




PRODUCTION ENGINEERING ARCHIVES

ISSN 2353-5156 (print)
ISSN 2353-7779 (online)Exist since 4th quarter 2013
Available online at <https://pea-journal.eu>

Predicting the mechanical properties of stainless steels using Artificial Neural Networks

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Article history

Received 29.02.2024

Accepted 15.04.2024

Available online 31.05.2024

Keywords

Stainless steel,

Yield stress,

Tensile strength,

Hardness,

ANN.

Abstract

Knowing the material properties is of a crucial importance when planning to manufacture some structure. That is true for the steel structures, as well. Thus, for the proper planning of a certain steel part or a structure production, one must be aware of the properties of the material, to be able to make a qualified decision, which material should be used. Considering that the manufacturing of steel products is constantly growing in various branches of industry and engineering, the problem of predicting the material properties, needed to satisfy the requirements for the certain part efficient and reliable functioning, becomes an imperative in the design process. A method of predicting four material properties of the two stainless steels, by use of the artificial neural network (ANN) is presented in this article. Those properties were predicted based on the particular steels' known chemical compositions and the corresponding material properties available in the Cambridge Educational System EDU PACK 2010 software, using neural network module of MathWorks Matlab. The method was verified by comparing the values of the material properties predicted by this method to known values of properties for the two stainless steels, X5CrNi18-10 (AISI 304), X5CrNiMo17-12-2 (AISI 316). The difference between the two sets of values was below 5% and, in some cases, even negligible.

DOI: 10.30657/pea.2024.30.21

1. Introduction

Application of steels in technics began to grow with the discovery of Bessemer's process, back in 1856. From then on, almost all new structures and machines began to incorporate steel parts, extending the service life of parts in that way. Nowadays, in the so-called conventional engineering, such as mechanical, civil, automotive etc., steel is still the most applied material. One of the reasons for such a situation is the significantly lower price of steels, as compared to other metal materials, such as aluminum or titanium, or composite materials, new-nano materials and others. However, there exist some disadvantages that are limiting their even wider application. The first and definitely the biggest is phenomenon of corrosion, i.e., reacting of steel with oxygen, forming the corrosive layer on the components surface, and, in the more severe cases, penetrating deeper into the material bulk. The corrosion, to put it simple, is an irreversible process of material destruction. Problems related to corrosion could lead to greater

problems, such as material loss, as well as sudden components' failures that can have catastrophic consequences, not only regarding financial losses, but endangering human lives, as well (Jovanović et al., 2017).

The solution to this problem was found in 1913 with discovering of steels that are resistant to corrosion, the so-called stainless steels. The resistance to corrosion comes as a consequence of those steels' chemical composition, consisting of minimum of 10.5 to 12% of chromium dissolved in steel solid solution. At present, there exist thousands of stainless steels grades, carefully engineered to meet the specific requirements of the parts that are to be made of them, all regulated by specific standards, (EN 10088-1:2005; EN 10088-2:2005; EN 10088-3:2005; EN 10088-4:2009; EN 10088-5:2009). Besides chromium, the stainless steels also contain other chemical elements, such as nickel, molybdenum, vanadium and others. Stainless steels with adequate addition of niobium are known as austenite (or austenitic) stainless steels, since their austenitic structure remains even at room temperatures. The



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reason for that is the action of Ni i Mn, which expand the region of stable austenite within the Fe-Fe₃C phase diagram.

The microstructure is the main criterion for classification of the stainless steels: ferritic, austenitic, austenitic-ferritic (the so-called duplex steels), martensitic, precipitation hardening. Differences between mechanical and physical properties of carbon and stainless steels are important for the structural safety. They include principal material properties (Young modulus, yield stress and ultimate strength), as well as stainless steel behavior (the stress-strain curve i.e., the σ - ϵ diagram, behavior during the cold working or at elevated temperatures). Those differences must be considered when the ultimate and serviceability limit states are being formulated during the structures design (Tylek and Kuchta, 2014).

When designing any steel structure, one must obey adequate standards (EN 1990:2002; EN 1993-1-1:2005; EN 1993-1-2:2005; EN 1993-1-3:2006; EN 1993-1-4:2006), respecting the material properties. The designer must be, in advance, aware of properties of different steels, so that he can decide which of the steels is the best for manufacturing the certain part or a structure. One of the methods for predicting some material properties of the two stainless steels is presented in this paper. The method is based on application of the artificial intelligence, precisely the artificial neural networks.

Artificial Neural Networks (ANN) are created from artificial neural cells (artificial neurons), which are modelled based on the principle of functioning of the biological neural cells (bio-neurons). Interpretation of the bio-neuron's working principle is the following: all the signals received on dendrites are summed in the neuron's body. If a sum of all the signal values exceeds the critical value, the signal is sent through axon to further layers and cells. Similar is the interpretation of working principle of artificial neurons. The difference between the two is that in the case of artificial cells, numbers values are used instead of signals. The artificial neuron's working principle is as follows: if the value of number received from other cells, multiplied by value of a weight coefficient, and added to a bias value, exceeds some critical value, the transfer function is activated and it sends the obtained value to the next layer.

It is of a great importance to emphasize that the artificial neural network's ability to predict some value is based on its training. The training of ANN means that adequate set of data is supplied to the network. Each data set has two parts, input and output. For each input there is a known output. Based on that, the ANN arranges weight and bias values so that the input data, after summing and multiplying through ANN, gives already known output. The smaller the difference (the error) between the known output and calculated output, the better is the ANN, i.e., the better it is constructed, (Lisjak, 2004).

Application of the ANNs covers a wide spectrum of areas (Qamar and Ali Zardari, 2023), such as medicine (Basheer and Hajmeer, 2000), text recognition and classification (Kim, 2023), railway transport (Bursać et al., 2022), geology (Varenina et al., 2018), solid mechanics (Sorić, Stanić and Lešičar, 2023), material types (Ciocan et al., 2000), material composition and microstructure (Kusiak and Kuziak, 2002), prediction of mechanical behavior of metal matrix composites

(Mukherjee et al., 1995), mechanical properties of steels (Dobrzanski and Sitek, 1999; Knap et al., 2008; Knap et al., 2014), influence of alloying elements on steel properties (Sitek et al., 2022), modelling of high-speed steels' properties (Sitek et al., 2004), etc.

2. Literature review

Qamar and Ali Zardari (Qamar and Ali Zardari, 2023) have recently summarized all the basic data on artificial neural networks, explaining the ANN's basics, the fundamental neuron and the artificial computer model. They described the network's 3-layer structure (input layer, hidden layer and output layer), and network learning and training methods. They emphasized the basic advantages of the ANN applications, adaptive learning, self-organization, real-time operation and the fault tolerance.

(Sorić et al., 2023) presented a review of machine learning methods employing the neural network algorithm, and discussed the most commonly used neural networks, such as feedforward NN, including deep learning, the convolutional NN, the recurrent NN, and the physics-informed NN, with special emphasis on their applications in solid mechanics. Based on application of ANNs on two simple examples authors concluded that the NN approaches show lower computational costs, as compared to the finite element method (FEM), simultaneously preserving the high accuracy of computing.

(Ciocan et al., 2000) have considered the recognition of different types of austenitic steels with an ultrasonic system that provided the necessary data for the two different neural networks. The input vector for the first ANN contained processed data (propagation velocity and ultrasonic attenuation), while for the second ANN it contained the amplitude of digitized radio-frequency signal and its numerical Fourier transform. Two thirds of acquired data for three kinds of steels were used in the learning process, while the last third was used in the testing process. Both neural networks gave similar results on input data, above 98% of steels classification probability.

(Kusiak and Kuziak, 2020) presented research of applying the ANN for predicting the volume fraction and mean size of the phase constituents in a steel subjected to the thermomechanical processing and cooling. The network was trained on the data obtained in the laboratory tests, and next validated using the data from the industrial measurements. Authors presented results which show that the prediction of the microstructure and mechanical properties of the considered steel is in a good agreement with the experimental data. They claimed that the ANN based model could predict, with good accuracy, such microstructural features as the ferrite grain size, ferrite fraction, as well as the steel's yield stress and ultimate tensile strength. The accuracy of values evaluated by the ANN model was much higher than that obtained from calculations using the classical, experimental models.

(Sitek et al., 2004) were modelling the relationship between the chemical composition and hardenability of structural alloy steels, using the artificial neural network and multiple regres-

sion models, and using large set of experimental data containing required information on the chemical compositions and corresponding Jominy hardenability curves for over 400 data steel sheets with variety of chemical compositions. Authors demonstrated the full practical usefulness of the developed model in selection of materials for particular applications with intended performance in the area of application. They also concluded that the developed ANN model can be used for simulations of the relationship between hardness at a given distance from the Jominy bar specimen face and the chemical composition of the steel, as well.

(Knap et al., 2008) were studying the possibility to predict the hardness profile – hardenability of the constructional steel, based on its chemical composition, using the ANN model. The database consisted of hardness profile measurements from the Jominy test samples and it contained almost twenty thousand data vectors, with extensive range of steels chemical compositions. The authors reported that, in spite of the great variations of the chemical compositions of each steel grade and the data base itself, the ANN made very accurate predictions of each steel’s hardenability.

In continuation of their research, (Knap et al., 2014) presented an attempt to model the effect of differences in chemical composition on material hardenability within one steel grade. They used very broad and heterogeneous database. They concluded that, if the database is big enough, predictions of hardenability would be accurate and of high quality. However, for a less comprehensive database there appeared differences in hardness predictions for various chemical compositions of the considered steel grade.

Application of artificial neural network has been proven to be reliable for use in diagnostics of various technical systems (Menasri and Aimeur, 2023).

3. Prediction of stainless steels mechanical properties using ANN

3.1. Input and output data preparation

Four properties, the yield stress, tensile strength, elongation and hardness, of the two stainless steels, X5CrNi18-10 (AISI 304), X5CrNiMo17-12-2 (AISI 316), were predicted using ANN. Input and output data for training of the artificial neurons were created using the Cambridge Education Software Edu Pack 2010 (CES EDU PACK 2010). As four properties were investigated, four input and four output data sets were needed. In all the four cases, properties were predicted based on chemical composition of 57 other stainless steels available in the used software, so the input set of data in all four cases was common. The four output sets consisted of values of each investigated property for those 57 other stainless steels. The complete process of properties prediction was conducted in MathWorks Matlab software using its Neural Network Module.

For the prepared data, four neural networks with three layers were prepared. The first (input) layer consisted of 18 neurons, each representing one element from the steel’s chemical composition. The second layer had 10 neurons. This value was

software default number of neurons for the second layer and it could be changed. However, for these purposes adequate precision was obtained, thus this number has not been changed. Number of neurons in the third (output) layer is equal to number of properties predicted by neural network. In all the cases that number was one, as only one property’s values were predicted.

Table 1. Chemical composition of the X5CrNi18-10 steel, wt%

1	2	3	4	5	6	7	8	9
C	Cr	Mn	Ni	N	P	Si	S	Fe
0.08	19.0	0	9.0	0.10	0.04	0.7	0.02	Bal.

Table 2. Chemical composition of the X5CrNiMo17-12-2 steel, wt %

1	2	3	4	5	6	7	8	9
C	Cr	Mn	Ni	N	P	Si	S	Fe
0.025	19.5	1.98	11.4	8.0	0.037	0.72	0.02	Bal.

Note: since the first layer has 18 neurons and the chemical composition contains 9 elements, the neurons 10 to 18 have been assigned the value of 0

3.2. Prediction of the yield stress values of austenitic stainless steels

The neural network was created according to previously explained construction, three layers, 18 neurons in the input layer, 10 neurons in the hidden layer and 1 neuron in the output layer – for the yield stress value. The activation function between the layers was chosen to be the same for activation between the first and the second layer, as well as for activation between the second and the third layer, the tan sigmoid tan function. The Bayesian Regularization algorithm was chosen as the training algorithm. Structure of this network is shown in Figure 1, where W is notation for the weight coefficient and b for the bias value.

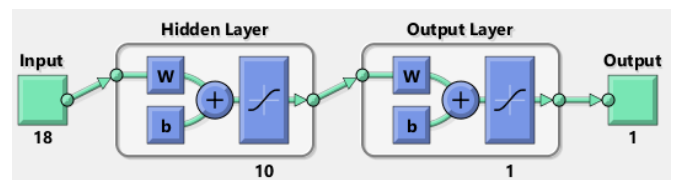


Fig. 1. Structure of the neural network for predicting the yield stress values

The created network was trained using parameters given in Table 3. Application of given parameters resulted with following regression displayed in Figure 2. Entering the chemical composition values of steels X5CrNi18-10 and X5CrNiMo17-12-2, predicted values of the yield stress, shown in Table 4 were obtained.

Table 3. Values of parameters used for network training

Parameter	Value
Maximum number of epochs	1000
Time	Infinite
Goal	0
Min gradient	0.0000001

Maximum number of fails	0
Initial momentum value	0.005
Incline momentum	0.1
Decline momentum	10
Maximum momentum value	10000000000

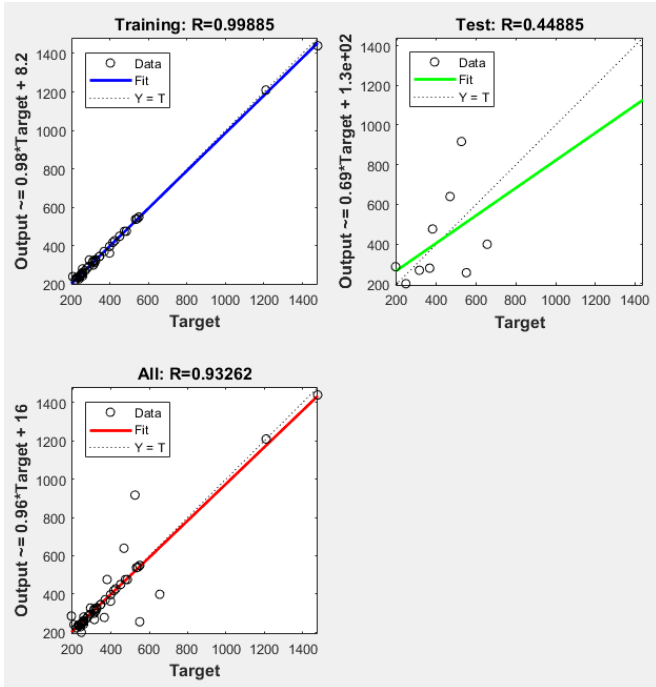


Fig. 2. Display of obtained regression values $r = 0.933$

The predicted values of the yield stress are graphically displayed in Figure 3. For the X5CrNi18-10 steel obtained value for the yield stress is 247.57 MPa, which is 10.43 MPa smaller than the experimental value (found in the CES software). As for the steel X5CrNiMo17-12-2, the predicted value of the yield stress is for almost 12 MPa smaller. Regarding the error percentage, for the first steel it is 4% , and for the second it is somewhat bigger, little below 5% Figure 4. Since the error values are lower than 5% for both steels, it could be concluded that the results predicted by the ANN are close to the real values. Thus, the constructed ANN provided for the reliable results and it could be used for predicting the yield stress values of other austenitic stainless steels.

Table 4. Predicted values of the yield stress, MPa

Steel	X5CrNi18-10	X5CrNiMo17-12-2
CES EDU PACK	258	240
ANN	247.5739	228.3207

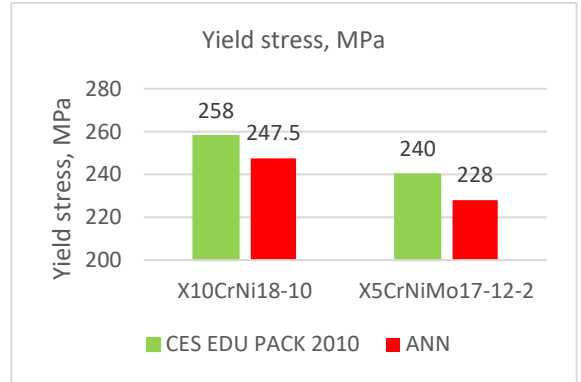


Fig. 3. Graphical display of predicted yield stress values

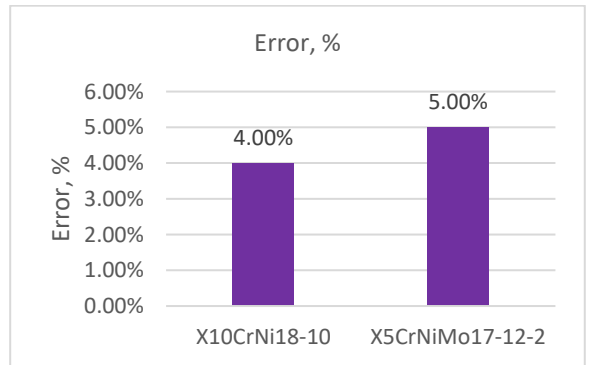


Fig. 4. Error values for the yield stress values prediction

3.3. Prediction of the tensile strength values of austenitic stainless steels

A special neural network was constructed for the tensile strength values predicting. The input data set was the same as for the case of yield stress prediction. The output data set was prepared from the tensile strength values for other stainless steels available in the CES software.

The neural network structure was built from three layers, as in the previous case. The activation functions between the layers were selected differently, with respect to the previous case. The tan sigmoid function was chosen as the activation function between the first and the second layer, same as in the first network. The linear function was selected for activation between the second and the third layer. The Levenberg-Marquardt algorithm was selected as the training algorithm for this neural network, the structure of which is presented in Figure 5.

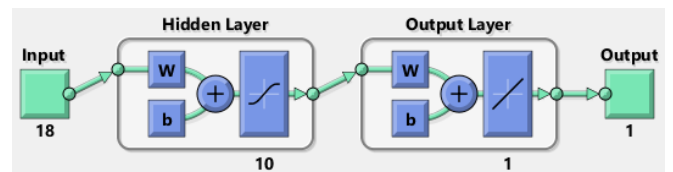


Fig. 5. Structure of the neural network for predicting the tensile strength values

Created network was trained using parameters given in Table 5. Application of given parameters resulted in the regression presented in Figure 6. The values of the tensile strength for the two considered steels were predicted by entering chemical composition values for steels X5CrNi18-10 and X5CrNiMo17-12-2 and using values of tensile strength from the CES EDU PACK 2010 software. Results are shown in Table 6.

Table 5. Values of parameters used for network training

Parameter	Value
Maximum number of epochs	1000
Time	Infinite
Goal	0
Min gradient	0.0000001
Maximum number of fails	6
Initial momentum value	0.001
Incline momentum	0.1
Decline momentum	10
Maximum momentum value	10000000000

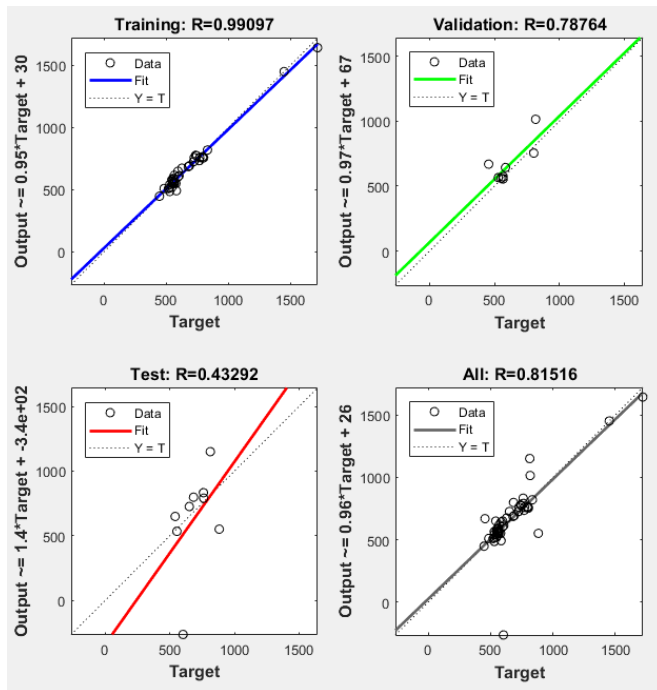


Fig. 6. Display of obtained regression values $r = 0.815$

Tensile strength values from the CES software and values predicted by the ANN are shown in Figure 7. For the X5CrNi18-10 steel the predicted value for tensile strength is 549.7284 MPa, which is almost 17 MPa smaller than the value obtained by experiment.

Table 6. Predicted values of the tensile strength, MPa

Steel	X5CrNi18-10	X5CrNiMo17-12-2
CES EDU PACK	565	570
ANN	549.7284	571.825

On the other hand, the predicted value for the steel X5CrNiMo17-12-2 is 571.825 MPa, which is almost 2 MPa

bigger than the experimentally obtained value. Regarding the error percentage of the predicted values, for the first steel it was little below 3% and for the second steel it was approximately 0.3%, Figure 8. Since in this case the error values are practically negligible, it can be concluded that this ANN is suitable for predicting the values of tensile strength for other austenitic stainless steels, as well.

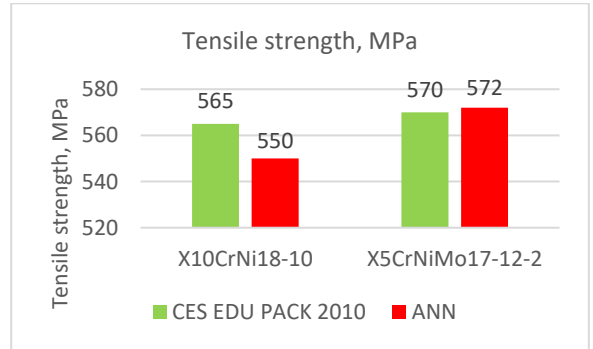


Fig. 7. Graphical display of predicted tensile strength values

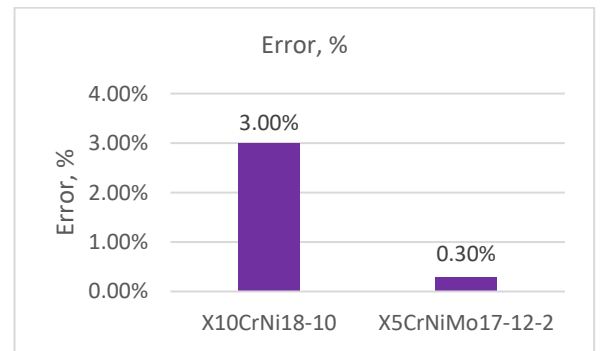


Fig. 8. Error values for prediction of the tensile strength values

3.4. Prediction of the elongation values of austenitic stainless steels

The neural network for predicting the elongation values of stainless steels was created in a similar manner as for the first two cases: three layers with 18, 10 and 1 neurons, respectively. The input data set, as mentioned, is the same in all the cases. The output data set is prepared from elongation values for other stainless steels from the CES software. The network structure, regarding the activation functions between the layers, is the same as for the case of predicting the yield stress values, in both cases the activation function is tan sigmoid function, Figure 1. The difference with respect to that case is that the training algorithm is selected to be the Levenberg-Marquardt algorithm.

The created network was trained using parameters given in Table 7. Application of given parameters resulted with the regression values displayed in Figure 9. After entering the chemical composition values for steels X5CrNi18-10 and X5CrNi17-12-2 in the neural network, elongation values were obtained, which are given in Table 8.

Table 7. Values of parameters used for network training

Parameters	Value
Maximum number of epochs	1000
Time	Infinite
Goal	25
Min gradient	0.0000001
Maximum number of fails	6
Initial momentum value	0.01
Incline momentum	6
Decline momentum	6
Maximum momentum value	10000000

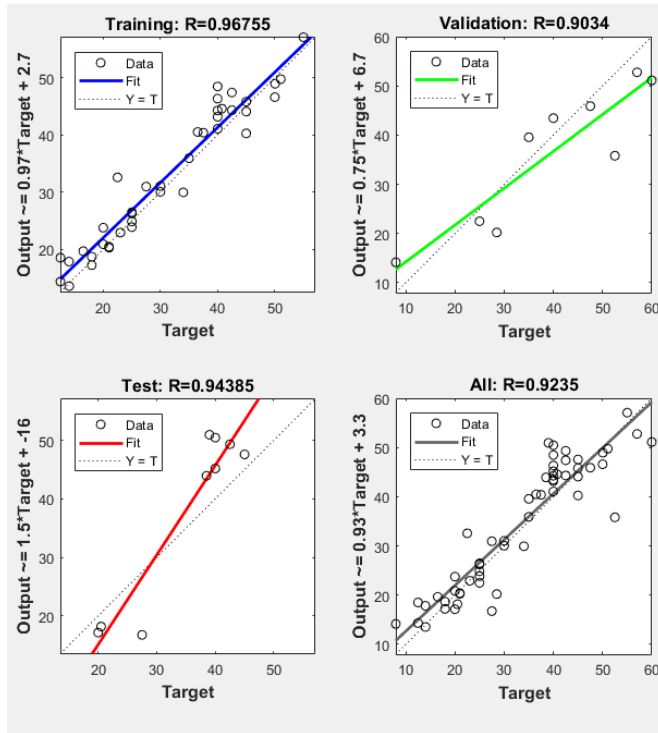


Fig. 9. Display of obtained regression values $r = 0.923$

Table 8. Predicted values of elongation, %

Steel	X5CrNi18-10	X5CrNiMo17-12-2
CES EDU PACK	52.5	40
ANN	47.9	42.1652

Graphical presentation of the predicted elongation values of the two stainless steels is shown in Figure 10. The predicted elongation value for steel X5CrNi18-10 is 47.9%, which is almost 4.6% smaller than the value obtained by experiment. For the steel X5CrNiMo17-12-2, the predicted elongation value is 42.17% and it is 2.17% bigger than the experimentally obtained value. The error value for the first steel is little below 10% (9.6%) and for the second steel it is 5%. Since the values predicted by this ANN have errors between 5% and 10%, it could be concluded that the predicted values are slightly off with respect to values obtained by experiments. Results obtained by this ANN need to be further investigated. The obtained error values are displayed in Figure 11.

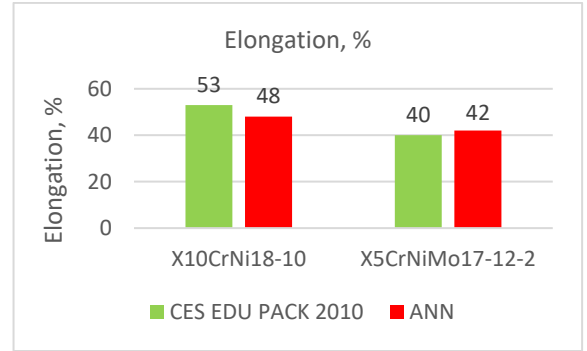


Fig. 10. Graphical display of predicted elongation values

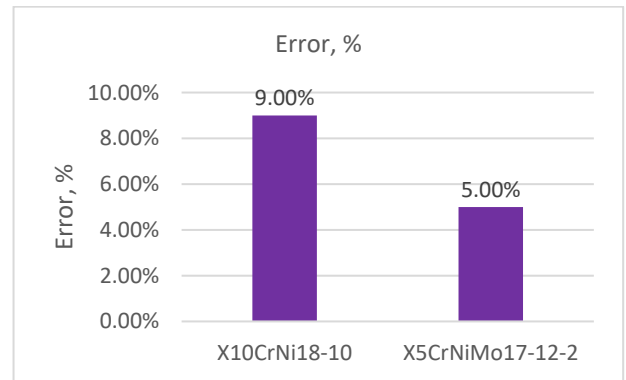


Fig. 11. Error values for elongation values prediction

3.5. Predicting the hardness values of austenitic stainless steels

The neural network for predicting the hardness values of stainless steels was created in the same way as in the previous cases, with the same set of input data and the output data set prepared from hardness values for other stainless steels from the CES software.

The neural network structure was the same as in the previous cases. Activation functions between layers were selected in the same way as in the case of predicting the tensile strength values, Figure 5. Between the first and the second layer the activation function was the tan sigmoid function, while between the second and the third layer the activation function was a linear function. The training algorithm for this case was the Bayesian Regularization algorithm.

The created network was trained using parameters given in Table 9.

Table 9. Values of parameters used for network training

Parameters	Value
Maximum number of epochs	1000
Time	Infinite
Goal	100
Min gradient	0.000001
Maximum number of fails	0
Initial momentum value	0.1
Incline momentum	10
Decline momentum	10
Maximum momentum value	1000000000

Application of given parameters resulted in the regression values displayed in Figure 12. Entering the chemical composition values for steels X5CrNi18-10 and X5CrNi17-12-2 in the neural network, hardness values were predicted for these two stainless steels that are presented in Table 10.

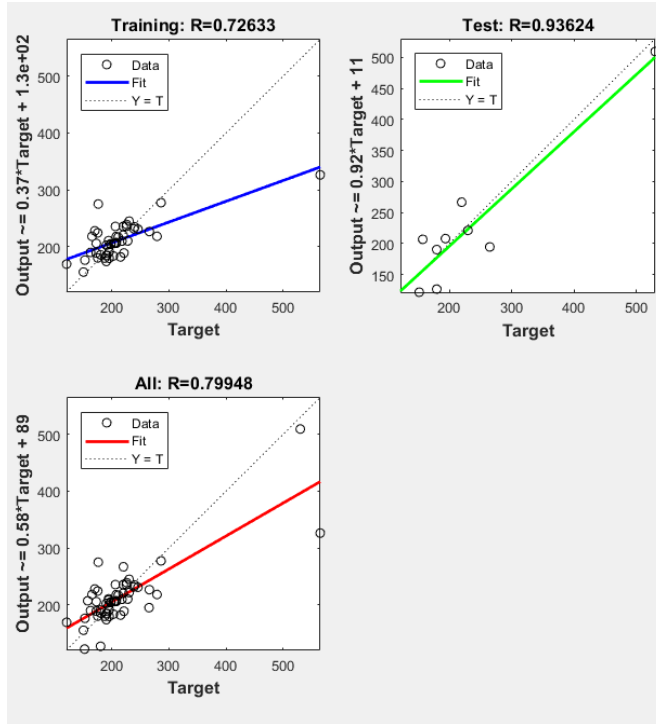


Fig. 12. Display of obtained regression values $r = 0.799$

Table 10. Predicted values of hardness, HV

Steel	X5CrNi18-10	X5CrNiMo17-12-2
CES EDU PACK	190	205
ANN	195.529	195.234

The predicted hardness values are shown in Figure 13. For steel X5CrNi18-10 the predicted value is 195.529 HV, which is for 5.529 HV bigger than the experimental value. As for the steel X5CrNiMo17-12-2, the predicted hardness value is 195.234 HV, which is for 9.76 HV smaller than the experimentally obtained value. Error value for the first steel is 3% and for the second steel it is somewhat below 5% (4.76%), Figure 14. Both error values are lower than 5%. Thus, it could be concluded that this ANN is suitable for predicting the hardness values of austenitic stainless steels.

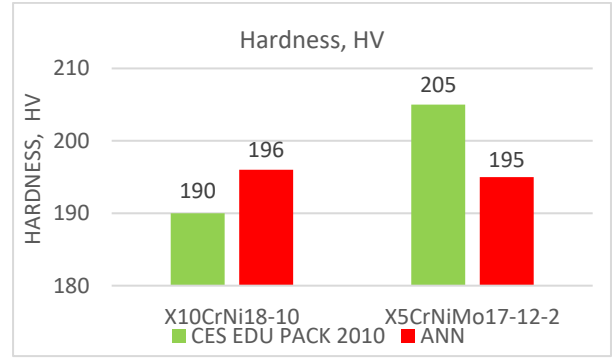


Fig. 13. Graphical display of predicted hardness values

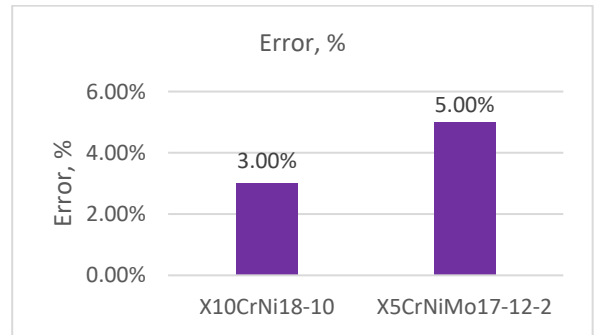


Fig. 14. Error values for hardness values prediction

4. Conclusions

Stainless steels were discovered in 1913 with idea to overcome one of the greatest disadvantages of structural steels – corrosion. It was found that addition of minimum 12% of chromium to steels solid solution enables steel to become corrosion resistant. Besides Cr, other alloying elements could be found in various steels chemical composition (Ni, Mo, V etc.).

One of the artificial intelligence methods for replicating human thinking process are the Artificial Neural Networks (ANN). They are made of multiple artificial neuron cells, which are connected in layers. The most frequent application of the ANN is for prediction of values based on known input values.

The topic of this paper was to investigate if the ANN could predict four mechanical properties (yield stress, tensile strength, elongation and hardness) of austenitic stainless steels, with sufficient accuracy. The data sets for the ANNs were created from *CES EDU PACK* software, in which information about various steels could be found. The input data set (with 18 neurons) consisted of chemical composition of considered steels and the output data sets (with 1 neuron for each network) were the investigated properties of those steels. The hidden layer consisted of 10 neurons, which was the default property of the used software and it was not changed since it provided for sufficient precision of the network(s).

After the data sets were prepared, the four neural networks were created and trained. Two stainless steels X5CrNi18-10 (AISI 304) and X5CrNiMo17-12-2 (AISI316) were used to validate results obtained from the ANNs. Based on obtained

results it can be concluded that for all properties obtained results were close to previously known experimentally obtained values, where the error for predicted values of considered properties were under 5% and in some cases negligible.

The slight exception was the result for elongation where the error values were between 5 and 10%, which are also low, but they cannot be ignored. If one would use this ANN to predict elongation of unknown steel it would be necessary to confirm results experimentally. This problem should be further investigated. Adding other input parameters besides the chemical composition of considered steels, would probably increase the precision of predicted values. As for the other ANNs, one could state that they are able to predict mechanical properties, with great precision, as the error values are low. Certainly, precision would increase if the number input variable types is increased.

Acknowledgements

Research presented in this paper was partially financially supported by the project of Operational Programme Integrated Infrastructure "Support of research and development capacities to generate advanced software tools designed to increase the resilience of economic entities against excessive volatility of the energy commodity market", ITMS2014+ code 313011BUK9, co-funded by European Regional Development Fund, and by the project TR35024 of the Ministry of Education, Science and Technological Development of Republic of Serbia.

Note: The shorter version of this research results was presented at the SEMDOK 2024 conference (reference Ivković et al., 2024).

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