Journal of Achievements in Materials and Manufacturing Engineering
International Scientific Journal published monthly by the World Academy of Materials and Manufacturing Engineering

The application of neural networks to analysis of the effects of chemical composition on hardenability of steel

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ABSTRACT

Purpose: The goal of the research carried out was evaluation of alloying elements effect on the development of artificial neural network models, allowing the determination of the Jominy hardenability curve based on the chemical composition of constructional and machine steels.

Design/methodology/approach: MLP neural network was used to learn rule for modelling the steels properties. Then the neural network used for computer simulation synergistic effect of alloying elements on the hardenability of steel.

Research limitations/implications: Results of the research confirmed that neural networks are a useful tool in evaluation the effect of alloying elements on the properties of materials compared to conventional methods. Additionally it confirms idea, that based on data from standards and catalogues is possible to develop the assumed model.

Practical implications: It has been demonstrated complete the practical usefulness of the developed models in the selection of materials designed machine parts, which allows the direct relationship during the melting process real time control of the desired hardness of the steel hardenability curve.

Originality/value: Based on the results of catalogues and standards with the used of neural networks developed and fully validated experimental model of the relationship between hardenability and chemical composition of the constructional and machine steels.

Keywords: Computational material science; Artificial intelligence methods; Materials design steels; Modelling; Simulation

Reference to this paper should be given in the following way:

W. Sitek, A. Jabłoński, The application of neural networks to analysis of the effects of chemical composition on hardenability of steel, Journal of Achievements in Materials and Manufacturing Engineering 72/1 (2015) 32-38.

ANALYSIS AND MODELLING

1. Introduction

Objects made of metal accompanied humanity since time immemorial, since then also came the development of knowledge concerning the preparation of metal products with the desired properties. This knowledge includes a huge resource of information about the phenomena occurring in metals in different states of aggregation and allows the technological control of the manufacturing process of products. The process consists of several stages, each of which indirectly affect the final properties of the product. The skillful conduct of the process, having a base in understanding the phenomena occurring in the material, allows you to control a range of material properties that determine the subsequent use of the resulting product [1-3].

Hardenability is one of the main criteria for selection of steel machine parts, thus is of great importance in the design of machines and therefore is of interest to technologists [4-6]. Almost any item made of metal in one of the processing steps has been subjected to such treatment. Therefore the skillful conduct of the process, having a base in understanding the phenomena occurring in the material, allows you to control a range of material properties that determine the subsequent use of the resulting product. Modelling and computer simulation helps to improve the properties of engineering materials and predict their properties even before manufacturing materials, with a significant reduction in expenses and time needed for their research and implementation. Today, the essence of modern technology involves the simultaneous and equivalent selection of the design features of the machines and their components, identifying their technological process, as well as a selection of the most appropriate materials, resulting in the most complete satisfaction of human needs [7-8].

The effectiveness of the element as an additive affecting the hardenability of the steel can be determined from the change of any measure hardenability due to change in the quantity of added element. However, almost all the published experimental data on the effect of the elements on the hardenability specified in terms of the relationship between the ideal critical diameter, coefficient of hardenability and the content of the element in the steel.

In the literature you can find an alternative, numerical methods for determining the hardenability [9-19]. Review and compare these methods have been in the works. Incomplete accuracy of the mathematical model adopted and mistakes made during the investigation hardenability method of cooling from the face in the Jominy test often result in a discrepancies the calculation results with the experimental data given in the literature, standards and catalogues of steel. The work shows the possibility of using neural networks to analysis of the effect of selected elements on the hardenability of steel. This paper presents results of research on the development of a universal, single neural network model to predict the Jominy hardenability curve.

Therefore, work was undertaken to develop its own new method of modelling hardenability.

2. Materials and methods

The basis for the design of neural networks are the results of the research includes information about the chemical compositions and the corresponding Jominy hardenability curves approx. 500 heats different steel grades. The data set includes the results of hardness to 13 points on a curve Jominy hardenability and information about a concentration of seven basic alloying elements, ie. C, Mn, Si, Cr, Ni, Mo and Cu. Ranges of the alloying elements occurring in analysed steels are presented in Table 1.

Finally used 472 series of experimental data, which were divided into two groups. The first one containing 446 series used to generate and learning neural network. The second group, representing the remaining 26 series, was used to test and choose the best network. The division was made in a random manner proportional basis, ie. To test the network uses approx. 25% of the available data from each species. The breakdown of data was performed to verify the operation of networks for data that have not been screened in the learning process or validation. This allows for the exclusion of randomness and the full credibility of the results.

To design, learning and testing neural networks were used STATISTICA Neural Networks version 4.0 F StatSoft. Divided into three sets of data: the learner, validation and testing done in two ways:

1. random, proportional basis,
2. assigned manually (was divided set by the steel grade).

In its application to generate tens neural network with a varying number of neurons in the hidden layer, which was subjected to various learning techniques.

There are eight nodes on the input of the network and 7 of them represent the values of the concentration of particular alloying element occurring in the analysed steels (C, Mn, Si, Cr, Ni, Mo, Cu). Next one input represent distance from the face of the sample. The node on the output network layer represents hardness 13 consecutive points on the Jominy curve.

Obtained in this way neural networks were verified on the basis of the data set, which provides 26 test series.

Table 1.
Ranges of mass concentrations of the alloying elements occurring in the analyzed steels

	Mass concentration of alloying element, %						
	C	Mn	Si	Cr	Ni	Mo	Cu
Minimum	0.12	0.36	0.12	0.09	0.04	0.0098	0.07
Maximum	0.7	1.4	0.41	1.92	2.739	0.43	0.34

After the calculation of hardenability curves using these neural network, compared with the experimental results for the different steel heats. Finally, to further calculations we selected one network, multilayer perceptron type with five hidden layers of structures 8-5-1 calculations showing the average error of 1.51 HRC. As a method for network learning was chosen QN (Quasi-Newton) on the number of eras 1120. The results obtained indicate their suitability for modelling hardenability.

3. Results

After completion of the learning process or during the observed graph of error learning each network. On the basis of verified whether the network has not overfitting, and network overfitting were removed from further analysis. As indicators of network quality imputing the average absolute error, the ratio of standard deviation and correlation coefficient. The models of neural networks (Fig. 1) were used to analysis of the effect of elements for hardenability.

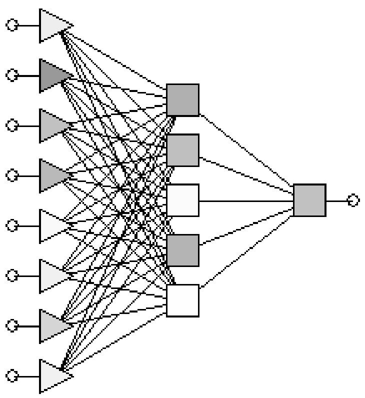

Fig. 1. A schematic presentation of a neural network with 3 layers; 8 input parameters, 5 neurons in the hidden layer and one output parameter

For this purpose, selected the group of steel, for which simulation was performed. Examples of the analyses carried out of the effect of alloy element with the fixed concentrations of the alloy elements given in Table 2 are presented in Figures 2-12.

Table 3-5 shows statistics for the training set, testing and validation for the entire data set.

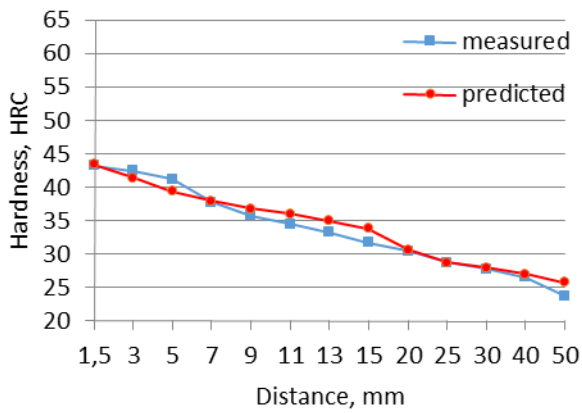

Fig. 2. The measured and predicted hardness profiles for steel grade 15CrNi6

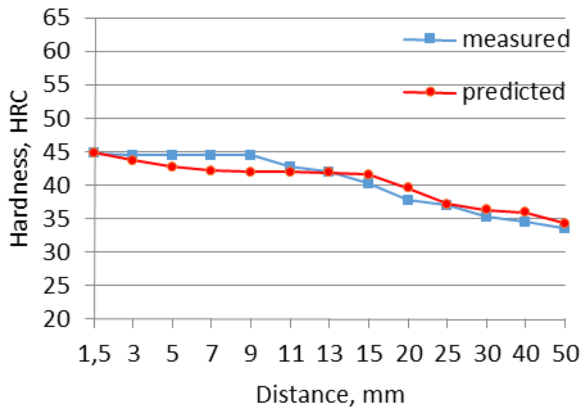

Fig. 3. The measured and predicted hardness profiles for steel grade 17CrNiMo6

Table 2.
Selected chemical composition of the constructional and machine steels used for modeling hardenability

Steel grade	Mass concentration of alloying element. %						
	C	Mn	Si	Cr	Ni	Mo	Cu
15CrNi6	0.14	0.58	0.12	1.6	1.51	0.05	0.14
17CrNiMo6	0.16	0.55	0.2	1.64	1.48	0.29	0.12
20MnCr5	0.2	1.19	0.26	1.11	0.23	0.06	0.22
25CrMo4	0.28	0.6495	0.22	1.04	0.159	0.1701	0.2
34CrMo4	0.32	0.68	0.32	1.01	0.17	0.17	0.19
37Cr4	0.37	0.67	0.28	0.99	0.13	0.03	0.34
41Cr4	0.39	0.75	0.34	0.98	0.09	0.04	0.13
46Cr2	0.48	0.74	0.27	0.53	0.14	0.03	0.18
50CrMo4	0.5	0.58	0.22	0.93	0.23	0.18	0.21
55Cr3	0.56	0.93	0.25	0.76	0.16	0.04	0.25
65Mn4	0.64	1.01	0.31	0.14	0.09	0.02	0.14

Table 3.
Network statistics for the training set

	x1.5	x3	x5	x7	x9	x11	x13	x15	x20	x25	x30	x40	x50
SD_HRC	6.50	5.86	6.69	7.86	9.09	9.08	8.98	8.60	7.59	7.33	6.47	6.30	5.98
SD_average error	0.99	1.09	1.39	1.60	1.52	1.44	1.28	1.33	1.35	1.39	1.25	1.37	1.55
average absolute error	1.01	1.26	1.44	1.58	1.78	1.79	1.56	1.56	1.55	1.69	1.69	1.75	2.00
correlation coefficient	0.98	0.96	0.96	0.96	0.97	0.98	0.98	0.97	0.96	0.96	0.95	0.94	0.91
Ratio of standard	0.15	0.19	0.21	0.20	0.17	0.16	0.14	0.15	0.18	0.19	0.19	0.22	0.26

Table 4.
Network statistics for the validation set

	x1.5	x3	x5	x7	x9	x11	x13	x15	x20	x25	x30	x40	x50
SD_HRC	6.14	6.40	7.11	8.68	9.17	8.49	8.82	8.87	8.31	6.69	6.25	6.08	5.47
SD_average error	0.89	1.11	1.49	1.47	1.66	1.45	1.53	1.34	1.24	1.25	1.26	1.34	1.60
average absolute error	1.00	1.30	1.58	1.59	1.85	1.88	1.89	1.57	1.58	1.50	1.46	1.65	2.11
correlation coefficient	0.98	0.97	0.96	0.97	0.97	0.97	0.97	0.98	0.97	0.96	0.95	0.94	0.88
Ratio of standard	0.14	0.17	0.21	0.17	0.18	0.17	0.17	0.15	0.15	0.19	0.20	0.22	0.29

Table 5.
Network statistics for the testset

	x1.5	x3	x5	x7	x9	x11	x13	x15	x20	x25	x30	x40	x50
SD_HRC	7.69	7.67	7.76	8.68	8.68	9.30	9.50	9.16	8.14	7.29	7.35	6.13	6.07
SD_average error	1.01	0.97	1.29	1.79	1.09	1.55	1.24	1.32	1.34	1.36	1.39	1.28	1.33
average absolute error	1.22	1.16	1.53	1.77	1.57	1.94	1.56	1.63	1.60	1.59	1.64	1.71	1.72
correlation coefficient	0.97	0.98	0.96	0.95	0.98	0.97	0.98	0.97	0.97	0.96	0.96	0.94	0.92
Ratio of standard	0.13	0.13	0.17	0.21	0.13	0.17	0.13	0.14	0.16	0.19	0.19	0.21	0.22

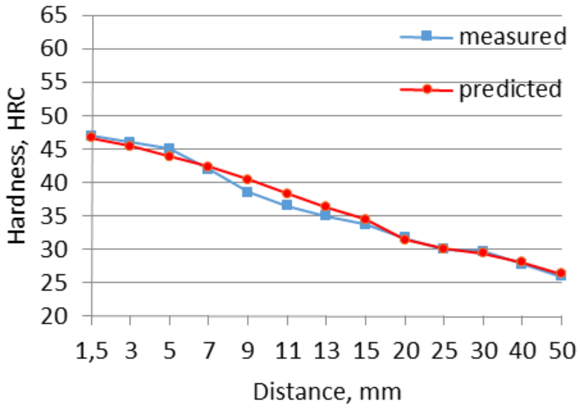

Fig. 4. The measured and predicted hardness profiles for steel grade 20MnCr5

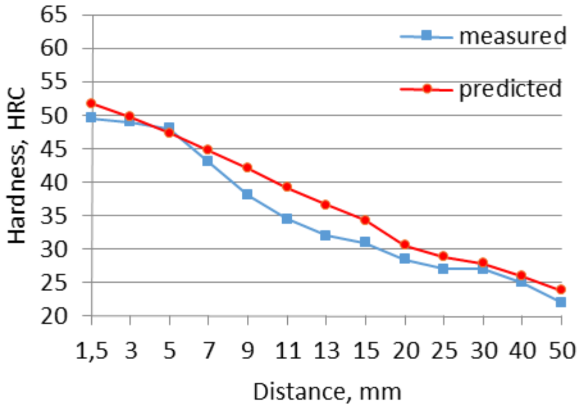

Fig. 5. The measured and predicted hardness profiles for steel grade 25CrMo4

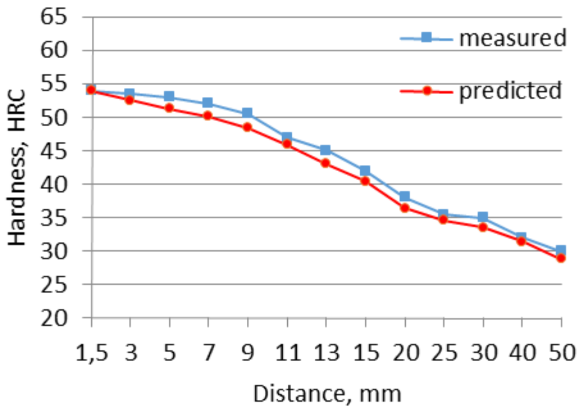

Fig. 6. The measured and predicted hardness profiles for steel grade 34CrMo4

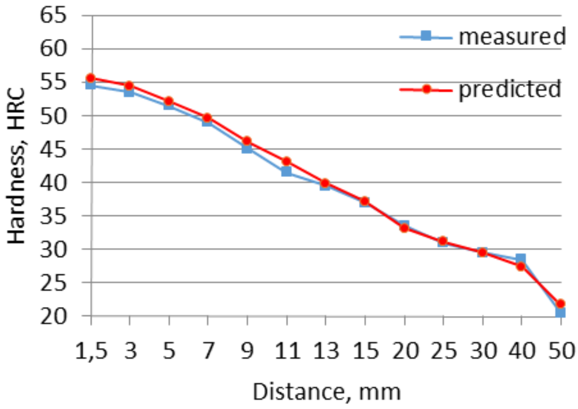

Fig. 7. The measured and predicted hardness profiles for steel grade 37Cr4

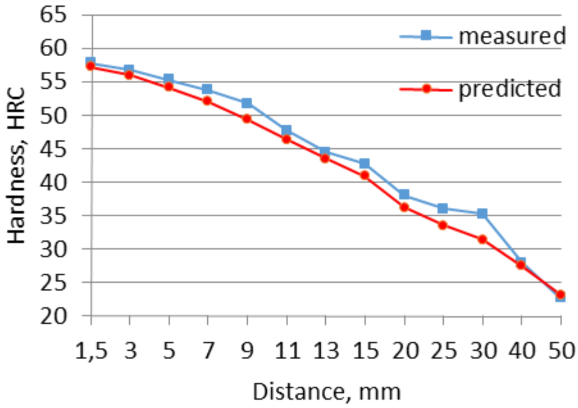

Fig. 8. The measured and predicted hardness profiles for steel grade 41Cr4

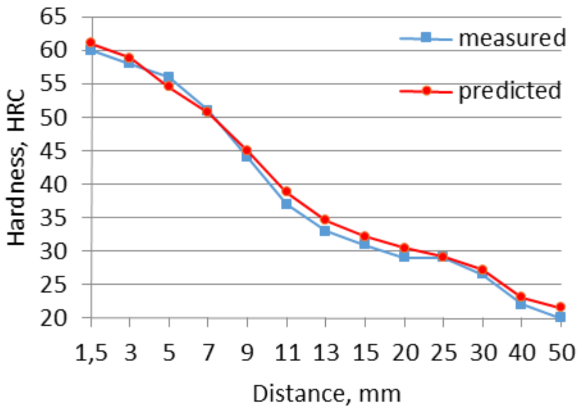

Fig. 9. The measured and predicted hardness profiles for steel grade 46Cr2

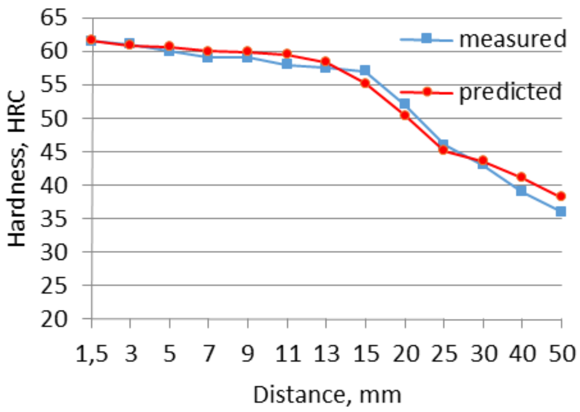

Fig. 10. The measured and predicted hardness profiles for steel grade 50CrMo4

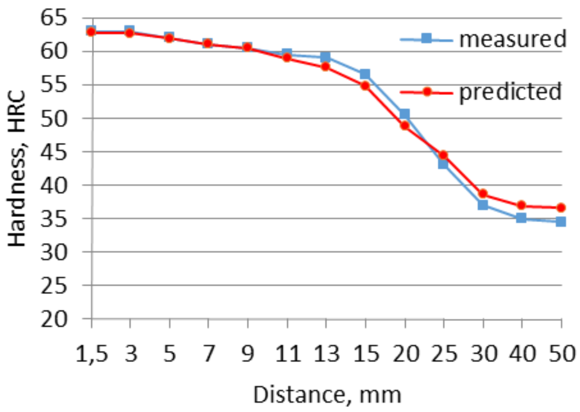

Fig. 11. The measured and predicted hardness profiles for steel grade 55Cr3

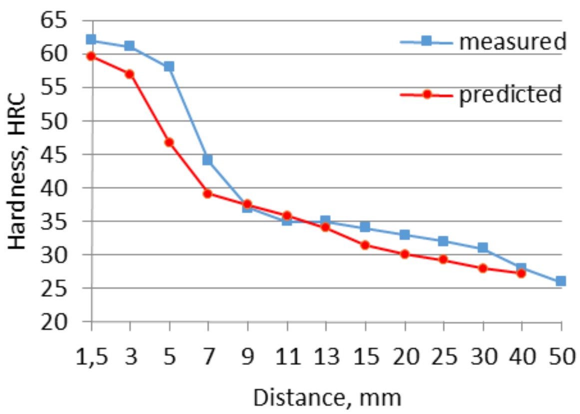

Fig. 12. The measured and predicted hardness profiles for steel grade 65Mn4

4. Conclusions

The paper presents models of neural networks for determining the Jominy hardenability curves for constructional and machine alloy steel based on chemical composition. Neural network models were developed based on approximately 500 data. Developed hundreds of network models, which have been revised. Finally, one model was considered ie giving satisfactory results. Designating hardenability curve with reasonable accuracy. Further demonstrated the usefulness of neural network models developed to analyze the influence of chemical composition on hardenability of steel. On the basis of calculations we found that artificial neural networks can be regarded as a very effective tool for computer-aided selection of materials. To design a neural network, which satisfactorily appoint hardenability curve is required relatively large number of experimental data used for learning and testing neural networks, so you can't stop carrying out experimental research.

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