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R. HONYSZ[1*]

OPTIMIZATION OF FERRITE STAINLESS STEEL MECHANICAL PROPERTIES PREDICTION WITH ARTIFICIAL INTELLIGENCE ALGORITHMS

The article presents a computational model build with the use of artificial neural networks optimized by genetic algorithm. This model was used to research and prediction of the impact of chemical elements and heat treatment conditions on the mechanical properties of ferrite stainless steel. Optimization has allowed the development of artificial neural networks, which showed a better or comparable prediction result in comparison to un-optimized networks has reduced the number of input variables and has accelerated the calculation speed. The introduced computational model can be applied in industry to reduce the manufacturing costs of materials. It can also simplify material selection when an engineer must properly choose the chemical elements and adequate plastic and/or heat treatment of stainless steels with required mechanical properties.

Keywords: Analysis and modelling; Numerical Techniques; Computational Material Science; Artificial algorithms, Stainless steel

1. Introduction

The development in material engineering has led to increased competition on the market, also for corrosion-resistant steels. The properties of these materials strictly depend on their chemical composition and type of processing. Therefore, to obtain the required mechanical properties and a relatively low production cost, it is necessary, that the chemical composition, as well as the appropriate heat and mechanical treatment conditions, should be selected following the client's requirements. The classic approach, i.e. the execution of a series of experiments with the production of the necessary number of samples to determine the properties of each of these steel grades, is a breakneck undertaking requiring an extremely large time and financial expenditure. Artificial intelligence methods, together with data obtained through experiments, allow developing a model that will allow predicting the mechanical properties of stain ferritic steels in a very short time with high accuracy. The main purpose of making such a model is to reduce the costs associated with materials testing of these steels and faster access to the results of calculations. The use of artificial intelligence enables the advancement of stainless steel technology in multiple ways, even though only a small number of definition vectors are available [1-7]. In recent years, many scientists from around the world have dealt with the topic of the application of artificial intelligence algorithms in material engineering. Many computational models were created describing the relationships between phenomena occurring in steels, their properties, chemical composition and processing conditions. In order to decrease production expenses of products, introduced models can be obtained in manufacturing industry. They can also simplify the selection of materials if the engineer has to correctly choose chemical elements and appropriate plastics and/or heat processing of stainless steels, having the necessary mechanical characteristics [8-17].

2. Materials and methods

Data for the construction of computation models for predicting steel properties were obtained by laboratory testing certain grades of ferritic stainless steels following PN-EN 10088-1: 2014. The main criterion for selecting steel grades was carbon concentration from 0.3 to 1.2%, chromium concentration from 10 to 14% and nickel concentration from 0.1 to 2% together with other alloying elements [19-25]. Steel was smelted in electric arc furnaces equipped with vacuum arc degassing (VAD) devices. The material was delivered in the form of round rods after normalization treatment at a specified temperature and time. From

[1] SILESIAN UNIVERSITY OF TECHNOLOGY, FACULTY OF MECHANICAL ENGINEERING, DEPARTMENT OF ENGINEERING MATERIALS AND BIOMATERIALS, 18A KONARSKIEGO STR., 44-100 GLIWICE, POLAND

* Corresponding author: rafal.honysz@polsl.pl

metallurgical approvals, values were read that were used as input variables in the process of teaching artificial neural networks: chemical element concentration, temperature and time of normalization treatment and rod diameter. Five mechanical properties were investigated: yield strength (Rp0.2), tensile strength (Rm), relative elongation (A), relative area reduction (Z) and hardness (HB) [26-29]. Values of these properties are output values for respective artificial neural network. Determination of strength properties consisted of carrying out a tensile test for steel samples following PN-EN 10002-1: 2002. Hardness tests were carried out using the Brinell method following PN-EN ISO 6506-1: 2002.

The results of laboratory tests were used to build a dataset with 3272 vectors. Input variables were:

- chemical composition of steel including concentrations of the thirteen, most common in steels, elements: carbon (C), manganese (Mn), silicon (Si), phosphorus (P), sulfur (S), chromium (Cr), nickel (Ni), molybdenum (Mo), tungsten (W), vanadium (V), titanium (Ti), copper (Cu) and aluminum (Al),
- three conditions of the normalization process, such as: the temperature to which the material was heated, the time of heating the material at this temperature, and the type of cooling medium in which the steel was cooled,
- diameter of the rod cross section.

Material tests were conducted in such a way as to obtain an even distribution of values in the range of variability of the given input value without excessive data clusters or empty spaces. Data uniformity was confirmed using the histogram tool. These vectors were randomly divided into three sets. Teaching set with 1635 vectors and a validation set with 818 vectors was used in network learning processes. The remaining vectors were included in the test file and were used to check the correctness of the network operation. The process of assigning cases to individual sets was repeated many times. After each new draw, the process of teaching artificial neural networks was repeated several times to obtain the best regression statistics. Artificial neural networks with a multi-layer perceptron (MLP) architecture with one or two hidden layers have been developed from such prepared data. Transfer functions in hidden and output layers were hyperbolic. The method of back error propagation and conjugate gradients were used for teaching. The back error propagation algorithm consists in changing the weight of the input signals of each neuron in each layer so that the error value for subsequent learning pairs contained in the learning set is as low as possible. For this purpose, the fastest gradient method is used. It is a generalization of the delta rule for perceptrons to multilayer feedforward neural networks. The conjugate gradients algorithm is an advanced method of learning multilayer perceptrons. It is especially recommended for networks with a large number of weights (more than a few hundred) and / or for networks with many output neurons. The conjugate gradients algorithm cumulatively modifies the weights. This means that the weight modification is carried out once at the final stage of the implementation of one era. During the application of the conjugate gradient algorithm, the average value of the gradient is determined (relative to all cases) on the error surface, which is the basis for a one-time weight modification carried out in the final phase of each epoch [22,27-28]. In the validation process, a number of material vectors cases are included in a separate group. Data belonging to this separate group are not directly used during network learning, but they are used to carry out independent control of the learning algorithm's progress. In each case, the initial network performance determined on the basis of the training and validation string is the same. It is obviously very poor because the network is unable to respond properly to any data prior to learning. During learning, the error made by the network decreases and, as long as the learning process minimizes the properly defined error function, the validation error also decreases. However, if the decrease in the validation error has stopped or this error is beginning to increase, it means that the network has started to adapt too much to the learning data and loses the ability to generalize the learning results. The final form of the network, taught using a learning set and verified using a validation set, is additionally tested using a test set. This additional check is practiced to make sure that the results obtained for the training set and validation set are consistent with reality, and are not just a mechanical product of the learning procedure. For the test set to fulfill this role correctly, it should be used only once [22,27-28]. The ranges of selected input variables are shown in Table 1. Separate networks were developed for each material property separate for two types of plastic treatment: free forging and rolling. The most important regression parameters that were used when selecting the neural network were average absolute error, standard deviations ratio and Pearson correlation.

The last step was to use a genetic algorithm to optimize the chosen artificial neural network. It consisted of creating the "mask" of variables to be used to model and examine the neural network's error. By adding to each variable penalty unit, the number of inputs can be reduced, which can have a beneficial effect on their regression statistics. The genetic algorithm parameters in each test were the same except for the penalty unit, which increased every time the algorithm was used. With

TABLE 1

The range of selected input variable values

	Chemical composition [mass %]							Normalizing	
	C	Mn	Si	Cr	Ni	Mo	Cu	Temp. [°C]	Time [min]
Minimum	0.03	0.42	0.18	10.60	0.10	0	0	600	50
Maximum	0.94	1.57	0.43	20.00	2.41	2.70	0.71	980	360

the amount of 200 generations, the algorithm population was 200 individuals. Standard values for Holland's classic genetic algorithm are the mutation probability of 0.1 and the crossover probability of 0.4. The sampling value was set to 0.3 to speed up modeling procedures. This reduced the search time five times from 10 minutes to about 2 minutes and allowed to increase the number of individuals in the population and the number of generations. Then artificial neural networks were built using genetic algorithm-suggested variables.

Besides, automatic neural networks developed using an automated designer was developed for comparative purposes. The use of this package simplifies network construction to the maximum. The user only needs to indicate the input and output variables. All important decisions in the learning process regarding the architecture, the number of variables used or the learning methods are made by the software. All calculations were made in the Statistica package [30] on desktop computer with an i5-3450 processor with 8GB Ram.

3. Results and discussion

Table 2 contains architecture, regression statistics for the test set, respectively, for the base neural networks, optimized by genetic algorithm and constructed automatically developed for steels after free forging. Table 3 presents architecture, regression statistics for artificial neural networks developed for rolled steels. Multi-layer perceptron architecture is described by three or four values, which are the number of input neurons, number of neurons in one or two hidden layers and single output neuron. For example, automated network used for hardness prediction of rolled steels is 12-6-1. This means 12 neurons in the input layer, 6 neurons in one hidden layer and 1 neuron in the output layer. The same network for forged steels has the architecture 11-7-4-1, this means 11 neurons in the input layer, 7 neurons in the first hidden layer, 4 neurons in the second hidden layer and 1 neuron in the output layer. Average absolute error E is the difference between the reference value and the value obtained at the output for the output variable. The correlation is determined by the standard Pearson R correlation coefficient for the set value and the value obtained at the output.

Figure 1 introduces a comparison of testing set mean absolute error of base, optimized and automated artificial neural networks developed for steels after free forging. Figure 2 introduces a comparison of testing set mean absolute error of artificial neural networks developed for rolled steels.

Figure 3 introduces a comparison of testing set Pearson correlation of base, optimized and automated artificial neural networks developed for steels after free forging. Figure 4 introduces a comparison of testing set mean absolute error of artificial neural networks developed for rolled steels.

Regression statistics analysis of yield strength prediction Rp0,2 showed that the optimized network has the lowest average absolute error and the lowest deviation ratio. Pearson correlation also achieves peak value for these networks for both types of treatment reaching 0.98 for forged steel. In the case of tensile stress Rm, optimization did not give satisfactory results for rolled steels, just as an automated designer. The best regression statistics has the base artificial neural network. Much better results were achieved for forged steels. The optimized network

TABLE 2

Regression parameters of artificial neural networks build for forged steels

Property	Non-optimized			GA optimized			Automated designer		
	MLP architecture	Average absolute error	Pearson correlation	MLP architecture	Average absolute error	Pearson correlation	MLP architecture	Average absolute error	Pearson correlation
$R_{p0,2}$ [MPa]	17-3-1	20.16	0.97	14-4-1	16.90	0.98	11-6-1	23.01	0.82
R_m [MPa]	17-10-1	18.50	0.96	8-5-1	18.50	0.94	11-7-1	17.61	0.94
A [%]	17-5-1	0.97	0.83	9-4-1	0.93	0.85	3-4-1	1.26	0.73
Z [%]	17-5-1	2.17	0.72	9-5-1	2.13	0.78	4-8-1	2.39	0.68
HB	17-5-1	13.03	0.61	4-8-1	10.21	0.69	11-7-4-1	11.48	0.68

TABLE 3

Regression parameters of artificial neural networks build for rolled steels

Property	Non-optimized			GA optimized			Automated designer		
	MLP architecture	Average absolute error	Pearson correlation	MLP architecture	Average absolute error	Pearson correlation	MLP architecture	Average absolute error	Pearson correlation
$R_{p0,2}$ [MPa]	17-3-4-1	20.69	0.86	13-8-1	17.65	0.89	12-4-1	19.45	0.86
R_m [MPa]	17-5-1	16.75	0.96	8-4-1	17.88	0.95	12-8-7-1	18.18	0.95
A [%]	17-4-1	3.77	0.70	7-1-1	3.52	0.75	15-9-1	3.58	0.71
Z [%]	17-7-1	4.71	0.74	9-7-1	4.06	0.84	12-5-1	4.59	0.82
HB	17-6-1	6.52	0.88	6-14-1	6.51	0.88	12-6-1	7.72	0.84

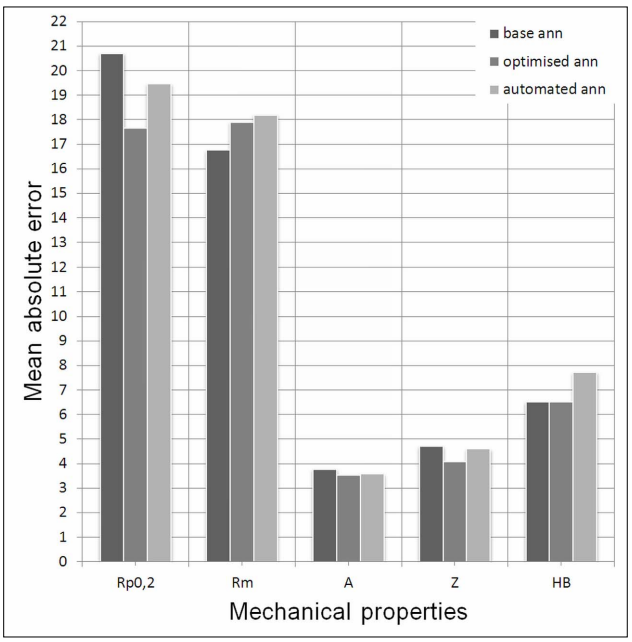

Fig. 1. Comparison of mean absolute error for base, automatic designed and genetic optimized neural artificial networks (testing set), build for forged steels

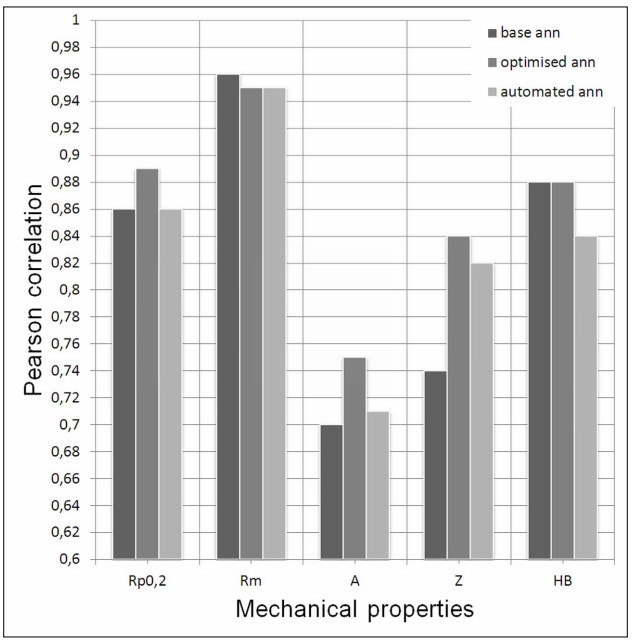

Fig. 3. Comparison of Pearson correlation for base, automatic designed and genetic optimized artificial neural networks (testing set), build for rolled steels

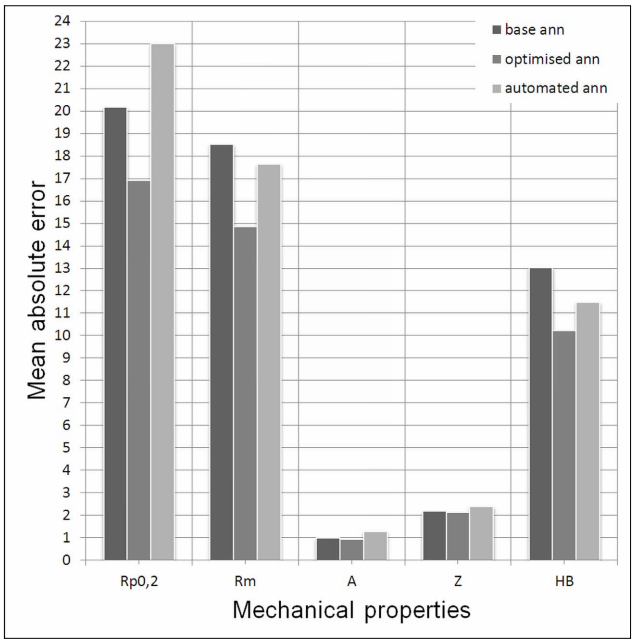

Fig. 2. Comparison of mean absolute error for base, automatic designed and genetic optimized neural artificial networks (testing set), build for forged steels

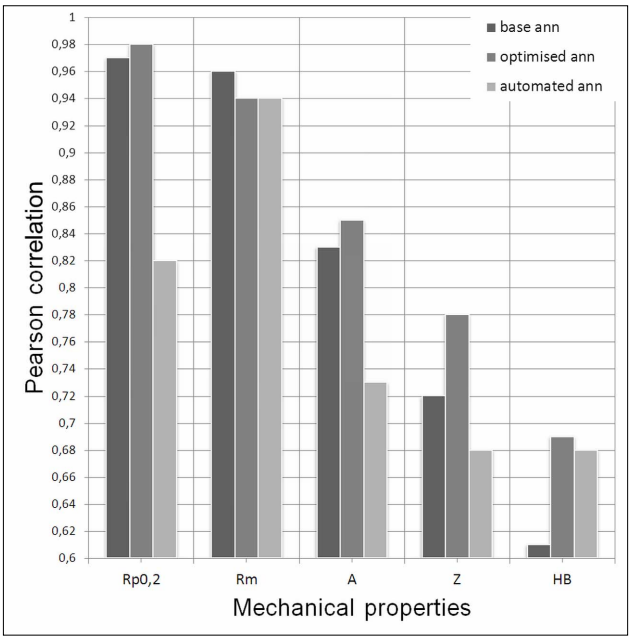

Fig. 4. Comparison of Pearson correlation for base, automatic designed and genetic optimized artificial neural networks (testing set), build for rolled steels

has the smallest average absolute error, but the correlation is slightly lower than in the base network. For the relative elongation A5 regression analysis shows that the smallest average absolute error has the optimized network, but the differences are small compared to other networks. Larger differences are in Pearson correlation, also in favor of the optimized network. A very similar situation occurs for the neural network optimized for the relative contraction Z. The optimized network has the best regression statistics for all sets, but the differences between the networks are insignificant. Slightly better than in the other networks is the Pearson correlation. Regression statistics for automated and optimized artificial neural networks build for prediction of Brinell hardness HB are very similar. Again optimized network has the Pearson correlation the highest along with the smallest mean average error for forged steel. For rolled steel regression statistics for the base and optimized artificial neural networks are identical. The automatic network has been left behind.

Summarizing, for all material property, optimization improved the mean absolute error, which is the smallest in optimized networks. Only in the case of Rm of rolled steels, deterioration of regression statistics was obtained, but the difference in and in Pearson's correlation is only 0.02 for the testing set. Only in the case of rolled steel hardness HB, the optimization did not change the regression statistics.

4. Conclusion

The objective of this study was to optimize the neural artificial networks after normalization treatment used to predict the mechanical properties of rolled and forged ferrite stainless steel and this objective has been reached. Artificial neural networks have been optimized to obtain better statistics on regression using the genetic algorithm. Optimization, except for rolled steel tensile strength Rm case, allowed the development of artificial neural networks, showing a better or comparable output in comparison to base networks, as well as a reduced input of variables. Modified artificial neural networks will allow the mechanical properties of the examined steels to be predicted more accurately and faster.

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