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Modelling and Analysis of the Synergistic Alloying Elements Effect on Hardenability of Steel

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Abstract

The paper presents a methodology of modeling relationships between chemical composition and hardenability of structural alloy steels using computational intelligence methods, that are artificial neural network and multiple regression models. Particularly, the researchers used unidirectional multilayer teaching method based on the error backpropagation algorithm and a quasi-newton methods. Based on previously known methodologies, it was found that there is no universal method of modeling hardenability, and it was also noted that there are errors related to the calculation of the curve. The study was performed on large set of experimental data containing required information on about the chemical compositions and corresponding Jominy hardenability curves for over 400 data steel heats with variety of chemical compositions. It is demonstrated that the full practical usefulness of the developed models in the selection of materials for particular applications with intended performance in the area of application.

Keywords: Hardenability, Artificial neural network, Multiple regression, Steel alloy composition, Modelling and simulation

1. Introduction

Steel is one of the most important materials used in all sectors of the economy. The reason for this is its good mechanical and physical properties, which can be improved by adding alloying elements.

The current research direction on heat-treatable steels concerns the optimization of the heat treatment parameters, in particular the cooling conditions using different cooling media and the cooling process itself in conjunction with numerical analyzes of the temperature distribution in the cooled element [1].

The properties of steel vary based on the composition of carbon and alloying elements present in it and the alloying elements give different properties depending on the concentration of each percentage ratio involved [2-3].

Another direction is to optimize the chemical composition of the steel to provide the desired properties or multiple properties simultaneously within a narrow range. Optimization of chemical composition of steel is the harmony of quality and price. A very important indicator of yesterday, today and tomorrow-even more. When chemical composition of alloy steel is optimized and intensively quenched, alloy elements in steel can be reduced more than two-times with simultaneous increasing service life of quenched machine components [4]. For example, in steels used in the automotive industry, the hardenability of the steel is an important property. In this case, customer requirements are often limited to a hardenability range narrowed in relation to the normative hardenability range of the grade and only within a certain distance of the quenched-end of the Jominy specimen. These customer requirements force the design of the chemical composition at the melt production stage. The task of ensuring the

chemical composition of the melt with guaranteed properties, narrowed down to those desired by the customer, must be carried out while maintaining the standard chemical composition for the species. Therefore, it is necessary to know already in the phase of metallurgical process how to correct the chemical composition.

The analysis of the influence of alloying elements on the properties of steel has been the subject of research for several decades. In most publications on this subject, the prevailing view is that the interaction of additional alloys is a superposition of the total concentration of elements in the steel. This first approach was proposed in the seminal work of M.A. Grossmann [5], who defined numerical coefficients describing the influence of elements on the hardenability of steel. This work is still the basis of the standard ATM A255 [6] for calculating the hardenability curves of steel.

Modelling and simulation plays immense role in improving engineering materials properties possible, as well as prediction of their properties like hardenability, even before the materials are fabricated, with the significant reduction of costs and time required for their investigation and application [7]. The mechanical properties of metal alloys have been predicted using machine learning models, which range from general models for elastic properties trained on data derived from first principles to models of macroscopic properties like hardness, toughness, and strength as well as phenomena like wear, fatigue, creep, hydrogen embrittlement, and crack initiation and propagation in particular alloy systems [8]. Similarly, predicting the effect of process parameters, quantitative structure-property relationships, using functional mappings of inputs to predict end-product quality, interpretability and the physical meaning of the computational intelligence methods were analyzed [9-11].

Determining hardenability enables to ensure the assumed decomposition properties in the cross section of the element [12-13]. Hardenability models proposed in the literature [5, 14-21] do not show the full relevance to the experimental data, probably due to incomplete verification, too small or even unrepresentative set of experimental data. Full adequacy of the mathematical model can be performed on a large number of melts with appropriately selected and exactly controlled chemical compositions exhausting all possible combinations of alloying elements present in the steel group [22-25]. This creates the necessity of seeking a new model—modern tools and computational methods, including artificial neural networks indicate the chances of solving this problem [26-31]. This indicates the advisability of taking methodological work aimed to develop such computer tools.

Previous work of our own [7, 22-23, 27, 30] as well as the results presented in this paper indicate that there is a synergy of the influences of the elements on hardenability. This fact should be taken into account when designing the chemical composition before melting or when correcting the chemical composition at the stage of control analysis of the melt. It should be noted that so far there are no research results on the synergistic effect of alloying elements on hardenability, which is probably due to the complexity of thermophysical phenomena that occur during the steel melting process.

In this paper we present the results of computer simulations in which the developed neural network model was used to calculate hardenability curves. The purpose of this model is to analyze the changes (increase) in hardness resulting from changes in the concentrations of elements and their combinations on the hardness of steel. Here, the hardness at different depths of the material cross-section were analyzed, represented by the hardness at the corresponding distance at the quenched-end of the Jominy specimen. The obtained results of the computer simulations show different quantitative increases in hardness depending on the proportion of each alloy component. This confirms the synergy of hardenability of the alloying elements and indicates the nonlinear nature of this synergistic effect.

2. Materials and Methodology

The basic reason for the design of artificial neural networks are the experimental results obtained from the standards, catalogs steel producers, trade literature, including information on the chemical compositions and the corresponding hardness on Jominy hardenability curve [32-37]. It was assumed that the heat treatment of steel for the collected data is made under optimal conditions, and the grain size is seven according to ASTM scale. The dataset contains information about measurements Rockwell Hardness scale C, respectively at distances of 1.5, 3, 5, 7, 9, 11, 13, 15, 20, 25, 30, 40 and 50 mm, and information about the concentration of the seven basic alloying elements present in the group of structural alloy steel, i.e. C, Mn, Si, Cr, Ni, Mo and Cu. The database contains the results finally 494 data series, which was created two disjoint sets of experimental data. The first of the sets (469 heats) is used to generate and training the artificial neural network modeling hardenability, and the second (25 heats) is used for testing and verification, by choosing the best network, of the derived model. The distribution of the data was performed to verify the act networks for data, which were not presented in the learning process or validation. This allows to exclude randomness and full credibility of the results. At this stage, it recycled note that within each of the sets get the large variety of chemical compositions of heats. The chemical compositions of heats are shown in Table 1.

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

Range	Mass fractions of element, %						
	C	Mn	Si	Cr	Ni	Mo	Cu
Min.	0.12	0.36	0.12	0.09	0.04	0.01	0.07
Max.	0.64	1.40	0.41	1.92	2.74	0.43	0.34

Made-to-date data selection, aimed at rejection of those for whom the results of experimental hardenability indicated the occurrence of any error or independent reasons connected with the experiment. Figure 1 shows the visualization of the range of occurrence of Chromium and Molybdenum data used in the analysis of steels, see Table 1.

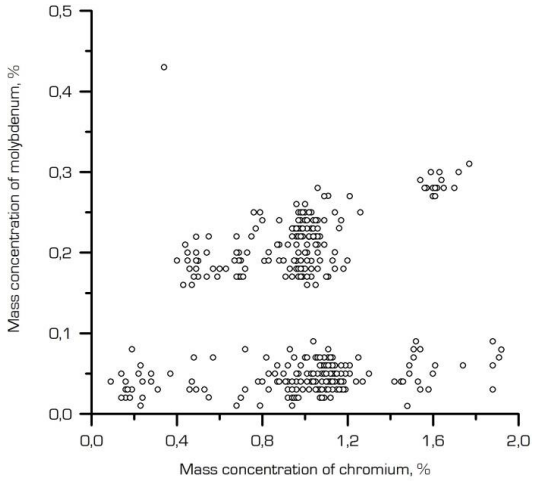

Fig. 1. Range of occurrence clusters of the alloying elements for whole mass concentrations of alloying elements

First developed in the working method of modeling hardenability used artificial neural networks. The selection of the type of network used have been guided by the circumstances which indicated task dictates the choice of the structure of your network. The rationale for this was continuity of the input signals compatible with hardness in the following distances from the front of the sample to the hardenability curves. Accordingly, the hardenability curves for modeling the neural network uses a unidirectional multilayer teaching method based on the error backpropagation algorithm and a Quasi-Newton method. The analysis of two-layer network type structure 7-x-13 and 8-x-1, where x is the number of neurons in the hidden layer. The general structure of the artificial neural network is shown on Figure 2.

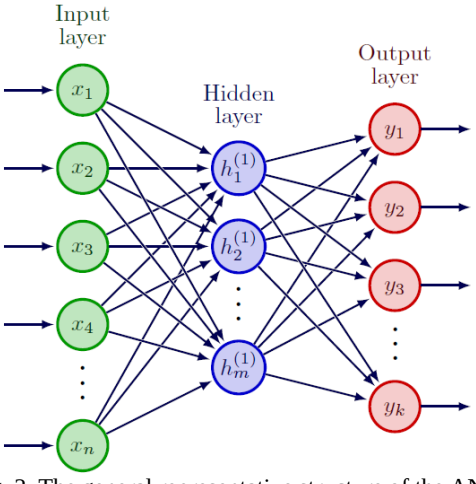

Fig. 2. The general representative structure of the ANN

In the first model it is assumed that seven basic alloying elements mainly affects hardenability which present in machine structural steels, such as: C, Mn, Si, Cr, Ni, Mo and Cu, whose concentration corresponds to the seven nodes of the input layer of the network. The nodes on the network output list correspond to the thirteen points where the hardness is measured on Jominy sample. In the latter model, as inputs were considered the mass concentrations of the seven major alloying elements and a point on the curve in the hardenability predetermined distance from the front. In the analyzed structure of the output signal has a hardness corresponding to the next points on Jominy hardenability curve. The choice of the second model is due to the result of the analysis of the results of error learning network.

In the second method, developed in the work hardenability modeling used equation derived by statistical stepwise regression. This method involves the sequential selection of variables in the model in order to obtain the best set of variables. The value of the Pearson correlation coefficient, standard error, and the ratio of standard deviations form the basis for assessing the significance of the resulting model. The Microsoft Excel with Analysis ToolPak is utilized to determine the coefficients of the regression equations. As with the training of the artificial neural network uses a set of experimental data to create the statistical models.

3. Results and Discussion

The choice of practical modeling methods of hardenability in the selection of steel components machine is based on the verification of each of the analyzed working methods of calculating the hardenability of experimental results. For this purpose, we selected two models developed using computer tools to evaluate the effect of chemical composition on hardenability of the steel. The purpose of this experiment is to compare the compliance impact assessments of chemical composition on hardenability obtained models for the artificial neural network model and the regression of experimental data and calculated. The comparison is shown in Table 2.

Table 2.
Comparison of statistics for the model of the neural network and regression

Neural network model		Distance from quenched end, mm		
		7	20	30
Average error, HRC	Training set	1.58	1.55	1.68
	Validating set	1.59	1.58	1.46
	Testing set	1.57	1.60	1.64
	Verifying set	1.58	1.58	1.56
Pearson correlation coefficient	Training set	0.96	0.96	0.95
	Validating set	0.97	0.97	0.95
	Testing set	0.95	0.97	0.96
	Verifying set	0.96	0.97	0.95
Quotient of standard derivation	Training set	0.20	0.18	0.19
	Validating set	0.17	0.15	0.20
	Testing set	0.20	0.16	0.19
	Verifying set	0.19	0.18	0.19

Mathematical model	Distance from quenched end, mm		
	7	20	30
Average error, HRC	1.69	2.37	2.08
Pearson correlation coefficient	0.96	0.95	0.95
Quotient of standard deviation	0.18	0.20	0.21

Similarly, the comparison of the model and the predicted hardness for the three distances from quenched end can be observed from Figure 3.

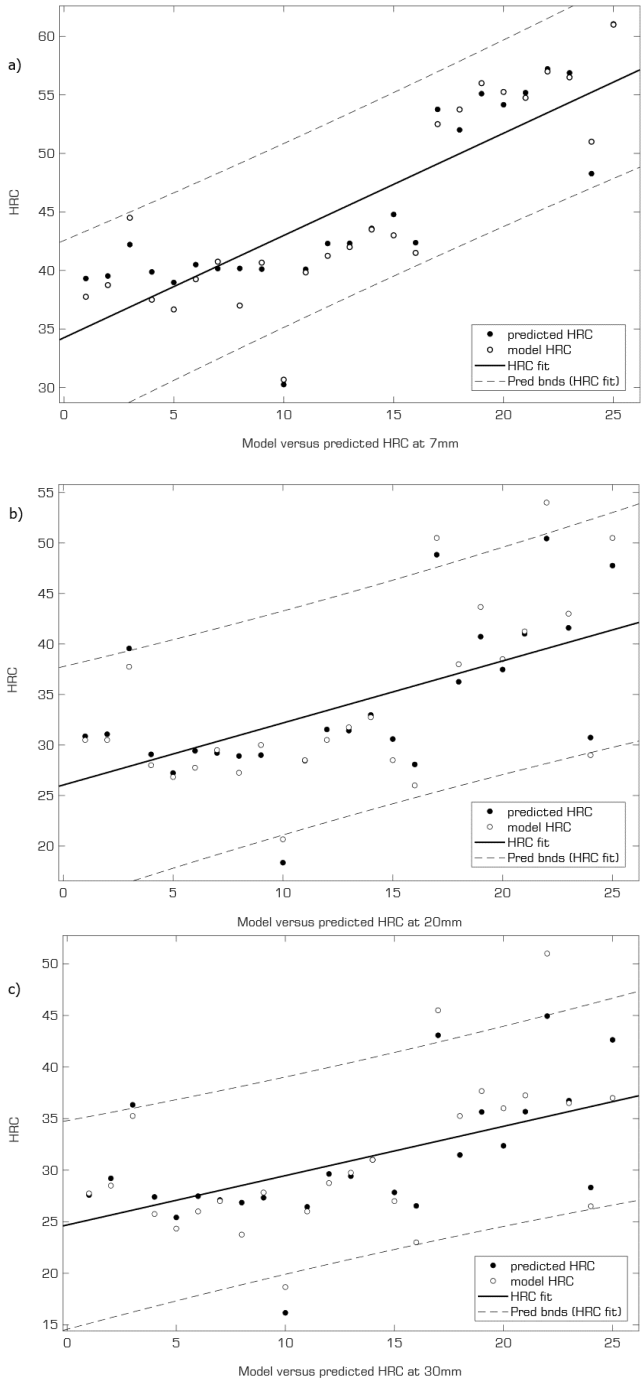

Fig. 3. The comparison of model HRC and predicted HRC for three distances from quenched end a) 7mm, b) 20mm, c) 30mm

Examples of the graphs of planned on the basis of statistical numerical experiments illustrate the effect respectively of a single element, pairs of element with range of clusters shown in Figure 1, and Figures 4 – Figure 6 for chemical composition 0.22% C, 0.7% Mn, 0.25% Si, 1.1% Cr, 0.25% Ni, 0.05% Mo, 0.16% Cu.

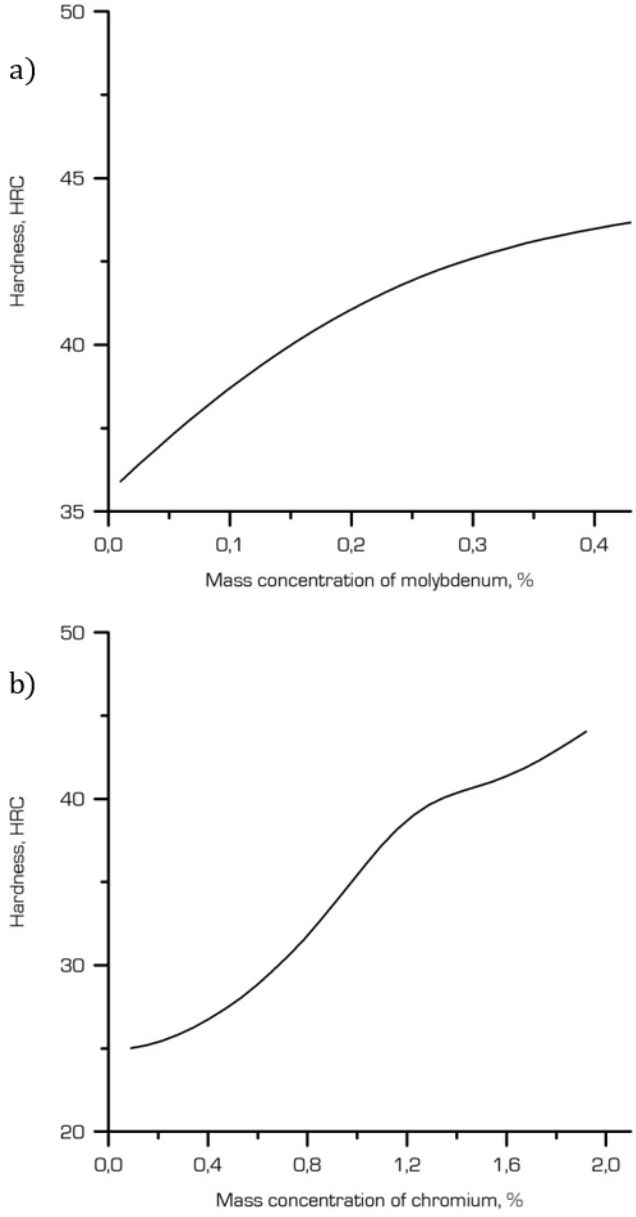

Fig. 4. The influence of alloying elements on the response function (hardness HRC) for the calculated data of the neural network model a) Mo, b) Cr

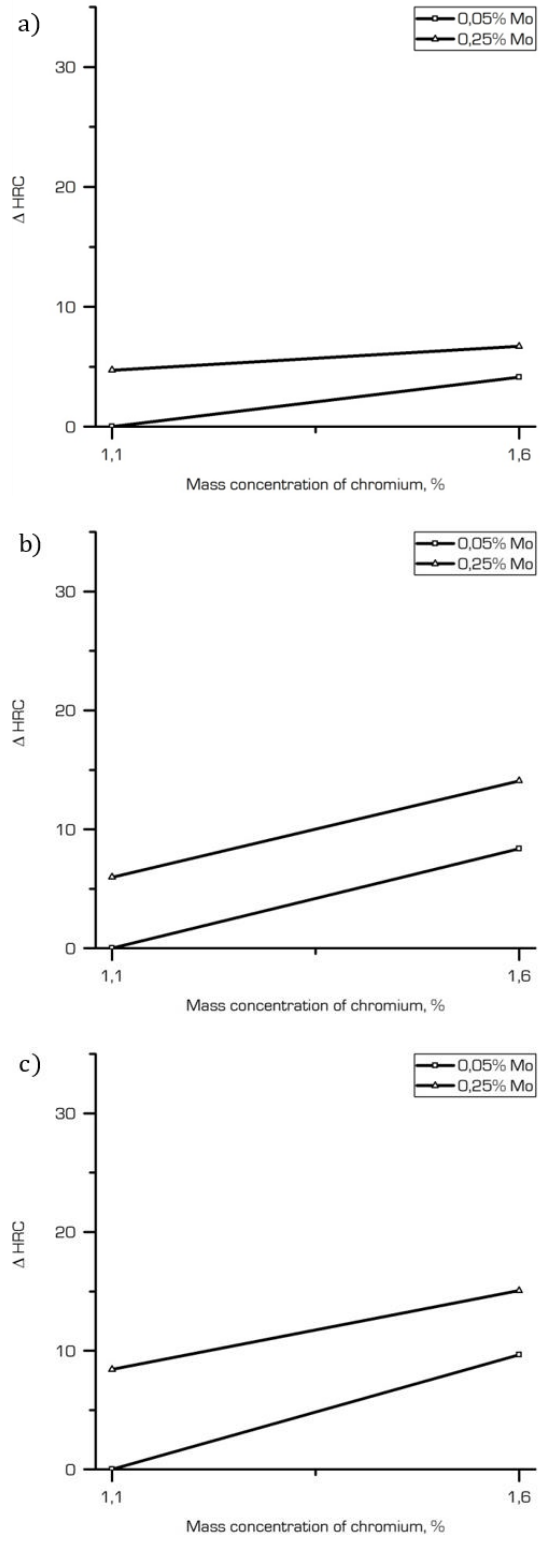

Fig. 5. Effect of concentration of chromium and molybdenum to increase the hardness at distance a) 7mm, b) 20mm, c) 40mm

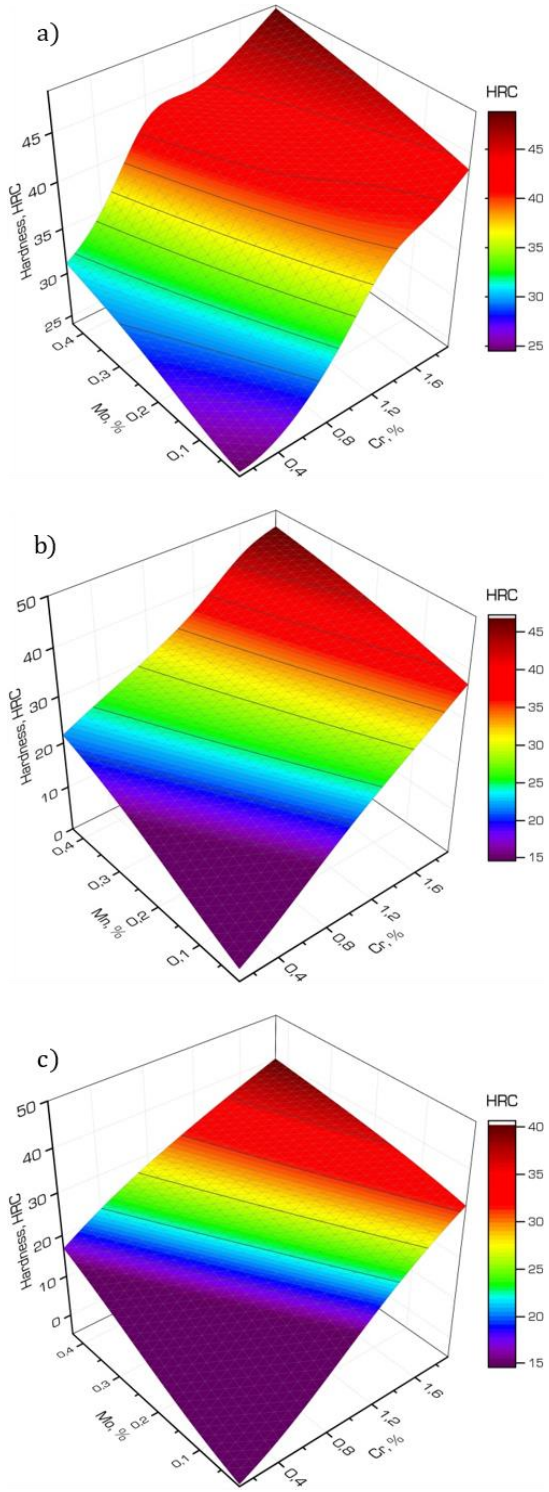

Fig. 6. Synergistic effect of Cr and Mo on the steels hardness at distance a) 7mm, b) 20mm, c) 40mm

Comparison of the data from Figure 1, and Figures 4 – Figure 6 with the results of classical methods [5, 7, 12-20] proves that the

conclusions concerning the subject presented in the works mentioned are correct. However, the results from the classical investigations do not provide evaluations of the effect of two or more alloying elements on hardenability. Therefore, it is possible to say that this is one of the main reasons for deficiency of the existing methods of evaluation of the effect of the composition of the elements on hardenability. Generally, based on the research conducted, and example presented, it is possible to determine which combinations of the alloying compositions elements considerably increase hardenability of steel.

4. Conclusions

The research addressed the application of the method of artificial neural networks and quasi-newton method in modelling hardenability of steel for evaluation of the synergistic effect of the alloying elements on its properties. The vast potential use of the computer tools developed was pointed out, and their practical usefulness was illustrated by examples. The developed artificial neural network model can also be employed for simulations of the relationship between hardness at a given distance from the Jominy bar specimen face and the chemical composition of the steel. This can be done in the entire range of concentrations of the main alloying elements occurring in constructional alloy steels. Application of the presented method, using the computer program developed, enables practitioners to make free analyses of the synergistic effect of the alloying elements occurring in heat-treatable alloy constructional steels using only computer simulation without carrying out time consuming and costly experimental investigations. The developed tool can be utilized to synthesis steel alloy with specific property for particular applications.

References

[1] Kobasko, N.I. (2018). Optimal hardenability steel for any size and form of machine components to increase their service life and decrease alloy elements in material. *International Journal of Current Research*. 10(02), 65867-65878.

[2] Grange, R.A., Hribal, C.R. & Porter, L.F. (1977). Hardness of tempered martensite in carbon and low-alloy steels. *Metallurgical and Materials Transactions A*. 8, 1775-1785. DOI: doi.org/10.1007/BF02646882.

[3] Bain, E.C., Paxton, H.W. (1961). *Alloying Elements in Steel, 2nd Edition*. Metals Park, Ohio: American Society for Metals.

[4] Kobasko, N.I. (2012). Correlation between chemical composition of steel, optimal hardened layer, and optimal residual stress distribution. In N.I. Kobasko & K.N. Prabhu (Eds.), Film and Nucleate Boiling Processes, STP1534 (61-80). West Conshohocken, PA: ASTM International.

[5] Grossmann, M.A. (1942). Hardenability calculated from chemical composition. *The American Institute of Mining, Metallurgical, and Petroleum Engineers*. 150, 227-255.

[6] ASTM A-255-02 (2002). Standard test methods for determining hardenability of steel. ASTM International. https://doi.org/10.1520/A0255-02.

[7] Sitek, W. & Trzaska, J. (2011). Numerical simulation of the alloying elements effect on steels' properties. *Journal of Achievements in Materials and Manufacturing Engineering*. 45(1), 71-78.

[8] Hart, G.L.W., Mueller, T., Toher, C. & Curtarolo, S. (2021). Machine learning for alloys. *Nature Reviews Materials.* 6, 730-755. https://doi.org/10.1038/s41578-021-00340-w.

[9] Schmidt, J., Marques, M.R.G., Botti, S. & Marques, M.A.L. (2019). Recent advances and applications of machine learning in solid-state materials science. *npj Computational Materials*. 5(83). https://doi.org/10.1038/s41524-019-0221-0.

[10] Lambiase, F., Di Ilio, A.M., & Paoletti, A. (2013). Prediction of Laser Hardening by Means of Neural Network. In 8th CIRP Conference on Intelligent Computation in Manufacturing Engineering, 18-20 July 2012 (pp. 181 – 186). Ischia, Italy: Elsevier Procedia. https://doi.org/10.1016/j.procir.2013.09.032.

[11] Chong, ZS, Wilcox, S, & Ward, J. (2005). The Use of Artificial Intelligence in the Modelling and Heat Treatment Parameters Identification for Alloy-Steel Re-Heating Process. In Proceedings of the ASME 2005 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. Volume 1: 20th Biennial Conference on Mechanical Vibration and Noise, Parts A, B, and C, September 24–28, 2005 (pp. 607-613). Long Beach, California, USA: ASME. https://doi.org/10.1115/DETC2005-84802.

[12] Hodge, J.M. & Orehoski, M.A. (1946). Relationship between hardenability and martensite in some low-alloy steels. *The American Institute of Mining, Metallurgical, and Petroleum Engineers*. 167, 502-512.

[13] Mangonon, P.L. (1982). Relative hardenabilities and interaction *effects* of Mo and V in 4330 alloy steel. *Metallurgical and Materials Transactions A.* 13, 319-320. DOI: 10.1007/BF02643323.

[14] Kramer, I.R., Hafner, R.H. & Toleman, S.L. (1944). Effect of Sixteen Alloying Elements on Hardenability of Steel, *The American Institute of Mining, Metallurgical, and Petroleum Engineers*. 158, 138-156.

[15] Doane, D.V. (1979). Application of Hardenability Concepts in Heat Treatment of Steel. *Journal of Heat Treating*. 1, 5-30. DOI: doi.org/10.1007/BF02833206.

[16] Doane, D.V. & Kirkaldy, J.S.G. (1978). Hardenability concepts with application to steels. *Transactions of the Metallurgical Society of AIME*. 12, 626-334.

[17] Jatczak, C.F. (1973). Hardenability in high carbon steels. *Metallurgical and Materials Transactions B*. 4, 2267-2277. DOI: doi.org/10.1007/BF02669366.

[18] Grange, R.A. (1973). Estimating the hardenability of carbon steels. *Metallurgical and Materials Transactions B*. 4, 2231-2244. DOI: doi.org/10.1007/BF02669363.

[19] Crafts, W. & Lamont, J.L. (1944). Effects of some elements on hardenability. *The American Institute of Mining, Metallurgical, and Petroleum Engineers*. 1(11), 157-167.

[20] Comstock, G.F. (1945). The influence of titanium on the hardenability of steel. *Transactions of the Metallurgical Society of AIME*. 12 (6), 148-150.
[21] Moser, A. & Legat, A. (1969). Die Berechnung der Härtbarkeit aus der chemischen Zusammensetzung. *HTM Härterei-technische Mitteilungen*. 24(2), 100-104. (in German)
[22] Sitek, W. & Jabłoński, A. (2015). 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), 32-38.
[23] Sitek, W. & Irla, A. (2016). The Use of fuzzy systems for forecasting the hardenability of steel. Archives of Metallurgy and Materials. 61(2), 797-802. DOI: dx.doi.org/10.1515/amm-2016-0134.
[24] Dobrzański, L.A. & Sitek, W. (1997). Comparison of hardenability calculation methods of the heat-treatable constructional steels. *Journal of Materials Processing Technology*. 64(1-3), 117-126. DOI: doi.org/10.1016/S0924-0136(96)02559-9.
[25] Dobrzański, L.A. & Sitek, W. (1999). Designing of the chemical composition of constructional alloy steels. *Journal of Materials Processing Technology*. 89-90, 467-472. DOI: doi.org/10.1016/S0924-0136(99)00140-5.
[26] Sitek, W. & Trzaska, J. (2021). Practical aspects of the design and use of the artificial neural networks in materials engineering. *Metals 2021*. 11(11), 1832. DOI: doi.org/10.3390/met11111832.
[27] Dobrzański, L.A. & Sitek, W. (1999). The modelling of hardenability using neural networks. *Journal of Materials Processing Technology*. 92-93, 8-14. DOI: doi.org/10.1016/S0924-0136(99)00174-0.
[28] Sitek, W., Trzaska, J., & Dobrzański, L.A. (2008). Modified Tartagli method for calculation of Jominy hardenability curve. *Materials Science Forum*. 575-578, 892-897. DOI: doi.org/10.4028/www.scientific.net/MSF.575-578.892.
[29] Sitek, W. (2010). A mathematical model of the hardness of high-speed steels. *Transactions of FAMENA*. 34(3), 39-46.
[30] Sitek, W., Dobrzański, L.A. & Zacłona, J. (2004). The modelling of high-speed steels' properties using neural networks. *Journal of Materials Processing Technology*. 157-158, 245-249. DOI: doi.org/10.1016/j.jmatprotec.2004.09.037.
[31] Sitek, W. & Dobrzański, L.A. (2005). Application of genetic methods in materials' design. *Journal of Materials Processing Technology*. 164-165, 1607-1611. DOI: doi.org/10.1016/j.jmatprotec.2005.01.005.
[32] Edelstahl Witten-Krefeld GmbH (2007). *THYROFORT: Heat-treatable steels* (Technical Information). Swiss Steel Group. https://www.swisssteel-group.com/fileadmin/user_upload/_SCHULUNG_/Sudafrika/Publications/heat_treatable_steel.pdf.
[33] EN ISO 683-2:2018 (2018). Heat-treatable steels, alloy steels and free-cutting steels - Part 2: Alloy steels for quenching and tempering (ISO 683-2:2016). ISO Standards. https://www.iso.org/standard/70643.html.
[34] Wever, F., Rose, A., Peter, W., Strassburg, W. & Rademacher, L. (1961). Atlas zur Wärmebehandlung der Stähle, Teil I and II. *Max-Planck-Institut für Eisenforschung in Zusammenarbeit mit dem Werkstoffausschuss des Vereins Deutscher Eisenhüttenleute*. Düsseldorf, Germany: Verlag Stahleisen m.b.H. (in German)
[35] Rose, A. & Hougardy, H. (1972). Atlas zur Wärmebehandlung der Stähle, Band 2. *Max-Planck-Institut für Eisenforschung in Zusammenarbeit mit dem Werkstoffausschuss des Vereins Deutscher Eisenhüttenleute*. Düsseldorf, Germany: Verlag Stahleisen m.b.H. (in German)
[36] Orlich, J., Rose, A. & Wiest, P. (1973). Atlas zur Wärmebehandlung der Stähle, Band 3: Zeit-Temperatur-Austenitisierung-Schaubilder. *Max-Planck-Institut für Eisenforschung in Zusammenarbeit mit dem Werkstoffausschuss des Vereins Deutscher Eisenhüttenleute*. Düsseldorf, Germany: Verlag Stahleisen m.b.H. (in German)
[37] Orlich, J., & Pietrzeniuk, H. (1976). Atlas zur Wärmebehandlung der Stähle, Band 4: Zeit-Temperatur-Austenitisierung-Schaubilder, Teil 2. *Max-Planck-Institut für Eisenforschung in Zusammenarbeit mit dem Werkstoffausschuss des Vereins Deutscher Eisenhüttenleute*. Düsseldorf, Germany: Verlag Stahleisen m.b.H. (in German)