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Deep learning in nickel-based superalloys solvus temperature simulation

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Abstract. Modeling the properties of complex alloys such as nickel superalloys is an extremely challenging scientific and engineering task. The model should take into account a large number of uncorrelated factors, for many of which information may be missing or vague. The individual contribution of one or another chemical element out of a dozen possible ligants cannot be determined by traditional methods. Moreover, there are no general analytical models describing the influence of elements on the characteristics of alloys. Artificial neural networks are one of the few statistical modeling tools that can account for many implicit correlations and establish correspondences that cannot be identified by other more familiar mathematical methods. However, such networks require careful tuning to achieve high performance, which is time-consuming. Data preprocessing can make model training much easier and faster. This article focuses on combining physics-based deep network configuration and input data engineering to simulate the solvus temperature of nickel superalloys. The used deep artificial neural network shows good simulation results. Thus, this method of numerical simulation can be easily applied to such problems.

Keywords: artificial neural network; framework; nickel-based superalloys; simulation; solvus temperature

1. Introduction

Nickel-based superalloys are complex alloyed metallic materials with unique properties such as high temperature resistance, corrosion resistance, high strength, etc. Alloying serves to achieve high resistance to mechanical and chemical degradation at high loads with prolonged exposure. Products made of these alloys operate at temperatures up to 1300°C and overcome a wide range of effects: thermal stress, corrosive media, contact stresses, strains from centrifugal forces, vibration bending stresses and torsional gas flow.

The major service properties of the alloys are heat resistance and structural thermal stability. Heat resistance is the ability of material to resist the load at elevated temperatures, without undergoing permanent deformation or fracture. To quantify the heat resistance, mechanical tests are carried out, the main of which is the test for long-term tensile strength, i.e., the greatest mechanical stress that the material could resist without breaking at a given temperature, exposure

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time and working atmosphere. The test temperatures range from 50 to 1200°C, the time of isothermal exposure varies from 50 to 10000 hours. Thermal stability is the ability of a material to retain properties during a period of prolonged isothermal exposures (Pollock 2006, Reed 2006).

The current level of heat resistance is achieved due to the optimization of the chemical composition, as well as the application of the most advanced technology of single crystal casting. These methods allow to enhance the temperature of the gases entering the turbine to 1580°C, which multiply the engine thrust by 15 ... 20% and its life by 1,5...2 times (Kuznetsov 2004). However, the desire to increase the characteristics of the gas turbines has led to a significant increase in their cost, especially due to alloying with expensive elements.

The main contribution to the strength properties of superalloys is made by γ' and γ'' precipitates. The γ'-phase constitutes the precipitate used to strengthen the alloy. It is an intermetallic phase based on $Ni_3(Ti,Al)$ which have an ordered **fcc** structure. The γ'-phase is coherent with the matrix of the superalloy having a lattice parameter that varies by around 0.5%. This phase solvus temperature highly correlates with the mechanical properties of the superalloys (Caron 2000). Along with direct modeling of the mechanical properties of superalloys, an indirect assessment is possible, which is useful if a direct model cannot be built for some reason. That is why the simulation of solvus temperature is an important task both from a physics and engineering point of view. However, there are certain difficulties. Although the data on the mechanical properties of nickel superalloys are fragmentary, in total they form a rather impressive sample that allows building various models. In contrast, information on the solvus temperatures of these materials is rather poor, which undoubtedly complicates the construction of traditional models.

Each of the several hundred developed alloys may contain up to two dozen chemical elements and even more. All this significantly complicates the modeling and simulation of the properties of these materials by traditional analytical methods, since the influence of each chemical element is so nonlinear that no unambiguous analytical dependences have been established so far. The more complex the composition of the alloy, the more difficult it is to determine the effect of each constituent element on one of the many mechanical and physical properties. The situation with nickel-based superalloys is exacerbated by the lack of sufficient mechanical test data and the variety of smelting technologies that can be accommodated in the models. In particular, the compositions of wrought, polycrystalline, directed crystallization and single-crystal alloys manifest themselves in completely different ways (Das 2010). During casting, small particles are dispersed in a nickel matrix, forming a kind of framework and acting as a barrier to the movement of dislocations (Zhou *et al*. 2012, Detrois *et al*. 2017). Paired, ternary, *etc*. compositions of superalloys are discussed in (Donachie and Donachie 2002, Pelleg 2013), however, with more complex alloying, the model cannot be created, yet.

Since the alloys are tested in fairly narrow time and temperature ranges, the lack of missing data is of great interest to practitioners who cannot independently conduct a series of demanding tests. Computer-aided experimental methods make it possible to extrapolate the results of tests for long-term strengths without the implementation of expensive and long-term full-scale experiments, by analogy with the vibration and acoustic tests supplemented and improved by computational methods (Olympio 2018, Biedermann 2019).

The researchers were helped by an alternative computational paradigm of artificial neural networks (ANN), which opened up new perspectives in solving problems characterized by high nonlinearity, fuzzy and implicit correlations. Neural network modeling made it possible to describe dependencies that were previously considered indescribable (Haykin 2009). This, of course, touched upon the issues of simulating the properties of superalloys. Nevertheless, since the

network itself is not able to build a good correlation, the success of its operation depends on the correctly chosen configuration, method and technology of training, and the appropriate format of the input and output data.

Previously, artificial neural networks were already used to analyze nickel-based alloys (Yoo *et al*. 2004, Nurgayanova, *et al*. 2006), however, the goal of these works was to synthesize new chemical compositions of heat-resistant alloys (Nurgayanova and Ganeev 2007), in modeling the change in the coefficient of thermal expansion (Bano *et al*. 2008, Bano and Nganbe 2013), in modeling energy hysteresis (Bano and Nganbe 2012), in the prediction of low-cycle fatigue energy (Bano *et al*. 2010a), in modeling the development of fatigue cracks (Bano *et al*. 2010b), in predicting the occurrence of material defects (Feng *et al*. 2019), in modeling the time to failure (Hasan *et al*. 2014). Moreover, it has done mainly about the same grade of alloy. The works devoted to the prediction of the solvus temperature on the basis of establishing the relationship between the chemical composition and experimentally obtained values of the alloys properties were not detected.

In this work, we apply the already tested deep artificial neural network and special data engineering taking into account physics and the known influence of elements to simulate such an important physical parameter as the solvus temperature of nickel-based superalloys based on information about their chemical composition.

2. Physical model and data preprocessing

The most important result of using ANNs is that they made it possible to extrapolate the results of tests without performing expensive and lengthy physical experiments. ANNs were previously used to simulate the properties of various superalloys, however, the main attention in these works was paid to the synthesis of new compositions. Only in some works ANNs were applied to establish the relationship between composition and properties (Hasan *et al*. 2014, Jones and MacKay 1996, Conduit *et al*. 2017). Earlier, we also worked in this direction and tried several variations of the networks (Tyagunov *et al*. 2019a, 2019b). The deep learning artificial neural networks have shown the best performance with simultaneously high speed. The programming and training of such models is initially rather complicated, however, for each specific task, significant optimization of these procedures is possible, based on the physics of the described process or object.

The main problem we faced from the very beginning of our attempts was the different scales of input and output data. We consider the use of mass percent (wt.%) when indicating the content of alloying elements to be a systemic problem in a huge number of studies. Each alloying element manifests itself in a different way, i.e., can impart both “positive” and “negative” characteristics to the alloy. Arguing about the stoichiometric composition of this or that phase included in the alloy, we naturally pass to the level of operating with atomic percentages. We have taken a similar approach here. However, it was developed so that we not only use the atomic percentages of the ligands, but also normalize them to the nickel content in order to remove the nickel itself from the model and thereby reduce the amount of input data.

It is convenient to explain the data preparation scheme using the example of the well-known superalloy CMSX-4. The composition of the alloy is given according to (Donachie and Donachie 2002), and the sequence of stages of transformation of the composition as it is applied for all alloys during simulation is shown in Table 1.

Table 1 The stages of alloying composition transformation from wt.% to atomic fractions for CMSX-4

#	Parameter	Ni	Cr	Co	Mo	Al	Ti	Ta	W	Re	Hf
1	wt.%	61.70	6.50	9.00	0.60	5.60	1.00	6.50	6.00	3.00	0.10
2	Atom. mass	58.60	52.00	58.90	95.96	27.00	47.90	180.90	183.80	186.21	178.49
3	(#1)/(#2)	1.0529	0.1250	0.1528	0.0063	0.2074	0.0209	0.0359	0.0326	0.0161	0.0006
4	Atom. fr.	0.6375	0.0758	0.0926	0.0038	0.1259	0.0127	0.0218	0.0198	0.0098	0.0003
5	Atom. fr./ Ni	-	0.1189	0.1453	0.0060	0.1974	0.0199	0.0342	0.0311	0.0153	0.0005

Line #1 - the nominal alloy composition according to the referenced source.
Line #2 - the reference data on the relative atomic mass of the alloying elements involved.
Line #3 - the result of dividing the data in row #1 by the data in row #2.
Line #4 - the atomic fractions of the alloying elements.
Line #5 - the fraction of the atoms of the given alloying element to the atoms of the nickel matrix.

Thus, in terms of 100 atoms of the nickel matrix, the CMSX-4 alloy contains approximately 12 Cr atoms, 14 Co atoms, 6 Mo atoms, *etc*. Thus, the variables characterizing the alloy composition are naturally normalized in such a way that their numerical values are automatically located in the range (0, 1) and this is a great advantage for simulation as it is believed (Haykin 2009, 4.6) that such a normalization favorably affects the operation of the error backpropagation algorithm during the network training. Thus, we came to the uniform scale in the model.

3. Framework

As noted, we have previously simulated the mechanical properties of superalloys based on their chemical composition. Initially, we used a conventional backpropagating multilayer perceptron network, however, then we had to develop a more complex model that expands the capabilities of the basic model and takes into account the difficulties associated with the contribution of a single element (Tyagunov *et al*. 2019c). A complicated network with Bayesian regularization gave encouraging results, however, an individual account of the contribution of each element can be carried out, it seems to us, only by a deep learning network (DLANN), in which each of the layers is responsible for a certain block of the studied characteristics. It is such a network that we simulate in this work.

Nevertheless, before starting building a neural network, one may use some steps to optimize the input information. This is intended to improve the training environment, make it easier for the network to find correlations, and increase the accuracy and speed of modeling. The performed normalization of the input variables makes it possible to effectively build practically any network architecture. We will use this, as well as, the known physical laws about the influence of certain elements on the parameters of the superalloys. This is nothing more than embedding a priori information into the model (Haykin 2009).

It is known that the addition of various elements to the alloy pursues different goals, while the compositions of the influencing elements intersect (Donachie and Donachie 2002, Pelleg 2013). So, for example, Al, Ti, Nb, Ta, Hf determine the precipitation hardening of the alloy by intermetallic phases of the Ni_3Al type, and Al and Ti, in addition, form a γ'-phase. Multilayer feedforward networks actually receive a differentiated signal at each successive layer, so it seems

reasonable to use this feature in conjunction with taking into account the influence of the elements. We form a deep network of the multilayer perceptron type, in which each introduced layer reflects some empirically discovered pattern and, in addition, we add an addition hidden differentiating layer transmitting a differentiated signal to the next layer of neurons combining it with a direct signal.

The advantage of a deep network built on the above principle over a multilayer fully connected perceptron is incomparably higher learning speed and, as expected, higher simulation accuracy.

We now describe the new information added to the model about the specific role of alloying elements in superalloys. We use the data from (Donachie and Donachie 2002) to account for the role of each element, which is presented in Table 2. We combine the information about the role of the elements in a "matrix of relationships" that reflects how each chemical element affects the properties of the alloy. This matrix is introduced into the deep learning model as a control element ("trigger"). The framework of the model is shown in Fig. 1. Actually, we build two models to compare. The first network has a differential layer, while the second does not. Each network uses concentrations of chemical elements in form of 16 groups according to Table 2 as the input data and (simulates) predicts the solvus temperature. Two input bias neurons with a preset opposite shift are used to increase the stability of the model and speed up its learning. This is a common practice in machine learning.

For the training, the input dataset is formed by the data (chemical composition and solvus temperature) on 79 nickel-based superalloys. The training method is a common error backpropagation with the Bayesian regularization.

In order to avoid the network overtraining, the fairly mild conditions (the target goal mean squared error, *MSE* (1) and the gradient) are empirically determined and set. In our case, y_i means

Table 2 Roles of alloying elements in superalloys

Group No	Effect	Alloying elements
1	Solid solution strengtheners	Co, Cr, Fe, Mo, W, Ta, Re
2	Carbide form MC	W, Ta, Ti, Mo, Nb, Hf
3	Carbide form M_7C_3	Cr
4	Carbide form $M_{23}C_6$	Cr, Mo, W
5	Carbide form M_6C	Mo, W, Nb
6	Carbonitrides M(CN)	C, N
7	Forms γ' Ni_3(Al, Ti)	Al, Ti
8	Raises solvus temperature of γ'	Co
9	Hardening precipitates and/or intermetallides	Al, Ti, Nb
10	Oxidation resistance	Al, Cr, Y, La, Ce
11	Improve hot corrosion resistance	La, Th
12	Sulfidation resistance	Cr, Co, Si
13	Improves creep properties	B, Ta
14	Increases rupture strength	B, if present in large amounts, borides are formed
15	Grain-boundary refiners	B, C, Zr, Hf
16	Retards coarsening	Re, Ru

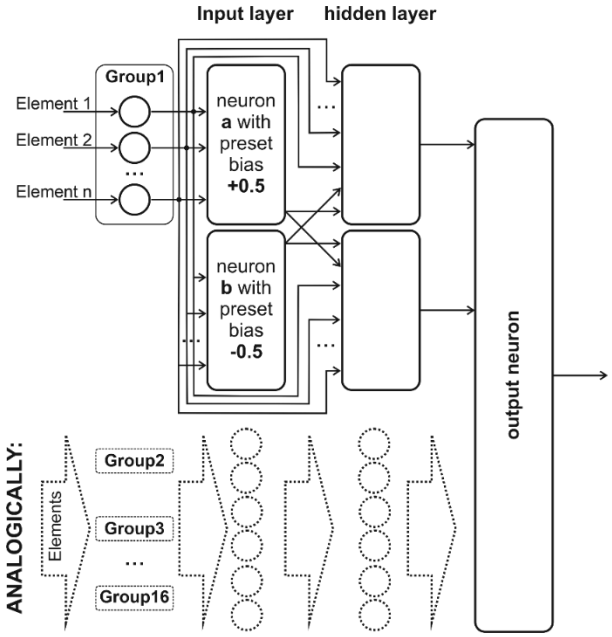

Fig. 1 The deep learning framework

the model output values or solvus temperatures. In the models, $y_{\text{predicted}}$ are the values obtained during the network prediction, y_{fact} are the known factual values of solvus temperature used in the network training.

$$MSE = \frac{\sum_{i=1}^{n}(y_{predicted\_i} - y_{fact\_i})^2}{n} \quad (1)$$

The training process is repeated several times until the condition *MSE*.test≤1.3×MSE.training is met. Here, *MSE*.training is the target function (1) value obtained at the training data set, *MSE*.test is the same regarding to the test data set. The initial data set is divided into training (75%) and test (25%) sub-sets randomly during the training procedure. For each new training repetition, the division is refreshed. The final model prediction ability is evaluated by the absolute value of the relative error (*RE*) between the model predictions and the real data from the verification sample (2).

$$RE_i = \frac{|y_{predicted\_i} - y_{fact\_i}|}{y_{fact\_i}} \quad (2)$$

As an independent verification sample, we engage 15 alloys, which do not take part in the training. Data on the solvus temperature of these alloys we compare with the network predictions.

4. Results and discussion

In the experiment, we train and test two different deep artificial neural networks. Their only difference is the presence of a hidden differential layer in the first one. The comparison of the results obtained might be done evaluating graphs in Fig. 2 where the predictions of the solvus

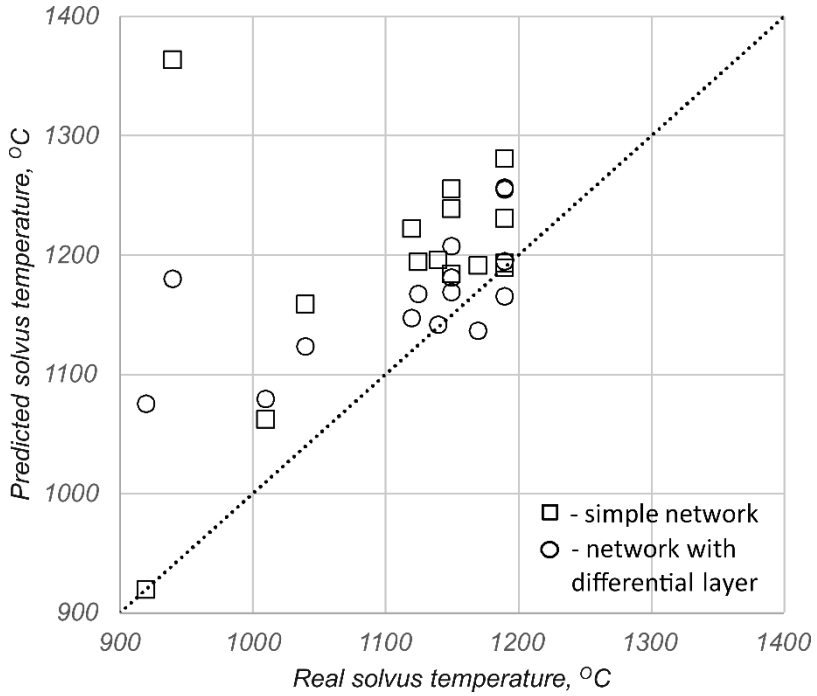

Fig. 2 Real solvus temperature *vs* ANN simulation (for two networks)

Table 3 Statistics of the related errors of predictions by two networks

Statistics	DLANN with differential layer	Simple DLANN
Mean	0.06	0.08
Median	0.04	0.05
SD	0.07	0.11

temperature *vs* real values for 15 superalloys from the verification set are shown. Obviously, a network with a differential layer shows a more "heap" result, although a simple deep network also performs well enough. For a more accurate assessment of the results, we turn to descriptive statistics. The statistics of the related errors are shown in Table 3.

Analyzing Table 3, we may deduce that the network with differential layer predicts better. Spending comparable time and computational resources on training, a deep network with a differential layer gives a standard deviation of at least one and a half times less. From a practical point of view, a prediction deviation of 7% is comparable to experimental methods (such as DTA), which achieve an accuracy of a few percent. An increase in the training sample and further optimization of the network configuration will further improve the forecast accuracy.

In addition, it is necessary to pay attention to a couple of "falling out" points in the temperature range of 920-940°C. Both models in this case seem to show not too convincing results. The fact is that among the alloys of the verification sample there were two alloys (In-901 and Nimonic 263), which, although they are considered nickel, should be more classified as iron/cobalt, since the nickel content in them is less than 50%. Naturally, these alloys demonstrate a different dependence of the solvus temperature on the chemical composition, which we observe on the graph.

5. Conclusions

In our work, we approve the possibility to simulate a physical feature of a nickel-based superalloy by a deep learning artificial neural network. The data preprocessing and a specially developed framework improves the accuracy. We may further improve the model by expanding the training dataset.

The overall evaluation of our work is follow:

- Our approach: simulating the solvus temperature of the complexly alloyed nickel-based superalloys using a specially developed deep learning artificial neural network with a differentiating layer. The choice of the network type and the preprocessing of the input data are based on physics of the alloys.
- In all respects a deep network is superior even to such an advanced feed-forward network as Bayesian. The differential layer improves a standard deviation of at least one and a half times.
- Adding a priori knowledge to the network about the individual influence of the elements on the alloy parameters give a positive effect on the modeling accuracy.
- We have achieved a high forecast accuracy (SD=7%).
- The forecast variance is small, which indicates the stability of the model.

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