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Prediction optimization of mechanical properties of ferrite stainless steels after rolling treatment with use of genetic algorithms

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ABSTRACT

Purpose: The article discusses the use of artificial neural networks for research and prediction of the impact of chemical elements and heat treatment parameters on the mechanical properties of stainless steels optimized by genetic algorithm.

Design/methodology/approach: To improve the quality of artificial neural network models and improve their performance the number of input variables of artificial neural networks has been optimized with use of genetic algorithms. Then a computational model build with optimised artificial neural networks were trained and verified.

Findings: Optimization, except of tensile strength R_m case, has allowed the development of artificial neural networks, which either showed a better or comparable result from base networks, and also have a reduced number of input variables. As a result, in computational model constructed with use of these networks the noise information is reduced.

Research limitations/implications: Data analysis was needed to verify if obtained data used for modelling are relevant to use them in artificial neural networks training processes.

Practical implications: The use of artificial intelligence allows the multifaceted development of stainless steels engineering, even if only a small number of descriptors is available. Constructed and optimised computational model build with use of optimised artificial neural networks allows prediction of mechanical properties of rolled ferritic stainless steels after normalization.

Originality/value: Introduced model can be obtain in industry to reduce manufacturing costs of materials. It can also simplify material selection, when engineer must properly choose the chemical elements and adequate plastic and/or heat treatment of stainless steels with required mechanical properties.

Keywords: Numerical techniques; Computational material science; Artificial algorithms; Stainless steel

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ANALYSIS AND MODELLING

1. Introduction

One of the main tasks of the modern engineer is the appropriate choice of material engineering, which will meet all the required conditions. It is also important, that a technological process of material manufacturing does not damage the natural environment. Therefore, to take into account all these problems and requirements, materials engineering are using computational models of material properties.

The development of materials engineering has led to increased competition in the market, also for stainless steels. Anti-corrosion coatings applied to the material are very stable and have high aesthetic characteristics. However, the use of conventional corrosion-resistant materials isproviding the structure durability even if delamination of the coating occurs. Mechanical properties of these materials are dependent on their chemical composition and the nature of their treatment. Therefore, to obtain the required mechanical properties and relatively low manufacturing costs of these materials, the engineer must properly choose the chemical elements adequate plastic and/or heat treatment. The classic approach, i.e. preparation of samples and performing a series of experiments to determine the properties of each of the species of these steels is a risky undertaking, requiring significant investment of time and money. The use of artificial intelligence allows the multifaceted development of stainless steels engineering, even if only a small number of description vectors is available [1-7].

2. Material

Ferrite stainless steels after rolling treatment structural steels were selected for examinations as example material. As the main criterion for selection of steel types was the chromium concentration, which for stainless steel exceed 10.5% [8-10]. Further criteria for minimal and maximal chemical elements concentration, conditions of heat and plastic treatment were taken from literature: the selection of mechanical properties, which were examined was based on analysis of the steel markets and literature studies [11-15].

For the description of stainless steel, five mechanical properties present in the metallurgical certificate have been selected. To describe the above properties set of descriptors characterizing steel in manufacturing process has been developed. It consists of chemical composition described by concentration of thirteen of the most common elements in steels temperature and time of normalizing treatment and the diameter of the final product. Steel was manufactured in electric arc furnaces with devices for steel vacuum degassing (VAD). The material was supplied in the form of long rods after rolling and normalising.

3. Investigation mythology

Methods of artificial intelligence, together with data obtained on the way experiments, make possible the development of computational model. This model will allow prediction of mechanical properties of mechanical properties of ferrite stainless steels after rolling treatment based on input variables such as chemical composition and treatment conditions [16-23].

First stage of researches was the development ofcomputational modelbuilt with the use of artificialneural networks. On the basis of input values, such as :

- chemical elements concentration,
- normalizingtemperature and time,
- rod's diameter,

five mechanical properties are predicted:

- yield strength ($R_{0.2}$)
- tensile strength (R_m)
- relative elongation (A_5)
- relative area reduction (Z)
- hardness (HB)

This model was obtained with use of all input parameters.

To improve the quality of artificial neural network models and improve their performance, in the second stage of investigation, the number of input variables has been optimized with use of genetic algorithms. Then a second model build with optimised artificial neural networks were trained with modified set of input variables with use of the same set of data.

For comparison purposes a third model was build. This time for the selection of input variables an automatic designer placed in the modelling software was used.

Preparation of data used for modelling was performed using Excel from Microsoft Office [24]. Training of artificial neural networks and genetic algorithms optimization were performed using Statistica. Neural Network developed by Statsoft [25].

4. Modelling of ferrite stainless steels mechanical properties after rolling treatment

To build an artificial neural network, which will deliver results with a high correlation to laboratory measured values, an appropriate number of variables affecting the network is required. Too many variables may adversely affect obtained results, causing noise information. These less significant variables should be removed. Removing of variable, that significantly affects the output, will result in larger error.

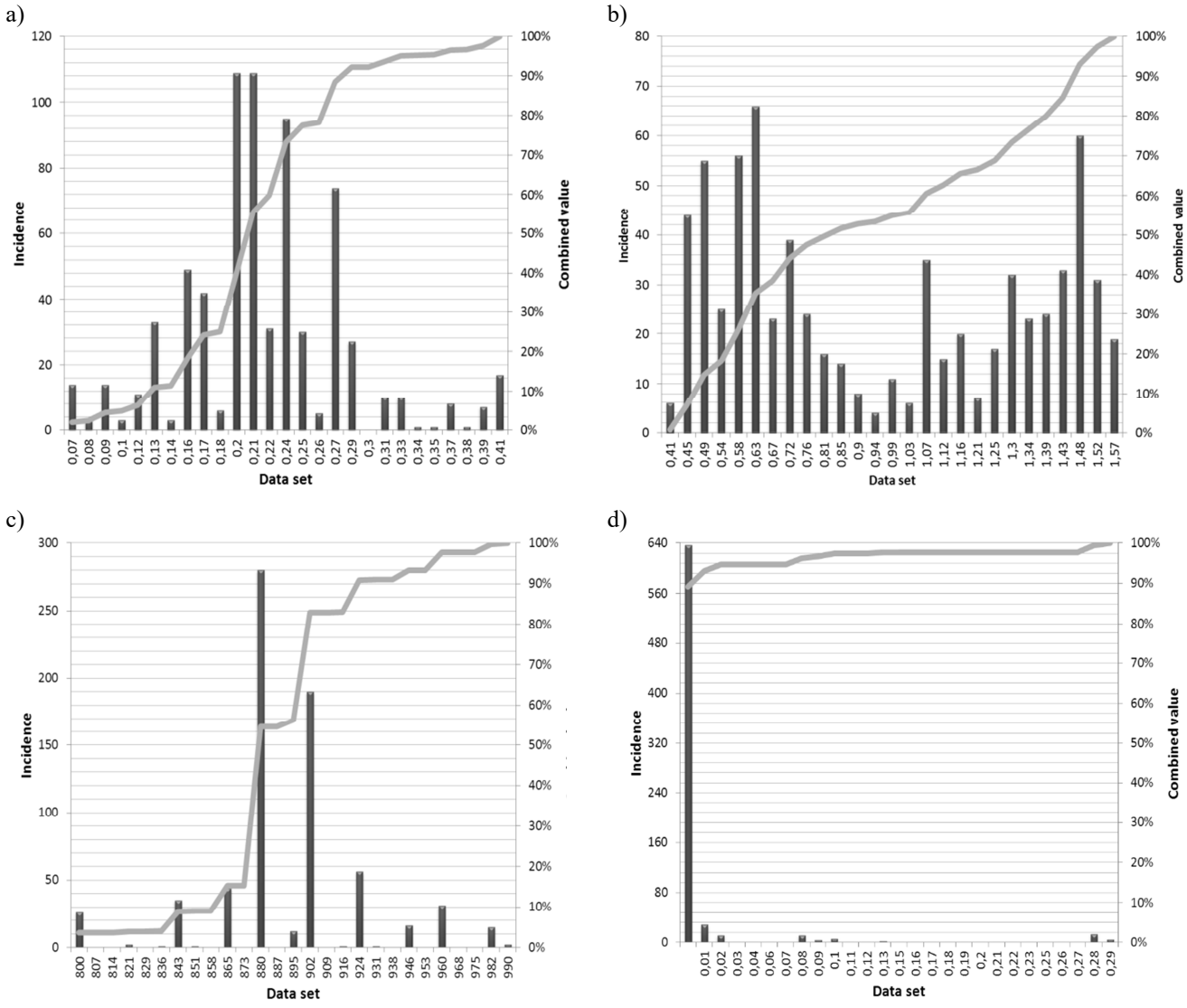

Fig. 1. Data set histograms for a) manganese concentration, b) carbon concentration, c) normalisation temperature, d) vanadium concentration of examined stainless steels

One way to select the relevant variables is to use the "automatic designer" for artificial neural networks, which select random topographies having the smallest statistical error and the best quality based on its search algorithms. Another way is to use a genetic algorithm. It indicates which variables have a major impact on output values, and which have no impact at all.

4.1. Input data analysis

Data analysis is needed to verify if data suitability to use them in artificial neural networks training. At the beginning from the data ranges of variables for artificial neural network model was obtained. The best distribution of data, which should be used for artificial neural network training is evenly distributed number of variables in the whole range. Unfortunately, such distribution for all variables is hard to achieve. Variables with all values at one point may have no effect at all on the artificial neural network model, it was recommended to remove such variables before building a model. Because of the project, such variables will be used for verification. It is assumed that the genetic algorithm should remove these variables from the set of input variables.

Then the distribution of the variable within these ranges was determined with use of the histogram tool in Microsoft Excel, which allows further to illustrate the results in a graph. The best values distribution was observed for: time of normalising, carbon (Fig. 1a), manganese (Fig. 1b.), silicon, copper, and diameter. Histograms, which show that variables can affect in limited range are: the treatment temperature (Fig. 1c), phosphorus, sulphur, chromium, nickel, molybdenum. Variables most focused, which probably will not affect at all on the model are: aluminium, titanium, vanadium (Fig. 1d) and tungsten.

4.2. Construction of base artificial neural networks

First model was built with use of all seventeen input variables without any optimisation. Ranges of input variables and their distribution are introduced in Table 1. The set of all vectors were divided into three subsets in relation 2-1-1. With half of all vectors a set of vectors used to modify the neuronal network weights (training set) were created, one quarter of vectors was assigned to evaluate the prediction error during learning process (validation set), and the remaining part was used to independent determination of the prediction accuracy at the end of the network training process (testing set).Assignment of vectors to the appropriate sets was random. The required accuracy of prediction is different among applications. The most important artificial neural networks parameters, which were taken into consideration when selecting best available network, was the average absolute error, deviation ratio and Pearson correlation [21]. Architectures and regression statistics for best artificial neural networks are introduced in Table 2. This model was selected for optimisation with use of genetic algorithm.

4.3. Optimization of artificial neural network using genetic algorithm

The next step was to optimize the selected artificial neural network using genetic algorithm. It consisted in generating the "mask" of variables, which will be used to model the neural network and to examine its error. By adding to each variable penalty unit, it is possible to reduce the number of input variables, which may have a positive impact on its regression statistics. The parameters of the genetic algorithm in each test were the same except the penalty unit, which increased at each use of the algorithm. Algorithm population was 200 individuals with the number of 200 generations. Mutation ratio of 0.1 and crossing ratio of 0.4 are standard values for Holland's classic genetic algorithm. To speed up modelling processes, sampling value was set to 0.3. This reduced the search time for about 2 minutes and allowed to increase the number of individuals in the population and the number of generations. Then, artificial neural networks were constructed with use of variables suggested by genetic algorithm. Architectures and regression statistics for best artificial neural networks in this model are introduced in Table 3.

4.4. Construction of the artificial neural networks using automatic designer

For verification purposes, third computational model was developed. Artificial neural networks for this model were created using the automatic designer who supports the critical design stages of construction. It has many tools that make it easy to automatically select the appropriate network architecture and optimize the number of input variables. Automatic designer also automatically stores the best artificial neural network created in during the development Model constructed from these artificial neural networks will be used to evaluate the effectiveness of a genetic algorithm. Architectures and regression statistics for best artificial neural networks used in this model are introduced in Table 4.

Table 1.
Ranges of input values

range	diameter [mm]	chemical composition [%]													normalising	
		C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al	temp. [°C]	time [min]
min.	25	0.03	0.22	0.15	0.01	0	10.60	0.10	0	0	0	0	0	0	800	30
max.	225	0.41	1.57	0.56	0.13	0.21	21.06	10.16	4.69	0.02	0.29	0.19	1.05	0.04	990	480
distribution	good	good	good	good	mean	mean	mean	mean	mean	poor	poor	poor	good	poor	mean	good

Table 2.
Parameters of non-optimized artificial neural networks.

variable	MLP network architecture	training set			validation set			testing set		
		average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation
$R_{0,2}$	17-3-1-1	21.13	0.58	0.82	18.59	0.52	0.85	20.69	0.51	0.86
R_m	17-5-1	15.03	0.26	0.97	14.84	0.25	0.97	16.75	0.29	0.96
A_5	17-4-1	3.38	0.69	0.72	3.36	0.66	0.75	3.77	0.72	0.70
Z	17-7-1	4.24	0.56	0.83	4.53	0.56	0.83	4.71	0.69	0.74
HB	17-6-1	7.16	0.47	0.88	7.52	0.53	0.85	6.52	0.47	0.88

Table 3.
Parameters of artificial neural networks build with use of automatic designer.

variable	MLP network architecture	training set			validation set			testing set		
		average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation
$R_{0,2}$	13-8-1	20.81	0.55	0.84	19.54	0.51	0.86	19.45	0.51	0.86
R_m	8-4-1	17.35	0.30	0.95	16.55	0.27	0.96	18.18	0.30	0.95
A_5	7-1-1	3.11	0.66	0.75	3.20	0.67	0.74	3.58	0.71	0.71
Z	9-7-1	4.53	0.56	0.83	4.27	0.52	0.85	4.59	0.58	0.82
HB	6-14-1	7.83	0.58	0.82	8.96	0.62	0.78	7.72	0.55	0.84

Table 4.
Parameters of artificial neural networks optimized with use of genetic algorithms.

variable	MLP network architecture	training set			validation set			testing set		
		average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation
$R_{0,2}$	12-4-1	19.62	0.52	0.85	17.41	0.44	0.90	17.65	0.45	0.89
R_m	12-8-7-1	16.68	0.29	0.96	16.11	0.27	0.96	17.88	0.30	0.95
A_5	15-9-5	3.06	0.62	0.78	3.29	0.66	0.75	3.52	0.66	0.75
Z	12-5-1	4.06	0.54	0.84	3.95	0.52	0.85	4.06	0.54	0.84
HB	12-6-1	5.93	0.45	0.89	7.61	0.52	0.85	6.51	0.47	0.88

5. Modelling results discussion

Comparison between mean absolute error for base, automatic designed and optimised artificial neural networks (testing set) is introduced in Figure 2. Comparison between Pearson correlation for base, automatic designed and optimised artificial neural networks (testing set) is introduced in Figure 3.

Analysis of regression statistics of optimised artificial neural networks builded for prediction of yield strength

$R_{0,2}$showed, that the best performance has the optimised network with the smallest average absolute error and deviation ratio. Also Pearson correlation for this network achieves peak value.

In case of tensile stress R_m genetic algorithm has not advised with assigned task, just as automatic designer. The best regression statistics has the base artificial neural network.

For the relative elongation A_5 regression analysis shows that the best performance have the artificial neural network optimised with use of genetic algorithm. In comparison with the base network, it has a lower Pearson correlation and deviation ratio in validation set, but for all other sets regression statistics are similar or better parameters that are set to be higher than the ratios of other collections of the core network.

Neural network optimized for the relative contraction Z has the best regression statistics for all sets, slightly better than statistics of the other networks. Its another advantage is the smallest number of variables.

Regression statistics for base and optimized artificial neural networks build for prediction of Brinell hardness HB are very similar. Deterioration of statistics for a network constructed using an automatic designer is due to the rejection of a large amount of input variables.

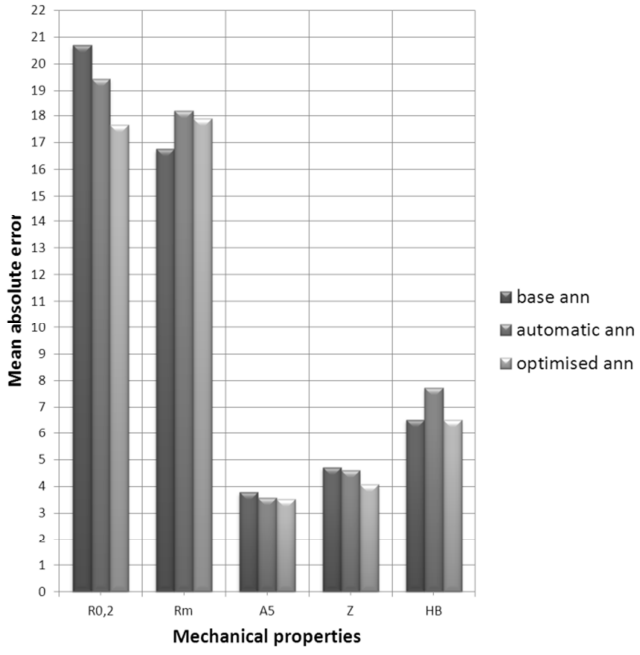

Fig. 2. Comparison between mean absolute error for base, automatic designed and optimised artificial neural networks (testing set)

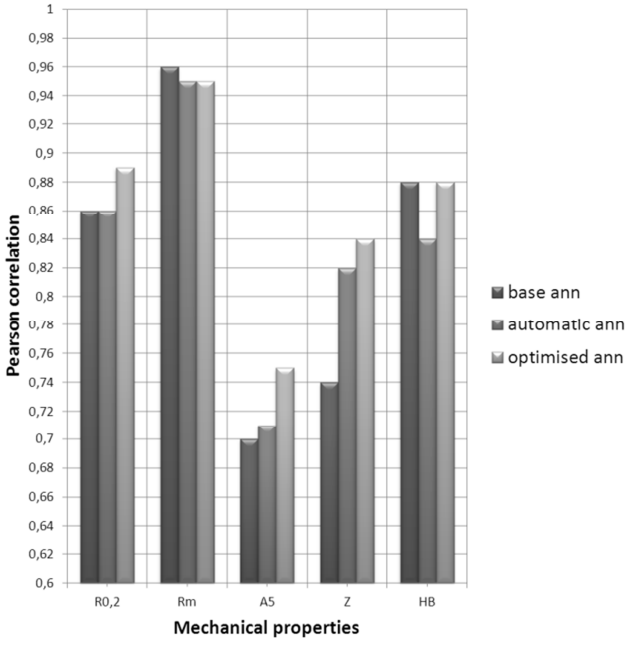

Fig. 3. Comparison between Pearson correlation for base, automatic designed and optimised artificial neural networks (testing set)

Table 5.
Chemical composition, shape and heat treatment conditions of examined stainless steels used in verification

sample	Diameter [mm]	Chemical composition [%]													Normalising		
		C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al	Temp. [°C]	Time [min]	medium
1	41	0.19	1.53	0.40	0.02	0.01	11.22	0.91	0.15	0	0	0	0.23	0.10	880	270	
2	131	0.25	1.47	0.28	0.02	0.01	11.58	0.10	0	0	0	0	0	0.02	920	80	- air
3	57	0.41	0.89	0.31	0.01	0.02	15.31	1.01	0.18	0.01	0.02	0.09	0.3	0.04	800	210	

Table 6.
Comparison between measured and predicted mechanical properties of examined stainless steels

sample	model	$R_{0.2}$		R_m		A_5		Z		HB	
		measured	predicted	measured	predicted	measured	predicted	measured	predicted	measured	predicted
1	base	379	380	583	583	30.7	31.9	46.3	46.9	158	160
	automatic		378		583		30.3		43.9		157
	optimised		379		581		31.6		46.0		158
2	base	372	368	569	570	19.1	20.4	55.9	54.4	153	156
	automatic		369		581		22.8		58.7		163
	optimised		372		572		18.5		55.7		151
3	base	333	362	553	553	30.6	29.9	67.8	42.8	144	143
	automatic		342		555		31.0		61.6		147
	optimised		334		542		30.5		68.1		146

6. Experimental verification

For verification purposes, an experimental set of three ferritic stainless steel samples has been developed. Their chemical composition and normalisation parameters are introduced in Table 5. To exclude the possibility of adjusting the artificial neural network only to the products of one manufacturer's material vectors, verification samples were collected from a different manufacturer. Samples, produced from these types of steel, were examined in order to obtain verification vectors. To minimize differences between training and verification data, material researches has been performed in the same way and using the same equipment, that were used in the main researches. The results obtained experimentally in a real laboratory have been compared with those obtained from computational models. All are introduced in Table 6. It was found, that all estimated results are correct for all examined steel samples. Differences among predicted and measured values of mechanical properties are very small and predicted results did not exceed the artificial neural network tolerance values in all models for corresponding property.

7. Summary

The aim of this study was to optimize artificial neural networks used to predict the mechanical properties of rolled ferritic stainless steels after normalization. Artificial neural networks were optimized with use of genetic algorithm to achieve better regression statistics. Optimization, except of tensile strength R_m case, has allowed the development of artificial neural networks, which either showed a better or comparable result from base networks, and also have a reduced number of input variables. As a result, in computational models constructed with use of these networks the noise information is reduced. Results of computational researches performer with use of these models were fully verified by experiment conducted in a real laboratory.

Additional information

Selected issues related to this paper are planned to be presented at the 22nd Winter International Scientific Conference on Achievements in Mechanical and Materials Engineering Winter-AMME'2015 in the framework of the Bidisciplinary Occasional Scientific Session BOSS'2015 celebrating the 10th anniversary of the foundation of the Association of Computational Materials Science and Surface Engineering and the World Academy of Materials and Manufacturing Engineering and of the foundation of the Worldwide Journal of Achievements in Materials and Manufacturing Engineering.

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