Development of computational system based on artificial neural network for prediction of high temperature deformation behaviour in steels

***A. Yu. Churyumov**, Cand. Eng., Associate Prof., Dept. of Physical Metallurgy of Non-ferrous Metals [1], e-mail: churyumov@misis.ru*

[1] NationalUniversity of Science and Technology "MISiS" (Moscow, Russia)

A significant number of the data about the hot deformation behaviour of the metallic materials is published up to date in the scientific sources. As a result, the systematization and formalization of such big datasets using mathematical modeling is required. However, the accuracy of the usual regression models is not enough for this purpose. The artificial neural network (ANN) based model for prediction of the steel flow stress under the hot deformation conditions was constructed. The model has shown a high accuracy on the training dataset such as on the independent additional compression tests of the stainless 13Cr11Ni2W2MoV steel. The compression tests were carried out in the strain rate range of 0.1, 1, and 10 s^{-1} and the temperature range of 1000 – 1200 ºC using thermomechanical simulator Gleeble 3800. The steel has a two-phase ferritic/austenitic microstructure in the hot deformation range. The average relative errors for the training dataset and approvement tests were about 8.8 and 9.5 %, respectively. The constructed model may be used for the determination of the different element influence the flow stress of the steel, which may allow fast correction of the hot deformation conditions. Special software was developed for the use of the built ANN-based model.

Key words: artificial neural network, steel, hot deformation, microstructure, flow stress, thermodynamic calculations, thermomechanical simulator Gleeble.

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Introduction

The hot deformation of the metallic semi-products is an essential part of a full producing cycle. The energy and materials consumption at this stage may significantly influence the price and concurrency of finished products. As a result, it is important to optimize the technologies of hot processing.

The rheological properties of the steel are the parameters that control the hot deformation behaviour during thermomechanical processing. The accurate determination of its values at different deformation conditions is necessary for the optimization of the production technology using modern techniques such as finite element simulation [1–5]. This method has rapidly spread due to a significant increase in the computation power and may be operatively applied for the correction of the technological process even in real-time.

The high-temperature mechanical properties of the steel are dependent not only on temperature, strain rate, and strain but primarily on the chemical composition. This influence may be significant even within the same steel grade [6–8]. Currently, a large number of constitutive models that connect the stress and thermomechanical parameters such as temperature, strain rate, and strain were developed [9–14]. However, they were constructed only for specific materials and do not consider the influence of the chemical composition. Due to the complex alloying of modern steel, it is not possible to construct such models using a classical approach. Machine learning is an effective method to find the links between properties and parameters in the case of the absence of the physical laws connecting them. This approach is usually realized through the construction of artificial neural networks (ANN). Such an approach was applied by R. Honysz for the modeling the chemical composition of ferritic stainless steels with the determined mechanical properties [15], P. L. Narayana et al have calculated high-temperature mechanical properties of austenitic stainless steels [16], P. Pourabdollah and S. Serajzadeh developed the model to assess thermomechanical behaviour of the 304L steel during and after rolling [17]. In most cases, the ANN-based models show a higher accuracy in comparison with the classic regression models due to their high flexibility.

In the paper, the new ANN-based model for prediction of the steel hot deformation behaviour under is described. The constructed model shows high accuracy for both the training dataset such as for the independent control experiments.

Materials and methods

For the construction of the ANN-based calculation system, the database of the hot deformation mechanical properties of the steels with different chemical compositions was collected using the scientific papers devoted to the investigation of the steels' hot deformation behaviour. The ranges of the deformation conditions (temperature, strain rate, and strain degree) and alloying elements concentrations in the database are presented in the **Table 1**. The overall number of records in the database was 33,937. The dataset was randomized and divided into groups: the training group (60 % of the dataset), the cross-validation data (20 %), and the testing entries (20 %). The temperature, strain degree rate, strain, and con-

Table 1. **The ranges of the elements' concentration (wt. %), deformation temperatures, strain rates, and strains in the constructed database**

C	Si	Mn	Cr	Ni	S	P	Cu	Mo	V	N	Ta
0–1.79	0–6.5	0–30.5	0–28	0–33	0-0.086	0-0.045	0–1.96	0–8.95	0–1.32	0–0.86	0–2.5
W	Nb	Al	Ti	Co	Zr	B	Temperature, °C		Strain rate, s^{-1}		Strain degree
0–3.11	0–1.1	0–15.9	0–6.36	0–17	0-6	0-3.2	500–1300		10^{-4}–100		0–1.3

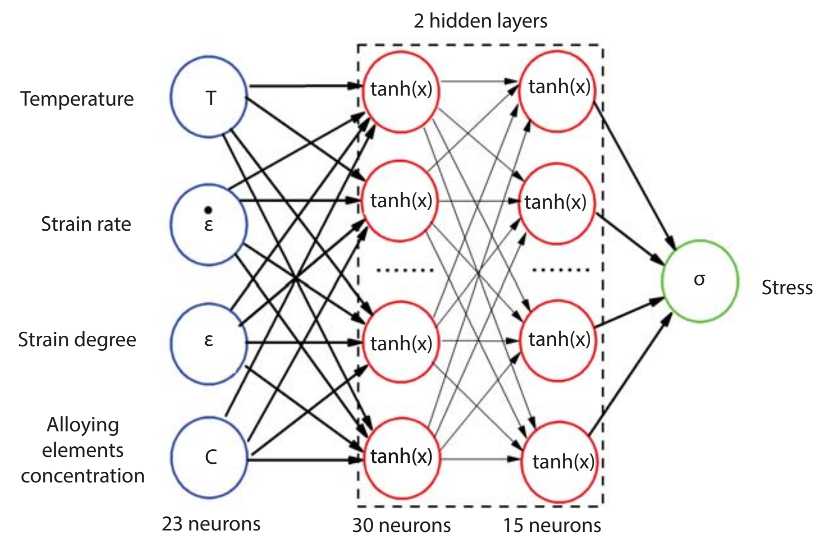

Fig. 1. The structure of the constructed ANN

tent of the elements were input parameters. The flow stress was an output of the model. The transformation of the data in the neurons was made by the hyperbolic tangent function. For the modelling, the perceptron with two hidden layers was used. The scheme of the ANN is shown in **Fig. 1**. The model's training was made by the static backpropagation algorithm. The constructed ANN-based computation system was realized as computer software.

The approvement of the calculation system accuracy was made by the conduction of the additional hot compression tests of the 13Cr11Ni2W2MoV steel. The ingots of the steel were obtained by vacuum induction melting with the following annealing and forging to the cylinder bars. The nominal chemical composition of the alloy is presented in **Table 2**.

Axisymmetric compression tests were carried out using a Gleeble 3800 thermomechanical simulator. The specimens with a diameter of 8 mm and a height of 12 mm were heated at a rate of 5 °C/s to the deformation temperature (1000, 1050, 1100, 1150, and 1200 °C), held for 1 min, and compressed in a single hit to a true strain of 0.95 at a constant strain rate of 0.1, 1 and 10 s^{-1}. The true stress-strain curves were treated to consider the friction and adiabatic heating during the deformation with high strain rates [18,19]. The initial microstructure was investigated by electron backscattering detection method using a Tescan-VEGA3 LMH scanning electron microscope. Thermocalc software with a TCFe7 database was used to determine the phase composition of the steel in the hot deformation temperature range.

Results and discussion

The accuracy of the constructed ANN-based calculation system may be estimated by the distribution of the dots in **Fig. 2**. The quantitative precision of the model was determined using Pearson's correlation coefficient (R) and average relative error (*ARE*) [20]:

$$R = \frac{\sum_{i=1}^{N}(E_i - \bar{E})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{N}(E_i - \bar{E})^2 \sum_{i=1}^{N}(P_i - \bar{P})^2}} \quad (1)$$

$$ARE\,(\%) = \frac{100}{N}\sum_{i=1}^{N}\frac{|E_i - P_i|}{E_i} \quad (2)$$

Here, E, P, $\bar{E}$ and $\bar{P}$ are the experimental, predicted stress and those mean values, correspondently. N is the number of entries in the dataset.

The *ARE* has a satisfactory value of 8.2, 8.8, and 8.8 % for training, cross-validation, and testing datasets. A high value of Pearson's correlation coefficient (higher than 0.988 for all datasets) shows the constructed model's good accuracy. However, the presented parameters show the model's accuracy only for the hot deformation curves used for the ANN teaching, and an additional independent experimental check is required.

Independent additional hot compression tests of 13Cr11Ni2W2MoV steel were carried out to check the prediction ability and accuracy of the constructed ANN-based model. **Fig. 3*a*** shows an initial microstructure of the investi-

Table 2. **Chemical composition of the 13Cr11Ni2W2MoV steel (wt. %)**

C	Si	Mn	P	S	Cr	Ni	Mo	W	V	Cu	Fe
0.13	0.42	0.46	0.022	0.003	11.25	1.73	0.4	1.73	0.22	0.19	Balance

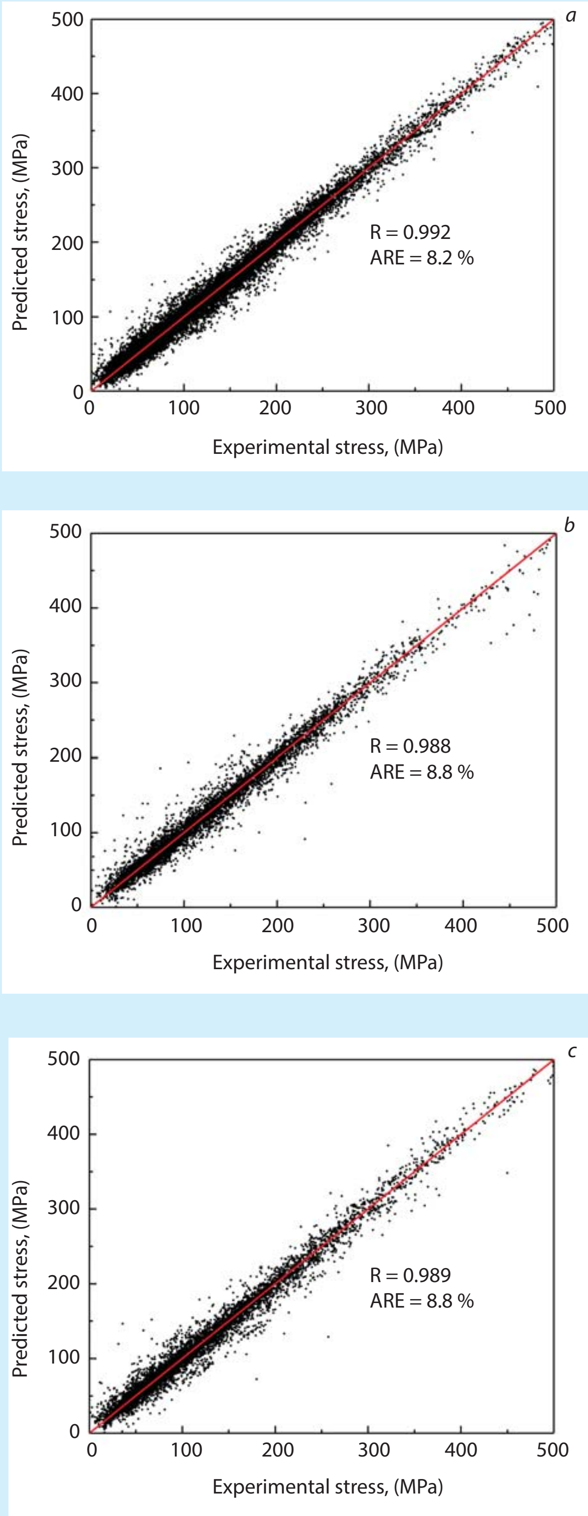

Fig. 2. Comparison between predicted using ANN-based calculation system and experimental stress values for (*a*) training, (*b*) cross-validation, and (*c*) testing datasets

gated steel. The microstructure consists of ferrite grains with an average size of 15±2.1 μm. Accordingly thermodynamic calculations, the microstructure of the investigated steel at elevated temperatures may contain austenite (FCC-(Fe)), ferrite (BCC-(Fe)), σ-phase, and liquid (Fig. 3*b*). In the current investigation, the deformation of the steel was carried out in the two-phase ferrite/austenitic region.

The 13Cr11Ni2W2MoV steel shows typical hot deformation behaviour during compression. The true stress increases with deformation temperature decreases and strain rate increases (solid lines in **Fig. 4**). A comparison between calculated and experimental stress-strain curves for the 12Cr3NiCu steel shows good accordance between them (Fig. 4). The *ARE* of the ANN-based model for the additional hot deformation test was 9.5 %. The largest error was shown at low temperatures due to the fact that most of the training data were obtained for temperatures higher than 1100 ºC. However, the constructed model may be used for the accurate prediction of the hot deformation behaviour of the steel.

A developed model may allow determining the influence of the different alloying elements on the hot deformation behaviour of the steel. As one can see in **Fig. 5***a*, the influence of chromium on the true stress of the 13Cr11Ni2W2MoV steel is insufficient in the wide range of concentrations. At the same time, the change in the tungsten content in the steel may significantly correct the stress-strain curve (Fig. 5*b*) that may influence the hot deformation technological process.

The constructed model was realized as a computer program (**Fig. 6**) that possesses the following possibilities:

- to predict the values of the stress at any deformation conditions and in a wide range of the concentration of the alloying elements;
- to analyze the hot deformation behaviour in terms of the effective activation energy for different steel;
- to construct the processing maps for the hot deformation of the steel;
- to plot 2D and 3D graphs with the dependences of the flow stress and effective activation energy on the deformation parameters and chemical composition.

The developed approach to the construction of the ANN-based calculation system may be applied for the modeling of the hot deformation behaviour not only for steel but also for other metallic materials such as aluminum, magnesium, and titanium alloys due to a large number of published experimental data and the increased computational possibility of the computers.

Conclusions

1. An artificial neural network model for predicting steel rheological properties during the hot deformation was constructed. The model shows high predictability for the training and testing datasets. An average relative error is in the range of 8.2 – 8.8 %.

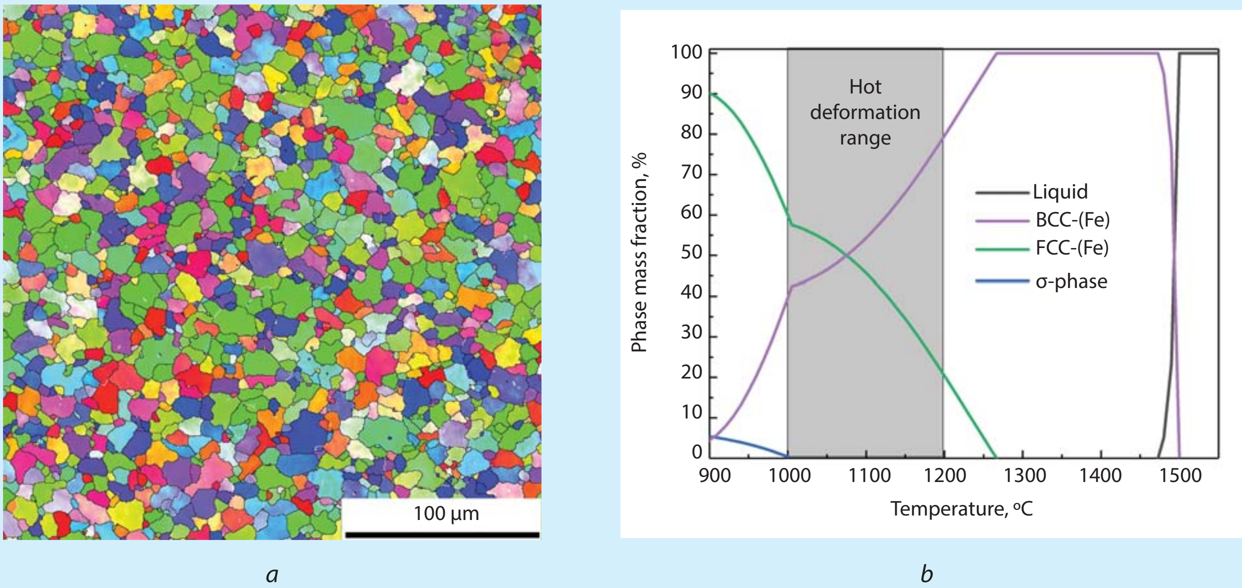

Fig. 3. Initial microstructure (*a*) and phase diagram (*b*) of 13Cr11Ni2W2MoV steel

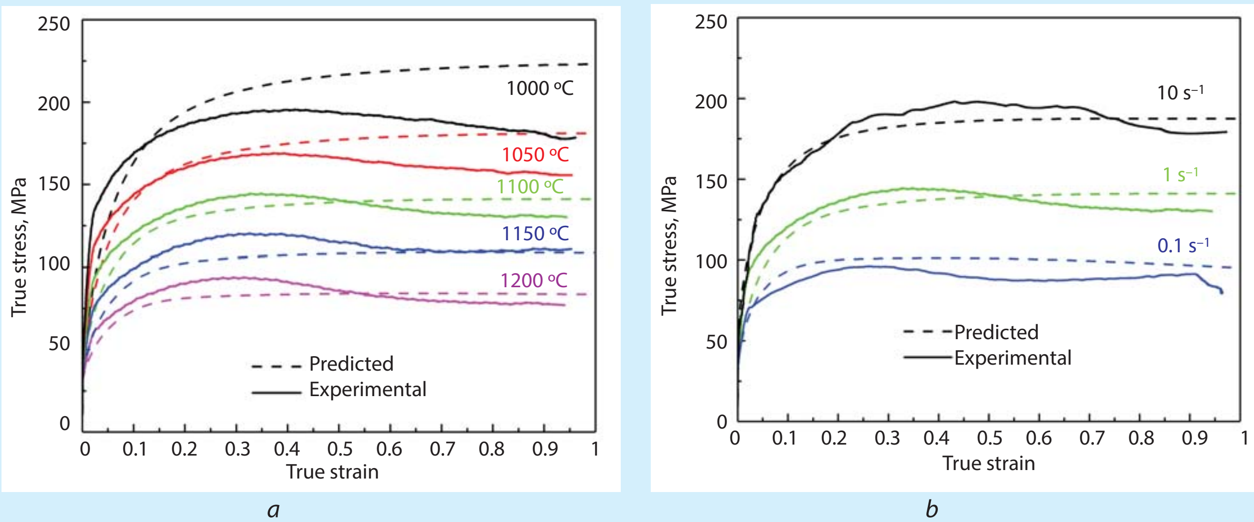

Fig. 4. A comparison of the experimental and predicted hot deformation curves for the 13Cr11Ni2W2MoV steel at a strain rate of 1 s^{-1} (*a*), and a temperature of 1100 °C (*b*)

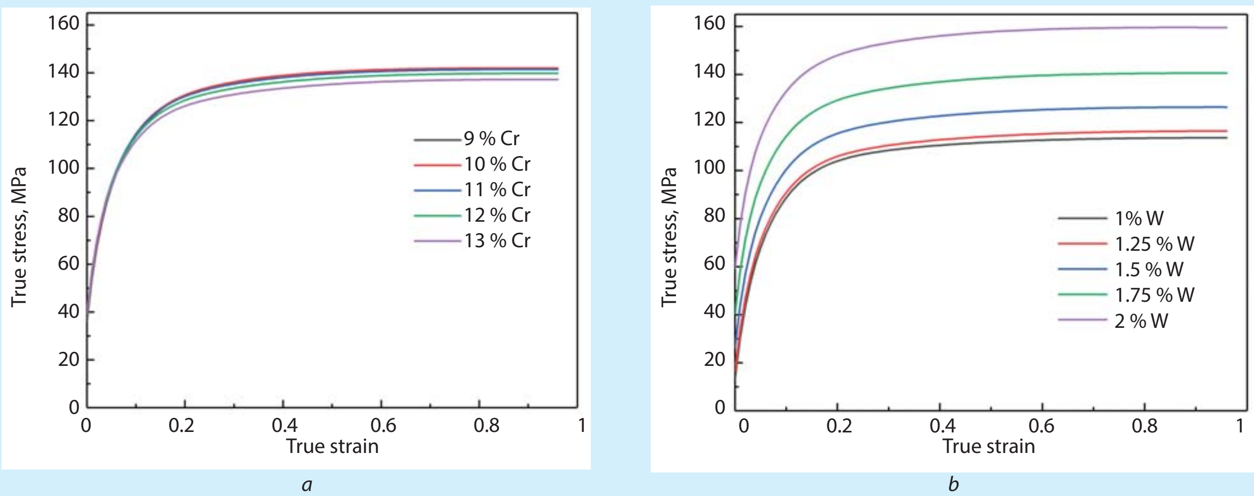

Fig. 5. Calculated stress-strain curves for the 13Cr11Ni2W2MoV steel of based composition (Table) with different concentration of Cr (*a*) and W (*b*) at a strain rate of 1 s^{-1}, and a temperature of 1100 °C

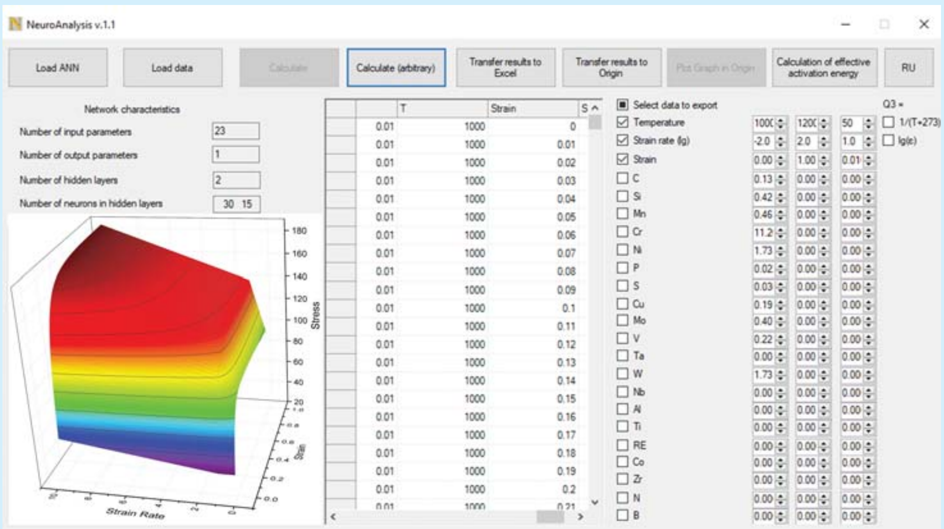

Fig. 6. An interface of the developed computer program for the prediction of the hot deformation behaviour of the steel using ANN-base models

2. The additional hot deformation tests of the 13Cr11Ni2W2MoV steel were carried out to approve the accuracy of the built ANN-based calculation system. The comparison of the experimental and calculated stress-strain curves shows a high model accuracy at temperatures higher than 1050 ºC.

3. The special computer software was developed for the use of the constructed ANN-based model. The program lets to predict the flow stress of the steels depending on deformation conditions and chemical composition in a wide range of their variation.

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