested at those temperatures and times for which it has been originally designed. This is a problem for manufacturers of motor equipment, since it significantly reduces the choice of alloys when designing new products. The inability to compare the tensile strength values obtained after various isothermal exposures is the problem for researchers, too.

The increase in the level of heat resistance is achieved by optimizing the chemical composition, as well as by the use of advanced technology of single crystal casting. These methods allow increasing the temperature of turbine gases up to 1580 °C, which magnify the thrust by 15...20% and the operation period by factor of 1.5...2 [3].

Due to the use of expensive alloying elements and because of the complex technological process of single crystal casting and subsequent heat treatment, nickel alloy products are becoming more and more costly. In addition, the development and creation of each alloy takes a lot of time and is associated with the load on the environment.

The desire to improve the characteristics of the gas turbine engine led to a significant increase in its cost, especially due to doping with expensive elements, such as Rhenium and Ruthenium. High value is reasonable when products are developed for aviation and space. In the case of the development of commercial goods, it is advisable to reduce the price of production, and hence the composition used. A complete informational picture of the content and service properties of alloys could significantly affect the choice of material for the manufacture of a particular product.

Mathematical modeling is an approach, which is able to substantially accelerate and reduce the cost of the process of analysis of existing alloys and of development new ones. When simulating alloys properties, the test temperature, the time and the content of the alloying elements are variable data in the model. The large number of variables also complicates the simulation task. Existing deterministic statistical methods make it possible to model the behavior of complex systems, though any nonlinearities complicate computation significantly.

The method of artificial neural networks (ANN) is a well-developed statistical method that allows solving complex problems associated with significant nonlinearities. Moreover, it is not demanding of computing power and is easy to apply. The use of artificial neural networks will make it possible to supplement the data and analyze the effect of the alloying elements content on the service properties of heat-resistant Nickel-based superalloys.

This work aims to establish relation between alloys content and heat resistance and to predict the absent values of tensile strength (σ, MPa) by artificial neutral network based on the chemical composition and exposure conditions (t, °C; τ, hours). The model might help to analyze existing and to create new alloys with reduced environmental load.

2 Approach and Experimental

The main objective of this work is to predict the unknown service properties of the Nickel-based superalloys based on the existing experimental data on the alloys content and tensile tests conditions. The secondary task is to analyze the effect of alloying elements on the basic service properties and to build an analytical dependence between the properties and test conditions. The computation method chosen is artificial neural networks.

2.1 The initial data description

The input data for the modeling are chemical compositions (25 alloying elements contents in percentage), tensile tests parameters (t, °C; τ, hours) and tensile tests results (σ, MPa). As an alloys sample, we have chosen a set of nickel-based superalloys with known chemical composition and test parameters. The alloys data has been collected from the open sources, dissertations and scientific literature. We selected the alloys with at least 5 values of tensile strengths under different test conditions. The sample size covered 210 Russian and Western alloys. Each alloy generates as many samples for network training as many different actual tests were carried out (the relevant information is available).

2.2 The preliminary network selection

The artificial neural network chosen for the modelling was multilayer perceptron with Bayesian regularization. Such a network has shown better results in similar experiments [4]. For the ANN creation, the MATLAB package was selected. The network structure is shown in Fig.1.

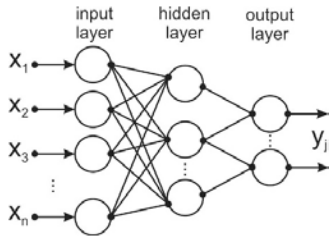

Fig. 1. Neural network structure

As the preliminary stage of the experiment, we applied a raw data for the modeling. In total, we applied 27 input parameters (x_i): 25 chemical elements content (%), test temperature t (°C); test duration τ (hours). The sub-sample size was 100 randomly selected alloys from the whole sample. The output (or target) parameter of the network (y_j) was the tensile strength σ (MPa).

The network structure has been selected in the following algorithm: the number of neurons in the hidden layer was varied from 4 to 20. Accuracy of predictions is characterized by the degree of coincidence of the values of the investigated parameters between the experimental measurements and calculated by ANN data.

In our work, the relative root mean squared error (1) was chosen as a criterion of prediction quality for the model.

$$RRMSE = \sqrt{\frac{1}{m}\sum_{t=1}^{m}\left(\frac{\sigma_{predict\ \ t}-\sigma_t}{\sigma_t}\right)^2} \times 100\% \quad (1)$$

The network training procedure is shown in the Fig.2. Each network processed the input set and predicted the output parameter. The error of prediction at each lap was evaluated and stored. The number of neurons in the network that showed the best performance was 15. The network training with initial raw data has led to minimal RRMSE=70%. Such an accuracy is unacceptable.

This mean that due to the high dispersion of initial data the correct evaluation of targets by the network is impossible. Therefore, one needs to pre-operate the raw data.

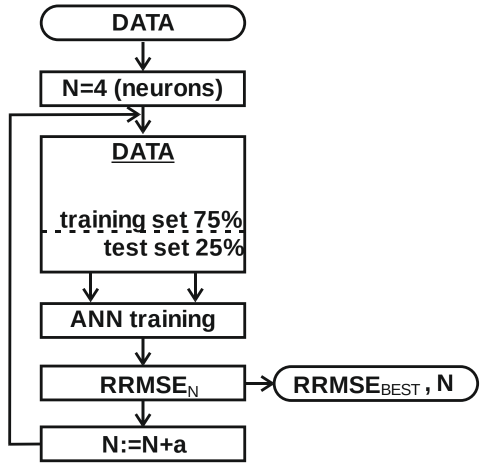

Fig. 2. Network training procedure

2.3 Operating the pre-processed data

The next stage of the experiment was carried out with input data pre-processing. The following transformations were performed to improve the network output and to reduce the prediction error: we took the whole sample (210 alloys); the temperature and tensile test time are replaced by the complex Larson–Miller parameter [5] (P_{LM}) (2); the chemical compositions of the alloys were converted from percentage into fractions; the results of the tensile tests were presented in their logarithms.

$$P_{LM} = \frac{(t+273)\times(20+lg\tau)}{1000} \quad (2)$$

We must note that in the Larson-Miller transformation the absolute temperature (K) is applied. The logarithm has a decimal base. Logarithm conversion resolve the following questions. The tensile test results cover the range of three orders of magnitude and logarithm transformation makes the error in relative mode. Back logarithm transformation allow one to avoid the negative prediction values that is physically impossible.

In order to carry out the training of the neural network on a statistically representative sample and take into account all possible strata of the initial data, the quartile partitioning of input data was applied. The algorithm was the follows: quartile division of input information into groups by the content of Ni; random division of each group into training (75%) and test (25%) samples; combination of training and test samples from each group into common training and test sets.

The described above data preprocessing does not negate the fact that with each separate training the neural network has a different quality of training. This is related to the automated selection of Bayesian regularization parameters and the parameters of the artificial neural network. Therefore, it is necessary to construct a set of neural networks to select the one that would meet the desired accuracy.

The algorithm for constructing a set of neural networks consisted in the sequential creation of 5 neural networks with the number of neurons 4, 8, 12, 16, 20 units in the hidden layer. After that, the best one corresponding to the smallest value of RRMSE was chosen. Accounting the above, the optimized network training procedure is shown in Fig.3.

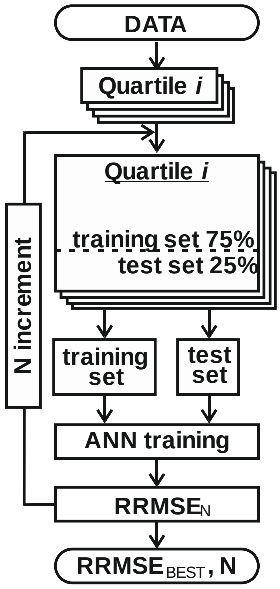

Fig. 3. Optimized network training procedure

The framework of the artificial neural network with the highest accuracy of predictions is presented in Fig. 4. It has 12 neurons in the hidden layer.

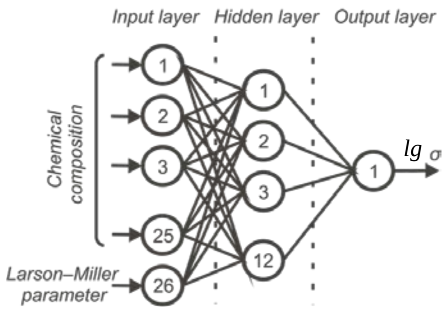

Fig. 4. Successive neural network framework

Input data preparation and neural network optimization reduced RRMSE down to 14%. Further reduction of this error is possible only by increasing the number of alloys in the input sample.

3 Results and Discussion

As a result of the optimization, the ANN with 12 neurons that demonstrates a minimal RRMSE was obtained. After loading the initial data (the chemical compositions of the high-temperature nickel superalloys and the known results of their tests for high-temperature strength after holding them in different temperature-time regimes) the tensile strength values were simulated. In total, the missing values of the tensile strength for 210 NBSA were predicted.

The obtained values indicate the same behavior of the tensile strengths of alloys vs temperature-time conditions. At the same time, the results demonstrate certain differences in the properties of alloys of different generations [6-17].

The most important feature of the approach is accessibility. It does not require expensive materials and tests to do. The predicted data might be of great interest for gas turbine engine designers in various applications. The proposed approach is, also, of great importance for materials scientists dealing with alloying materials, especially in the case when some of the properties of the material are well known and some not. The performed simulations made it possible to supplement the missing parameters with a database on the service properties of high-temperature nickel-based superalloys. After that, the dependences of the long-term tensile strength on the Larson-Miller parameter for all compositions of alloys contained in the database were constructed.

All alloys have the same exponential nature of the dependence of the tensile strength on the temperature and time conditions of testing, as shown in Fig. 5, where time and temperature are combined in the Larson-Miller parameter.

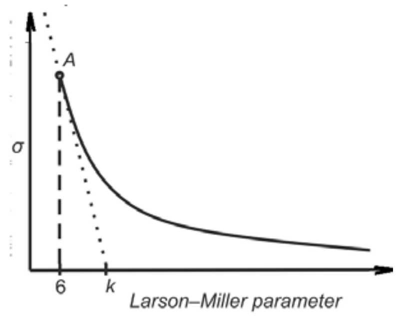

Fig. 5. Dependence of the tensile strength on the Larson-Miller parameter, typical for all nickel-based alloys

Accordingly, the nature of the dependence might be described by the following expression (3)

$$\sigma = e^{-\frac{P_{LM}}{K}} \quad (3)$$

The following characteristic features of each alloy are distinguished on the graph: A – calculated value of the tensile strength (σ) at P_{LM} = 6 that corresponds the room temperature, respective possible initial test conditions, characterized by an initial high-temperature strength of the alloy. The *K* coefficient characterizes how close the exponential curve is to the abscissa axis. This is the indirect indicator of the thermal stability. The larger the *K*, the longer the structure resists destruction.

In scientific literature, a lot of experimental data on the effect of alloying elements on the tensile strength of Nickel-based superalloys has been accumulated. For the validation of the predicted values of σ and thermal stability of the alloys (*K*), we selected some elements that make the main contribution to the hardening of alloys: Mo, Cr, Rh, Ru, Ta, Co, and W.

In MATLAB, we recalculated the dependencies of the elements content on the tensile strength and *K* coefficient (see Fig. 6 and 7) by using the prepared database.

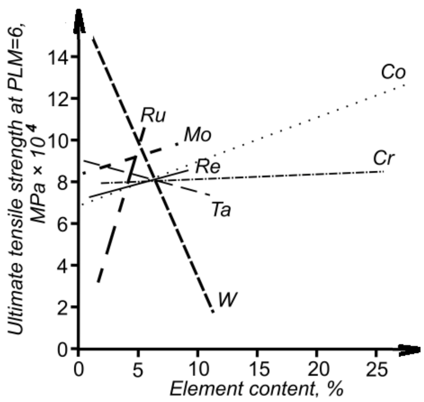

Fig. 6. Calculated data on the effect of certain alloying elements on the ultimate tensile strength of nickel alloys

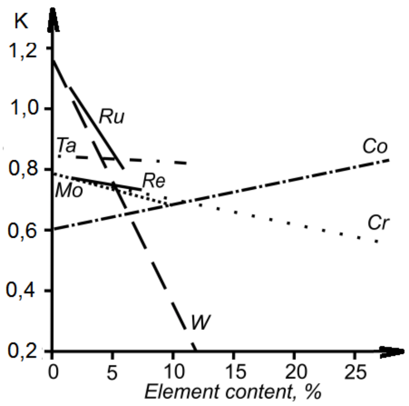

Fig. 7. Calculated data on the effect of certain alloying elements on the thermal stability of nickel alloys

The results of calculations show that Ta, Re, and Ru increase the high-temperature strength of alloys, while Cr and W reduce it. Mo and Co do not significantly affect the alloy features. These data are in good agreement with the experimental data given in [13], that confirms their adequacy.

Fig. 5 shows the calculated information on the effect of alloying elements vs thermal stability. As it follows from numerous studies, the overdeposition of high-temperature nickel alloys leads to an unbalanced phase composition and a decrease in thermal stability. The only elements Rhenium and Ruthenium block the development of embrittlement phases and substantially slow down the destruction.

4 Conclusion

High-temperature nickel-base superalloys are compositions with complex doping. The cost of both the materials themselves and the technology of single-crystal casting as a part of gas turbine engines building methods are high. At present, a large amount of data on the chemical compositions and service properties of NBSA has been accumulated. However, a significant part of information on alloys properties is absent as particular tests have not been carried out. The method of artificial neural networks is able to fill in the missing information in alloys catalogue by simulating it during the computational experiment.

The network framework might be developed during the preliminary experiment. In our case, we utilized a Bayesian neural network with 12 neurons in the hidden layer. As input parameters, information on the content of chemical elements in the composition of the alloys and experimental data of service properties are used. The tensile strength acts as an output parameter of the model. The initial data preprocessing significantly reduce the RRMSE and improve the accuracy of calculations. We combined the temperature-time exposures of alloy samples in the compex Larson-Miller parameter and further we applied a quartile decomposition of training data for the network. Thus, our model has 26 input and 1 output parameters.

As a result, a complete database for 210 nickel-based superalloys and their tensile strengths under different conditions was obtained. The previously obtained experimental data served as the basis for simulation of the missing values.

Thus, up-to-date simulating method of artificial neural networks has allowed substantiating a new approach to the analysis of service characteristics of metallic materials; taking into account previously accumulated experience.

The use of a database on the chemical composition of the alloys and their tensile strengths as input parameters of the ANN made it possible to obtain a series of plots of the dependence of the tensile strengths against the temperature-time conditions combined in the Larson-Miller parameter. We have described them by the exponential expression (3). Characteristic features for each composition of the alloy are the A and K parameters. They designate the initial heat resistance and thermal stability of the alloys respectively.

The computations made, also, have allowed to obtain dependences of tensile strengths and thermal stability on the content of the basic reinforcing elements. The results of the calculations coincide with the known experimental data, which confirms their adequacy.

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