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Application of artificial neural networks in modelling of normalised structural steels mechanical properties

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Analysis and modelling

ABSTRACT

Purpose: This paper presents the application of artificial neural networks for mechanical properties prediction of structural steels after heat treatment.
Design/methodology/approach: On the basis of such input parameteres, which are the chemical composition, type of heat and plastic treatment and geometrical dimensions of elements, mechanical properties, such as strength, impact resistance or hardness are predicted.
Findings: Results obtained in the given ranges of input parameters show very good ability of constructed neural networks to predict described mechanical properties for steels after heat treatment. The uniform distribution of descriptive vectors in all, training, validation and testing sets, indicate about the good ability of the networks to results generalisation.
Practical implications: Created tool makes possible the easy modelling of described properties and allows the better selection of both chemical composition and the processing parameters of investigated materials. At the same time the obtainment of steels, which are qualitatively better, cheaper and more optimised under customers needs is made possible.
Originality/value: The prediction possibility of the material mechanical properties is valuable for manufacturers and constructors. It allows preserving the customers quality requirements and brings also measurable financial advantages.
Keywords: Artificial intelligence methods; Computational material science and mechanics; Artificial neural networks; Mechanical properties

1. Introduction

From the beginnings of the computer usage in material engineering, effective simulating methods for prediction of engineer materials usable parameters were searched. Computer simulations became more effective and they started to assist in experiments or manufacturing. The prediction possibility of the material mechanical properties is valuable for manufacturers and constructors. It allows preserving the customers' quality requirements. Prediction of mechanical properties brings also measurable financial advantages, because expensive and time-consuming investigations are reduced to the indispensable minimum. Necessaries to execute are only to the investigations made for verification of computed results [1-2].

That is why, since many years' investigative centres make intensive investigations over mathematical models developing

methodology. Such models should enable the qualification of mechanical properties such as strength, impact resistance or hardness for numerous engineer materials (with various chemical composition and after heat and plastic treatment conducted with various parameters). Suitable tool, which allows the easy modelling of such properties will make possible the better selection both chemical composition and the parameters of the material processing. It makes possible at the same time the obtainment of steels, which are qualitatively better, cheaper and more optimised under customers needs [3-7].

The prediction of steels mechanical parameters after normalisation process is not an easy process at all. The determination of the chemical composition influence is particularly difficult, especially in the case of rolled sheet metal plates [8]. Because of the fact that there is no physical models allowing to connect the influence of the chemical compositions and the parameters of the mechanical and heat treatment on properties of manufactured steels, existing models are mainly based on the statistical analysis and have limited range of use. They are the most often prepared to describe one single steel species manufactured in equal conditions [7,16-18].

Application of artificial neural networks is considerably simplifies the modelling methodology. There is no need to posses the function of input and output parameters in evident form. If only such a function exists it will be established through the network during the training process and it will be written down as weights individual neurons. However it is important that this function exists and has the regular and unique character.

In most cases the failure of neural network creation is caused by the lack of the assignment function (output parameters are independent from input parameters) or the function is strong deformed by the noise, presented in descriptive vectors [9-12].

2. Investigated material

Structural non-alloy and alloy steels were chosen for investigations. They are used in manufacturing of steel constructions and devices and machines elements of the typical destination.

Structural steels are the most often species produced in polish metallurgy. They are delivered to the customer as semi-manufactured articles or ready articles in the form of long, round or squared bars, or (rarely) as sections, sheet metals and pipes.

Structural steels delivered as semi-manufactured articles are manufactured as normalised, they reach customers after the normalising rolling or without any thermal processing (directly after the hot rolling).

As ready products steels are delivered after heat treatment, manufactured according to conditions required by a customer or polish standards.

Mechanical properties of over 125 various structural non-alloy and alloy steel species were examined. Examples of those species are showed in table 1.

Examined material was delivered in a form of round and square rods. Steels were manufactured as normalised with various processing parameters. Ranges of chemical elements, temperatures, duration times, kinds of cooling mediums for normalisation treatment and geometrical parameters of manufactured elements are presented in table 2.

Table. 1.
Examples of steels selected for examination.

Non-alloy steels			Alloy steels			
Steel for general purposes [22]	**Steels for toughening [23]**	**Steels for pressure devices [24]**	**Steels for toughening [25]**	**Spring steels [26]**	**Steels for nitrogenising [27]**	**Steels for carburetting [28]**
E295	C22	P235T2	17CrNiMo6	52CrMoV4	31CrMo12	16MnCr5
E335	C30	P255G1	24CrMo4	45SiCrV6-2	31CrMoV9	16CrMo4-4
E360	C45R	P265GH	30CrNiMo8	51CrV4	33CrAlMo7-10	17Cr3
S235J2G3	C60E	P355N	36CrNiMo4	54SiCr6	34CrAlNi7	18NiCr5-4
S275JR	20Mn5	P355NL1	41Cr4	55Cr3	40NiCr6	20MnCr5
S355K2G2	28Mn6	P360N	50CrMo4	60Cr3	41CrAlMo7	20NiCrMo2-2

Table. 2.
Ranges of chemical elements, temperatures, times, kinds of cooling mediums for heat treatment and geometrical parameters of examined steels.

range	**size**	**shape**	**Chemical composition [%]**													**Mechanical treatment**
	[mm]		C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al	
min	30	- round	0.09	0.25	0.16	0	0	0	0	0	0	0	0	0	0	- rolling
max	220	- square	0.60	1.57	1.20	0.3	0.28	2.20	2.08	1.10	0.12	0.26	0.15	0.35	1.02	- forging

range	**Normalising**		
	Temperature [°C]	Time [min]	Cooling medium
min	180	30	-air
max	980	480	

3. Artificial neural networks

The name "artificial neural networks" describes the hardware or software simulators, which are realizing semiparallel data processing. They are built from many mutually joined neurons and they imitate the work of biological brain structures [15].

McCulloch and Pitts worked out the scheme of the neuron in 1943 and it was created as a building imitation of the biological nervous cell [11,12].

Input signals x_i coming from external receptors (for the input layer) or from the previous neurons layer (for hidden layers and exit layer) are attached to the network inputs. Every signal is multiplicated by numerical value w_i, which is interpreted as weight of the given neuron, ascribed to the neuron. This value has the influence in creation of the output value. The value of the weight can stimulate the neuron to operate, when its sign is positive, or can also hold on the neuron inactive , when the sign is negative. The sum of entrance signals multiplied through appropriate weights is the argument of the neuron's activation function φ. The value of this function is the output signal of the neuron y and is propagated to the neurons of the next layer or on the output of the network (for the neurons of the output layer).

The diagram representing the structure of single neuron is presented in Figure 1.

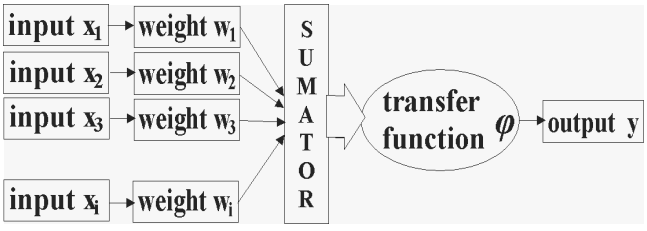


Fig. 1. The model of artificial neuron by [11,12]

Equation 1 describes the mathematical model, where *m* is a number of input signals of a single neuron

$$y = \varphi\left(\sum_{i=1}^{m} w_i x_i\right) \quad (1)$$

The fundamental difference between artificial neural networks and other analytical algorithms, which are realizing the data processing is the ability to generalise the knowledge for new given data, which were unknown earlier and which were not presented during the training process.

In distinction from expert systems, which require the permanent access to whole assembly of knowledge on the subject about which they will decide, artificial neural networks requiring only single access to this data set in the process of training.

Neural networks reveal the tolerance on discontinuities, accidental disorders or lacks of data in the descriptive vectors. This allows to use the networks for problems, that cannot be solved by any other algorithm or their implementation will not give any satisfactory results [10,12,15].

A creation of a model with utilisation of artificial neural networks is indicated where the precise physical and mathematical description of the considered phenomenon is not known and where input and output values in descriptive vectors are well determined, however its entries and exit are well qualified. An artificial neural network is able to learn how to recognise the analysed problem and quickly give the answer on the changing input parameters of the given problem [18, 19].

4. Modelling methodology

For property simulation of structural steels, the data set, consisting of over 14212 vectors was used. This data describes structural steels produced in the „Batory" foundry in Chorzów, Poland [20] after casting, mechanical and heat treatment. The intelligent processing of data was applied with the use of artificial neural networks for prediction of mechanical properties of steel materials. For every studied mechanical property the separate neural network was created.

Predicted mechanical parameters were: [1-3,7,13,14,16]

- yield stress R_e,
- tensile strength R_m,
- relative elongation A_5,
- relative area reduction Z,
- impact strength KV,
- Brinell hardness HB.

Input values, which are used for parameter prediction are:

- chemical composition,
- type of mechanical treatment,
- normalisation parameters (temperature, time and cooling medium),
- element shape and size.

The ranges of chemical elements, temperatures, times, kinds of cooling mediums for normalisation processes and geometrical parameters are presented in Table 2.

The set of all descriptive vectors was divided into three subsets in the relation 2-1-1. The first set contains the half of all vectors and was used for the modification of the neuron weights (training set). One fourth of the vectors were used for valuation of prediction errors by training process (validation set). Remaining vectors were used for the independent determination of prediction correctness, when the training process is finished (testing set).

Networks were trained with use of the back propagation and conjugate gradient methods. [10,12,15]

For the verification of networks usability for the aims of parameters prediction the following parameters of the quality valuation were used:

- average absolute error – difference between measured and predicted output values of the output variable,
- standard deviation ratio – a measure of the dispersion of the predicted values from their expected (mean) value. It is the most common measure of statistical dispersion, measuring how widely the values in a data set are spread,
- Pearson correlation – the standard Pearson-R correlation coefficient between measured and predicted output values of the output variable.

The kind of the problem was determined as the standard, in which every vector is independent from another vector. The assignment of vectors to training, validation or testing set was random. The search for the optimal network was restricted to architectures such as [6,9,10,18]:

- linear networks
- radial basis function network (RBF)
- generalized regression neural network (GRNN)
- multi-layer perceptron (MLP)

All computations were made by the use of Statistica Neural Network by Statsoft, the most technologically advanced and best performing neural networks application on the market. It offers numerous selections of network types and training algorithms and is useful not only for neural network experts. [21].

5. Modelling results

At the beginning only one multi-output network was trained for estimation of all parameters simultaneously, but the prediction quality was not satisfactory.

In order to improve results, all vectors were divided on two sets: the first one containing all vectors, which describes steels after normalisation and forging processes and the second - containing vectors coming from normalised and rolled steels. Then, another two multi-output networks were trained. Results were better, but still not satisfactory.

That is why it was decided to create separate network for every parameter, whose value has to be predicted. The best results were obtained for the multi-layer perceptron architecture with one and two hidden layers. The types of the net for individual properties among with the numbers of used neurons and the parameters of the quality valuation for all three sets for normalised and forged steels are introduced in the table 3. The parameters for steels after normalisation and rolling processes are in table 4.

For all trained networks the Pearson correlation coefficient has reached the value above 90% and comparatively low values of the standard deviation ratio. This is the very good representation of estimated properties. On special attention deserving two networks for yield stress (R_e) and strength stress (R_m) prediction. Correlation coefficient values over 98% and standard deviation ratio lower then 0,2 indicates very good regression performance.

For a graphical representation of networks quality comparative graphs among values predicted and measured of testing set are shown on figures 2 and 3. For every estimated parameter the vectors distribution is comparable for all three subsets. It speaks for correctness of the prediction process. Significant differences in vectors distribution among groups would mark the possibility of excessive matching to training vectors, and the bad quality of the network.

Trained neural networks made possible the analysis execution of the influence of the input parameters on predicted mechanical properties. In peculiarity the influence of alloying elements change on mechanical properties with no change of heat treatment. Then, the influence of heat treatment parameters change on mechanical properties with no modification to steel chemical composition was computed.

To introduce the influence of chemical composition and processing parameters on estimated parameter surfaces graphs were prepared. It allows to show the analysis results in graphical style. Several of processed graphs are introduced as examples (Figs. 4-9).

Table. 3.
Parameters of computed neural networks for steels after normalisation and forging processes

Variable	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
Re	MLP 18:18-5-1:1	15.439	0.1911	0.9817	16.623	0.1918	0.9814	18.146	0.1889	0.9820
Rm	MLP 18:18-4-1:1	17.077	0.1953	0.9807	15.139	0.1983	0.9801	16.022	0.1940	0.9811
A5	MLP 14:14-6-1:1	1.397	0.3451	0.9388	1.257	0.3822	0.9242	1.324	0.3648	0.9313
Z	MLP 16:16-10-1:1	1.984	0.2909	0.9567	1.926	0.3064	0.9511	1.894	0.3021	0.9533
KV	MLP 14:14-9-1:1	14.594	0.2884	0.9581	14.161	0.3100	0.9553	14.624	0.3096	0.9513
HB	MLP 11:11-5-1:1	5.243	0.3209	0.9482	5.595	0.3367	0.9423	4.743	0.2965	0.9563

Table. 4.
Parameters of computed neural networks for steels after normalisation and rolling processes

Variable	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
Re	MLP 17:17-9-3-1:1	6.433	0.1880	0.9826	6.932	0.1978	0.9803	7.132	0.2005	0.9800
Rm	MLP 17:17-12-6:1	12.412	0.1871	0.9823	13.148	0.1938	0.9811	13.155	0.1855	0.9827
A5	MLP 13:13-4-1:1	1.130	0.3064	0.9519	1.108	0.2993	0.9542	1.191	0.3116	0.9503
Z	MLP 15:15-9-1:1	1.343	0.2921	0.9563	1.385	0.3089	0.9519	1.474	0.3396	0.9410
KV	MLP 16:16-11-1:1	11.505	0.3344	0.9424	11.646	0.3664	0.9307	12.164	0.3849	0.9234
HB	MLP 8:8-5-1:1	4.884	0.2790	0.9604	4.730	0.2878	0.9579	5.841	0.3320	0.9441

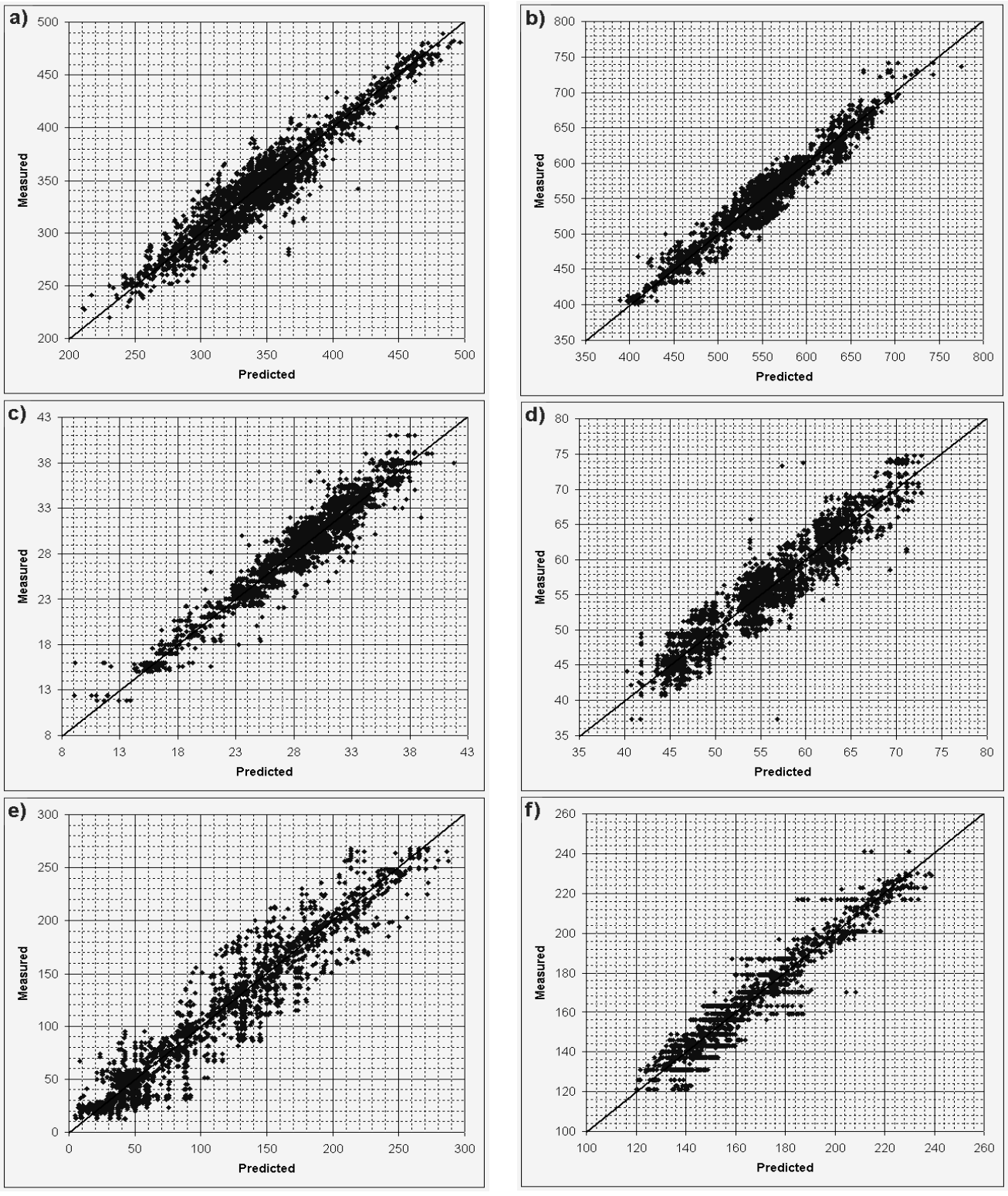
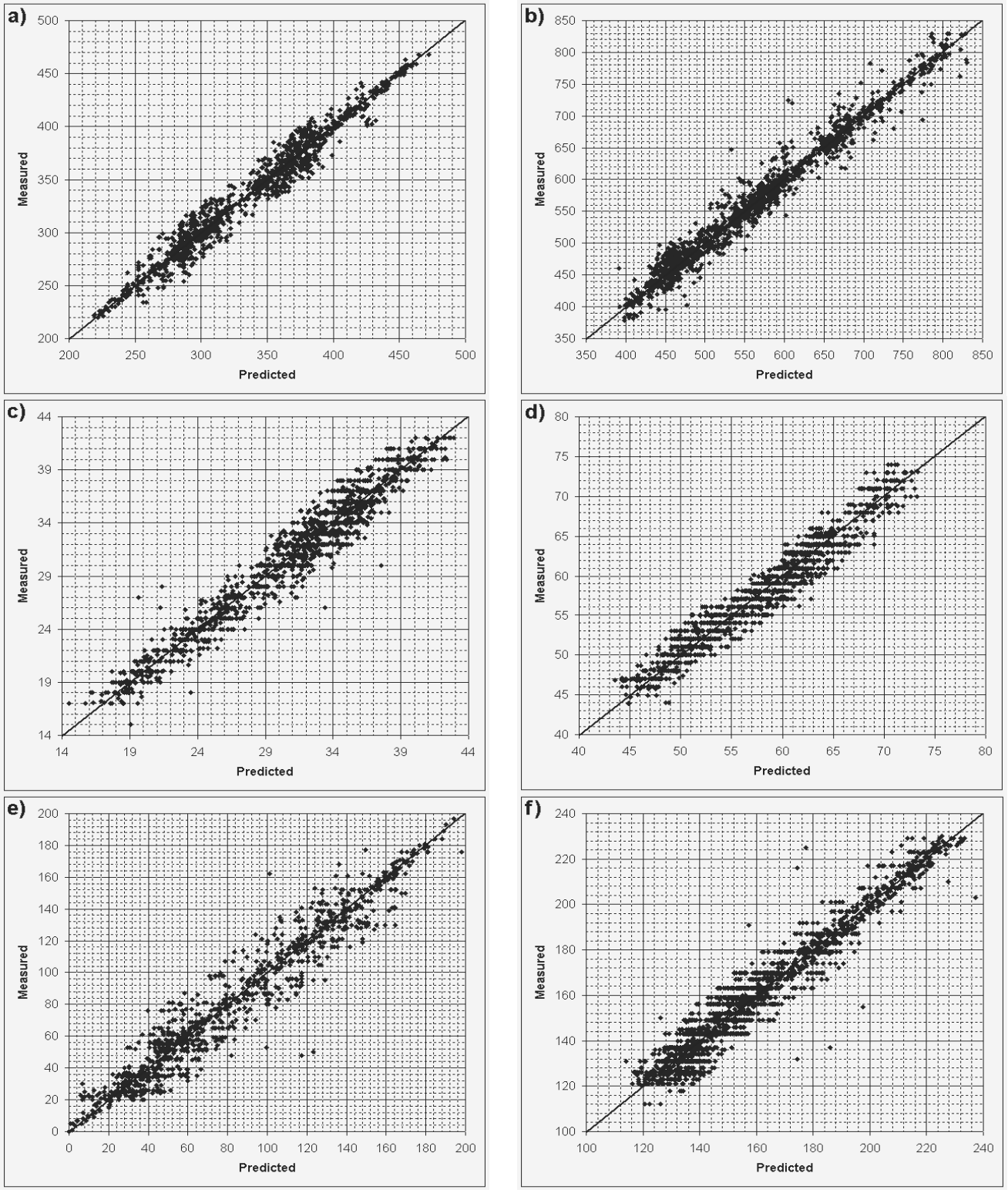


Fig. 2. Comparative graph of a) yield stress R_e, b) tensile strength R_m, c) relative elongation A_5, d) relative area reduction Z, e) impact strength KV, f) Brinell hardness HB, calculated with use of the neural networks (testing set) and determined experimentally for steels after normalisation and forging processes



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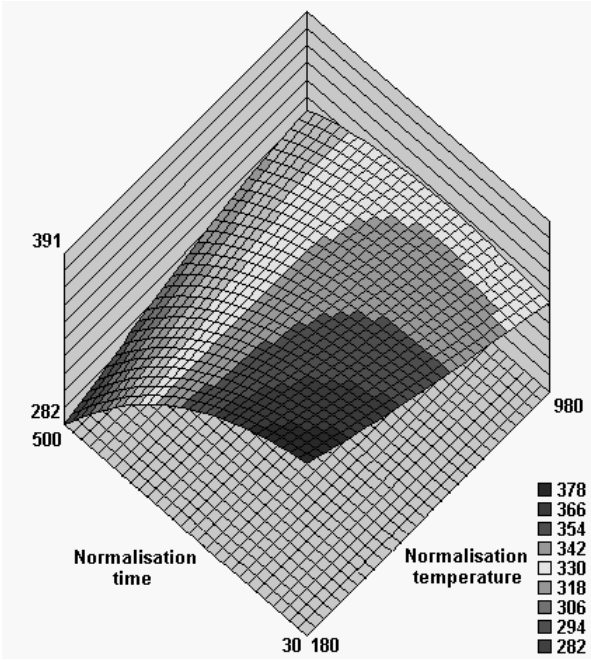

Fig. 4. Influence of normalisation temperature and time on yield stress. (shape: round, diameter: 135mm, 0.21%C, 0.74%Mn, 0.34%Si, 0.003%P, 0.002%S, 0.88%Cr, 0.34%Ni, 0.27%Mo, 0.12%Cu, 0,024%Al, rolling).

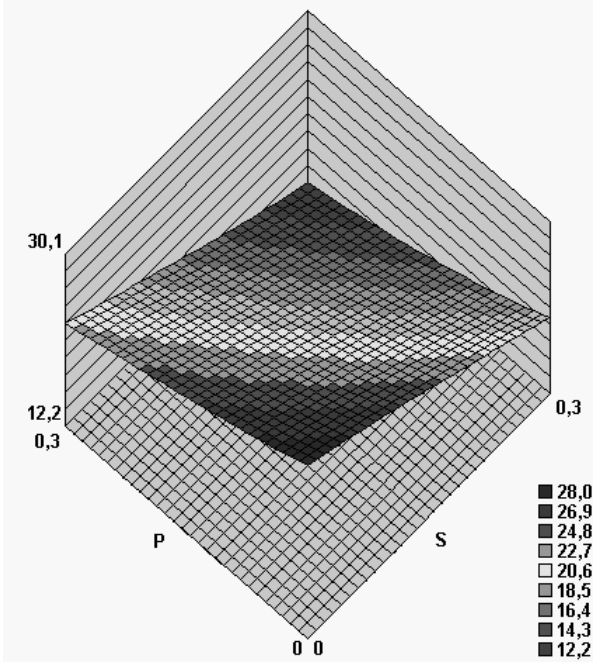

Fig. 6. Influence of sulphur and phosphorus concentration on relative elongation A_5 ,(shape: square, size:220mm, normalisation parameters: 980°C/180min/air, 0.13%C, 0.46%Mn, 0.22%Si, 0.34%Cr, 0.14%Ni, 0.52Mo, 0.23%V, 0.14%Cu, forging).

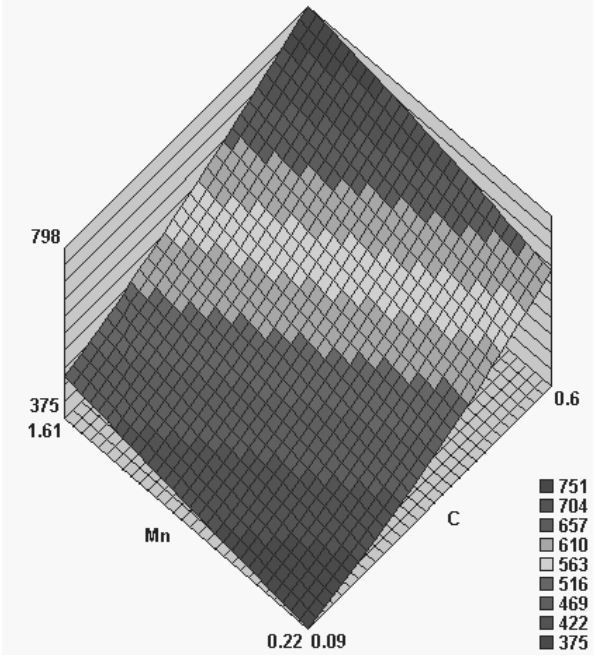

Fig. 5. Influence of carbon and manganese concentration on strength stress,(shape: round, diameter: 45mm, normalising parameters: 550°C/240min/air, 0.32%Si, 0.016%P, 0.005%S, 1.17%Cr, 1.05%Ni, 0.02%Mo, 0.001%V, 0.05%Al, forging).

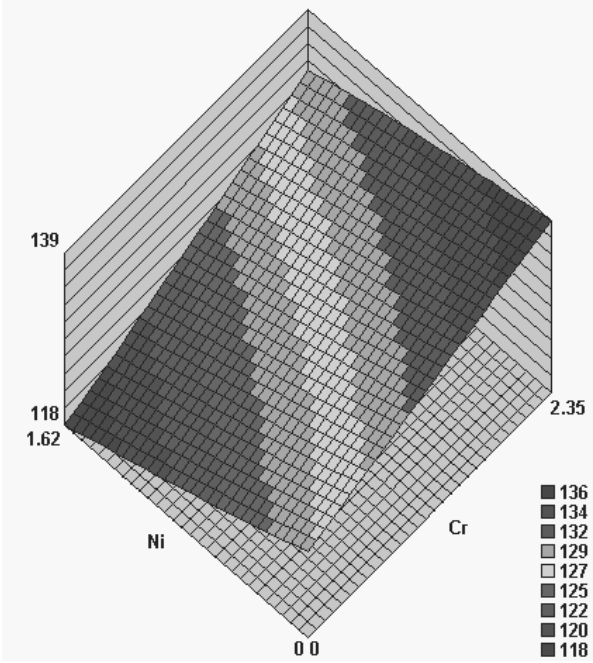

Fig. 7. Influence of nickel and chromium concentration on Brinell hardness, (normalisation parameters: 760°C/240min/air, 0.21%C, 0.56%Mn, 0.009%P, 0.021%S, 0.02%Mo, 0.03%Ti, 0.0035 Al, rolling).

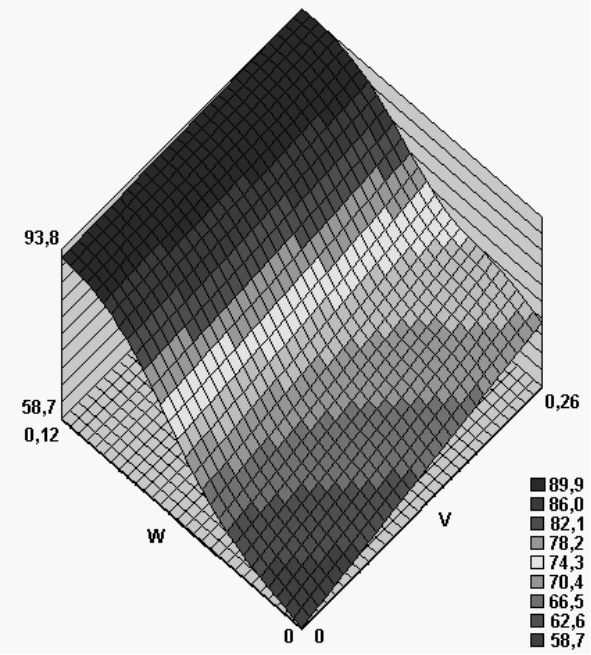

Fig. 8. Influence of tungsten and vanadium concentration on relative area reduction Z, (shape:round. diameter:35mm, normalisation parameters: 860°C/120min/air, 0.33%C, 0.91%Mn, 0.33%Si, 0.017%P, 0.009%S, 0.1%Cr, 0.06%Ni, 0.02%Mo, 0%Ti, 0.12%Cu, 0.02%Al, rolling)

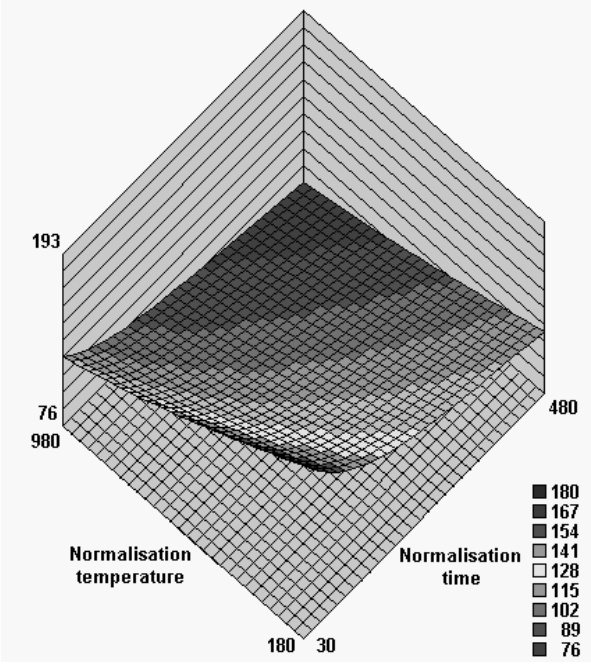

Fig. 9. Influence of normalisation temperature and time on impact resistance KV, (shape:square, size:160mm, 0.15%C, 0.56%Mn, 0.21%Si, 0.45%Cr, 0.08Ni, 0.52%Mo, 0.001%Ti, 0.027%Al, forging).

An example of neural nets, which are used to predict yield stress is presented on figure 10a. It is a four layer perceptron with 17 input values, 11 neurons in first hidden layer, 3 neurons in second hidden layer and one output value. Figure 10b shows the neural network used to predict impact resistance. It is a three-layer perceptron with 16 input values, 11 neurons in one hidden layer and one output value.

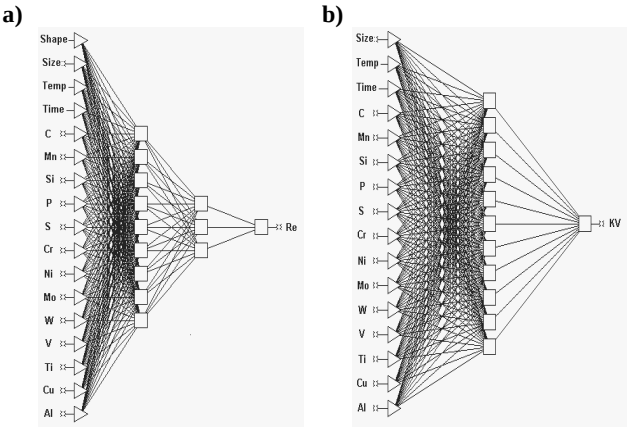

Fig. 10. Architectures of neural net used to predict mechanical parameters a) yield stress, four-layer perceptron 17:17-9-3-1:1, b) impact resistance , three-layer perceptron 16:16-11-1:1.

6. Conclusions

This paper introduces the property modelling methodology of structural steels after normalisation process. Parameters, which were determined through the use of artificial neural networks, are yield stress, tensile strength, relative elongation, relative area reduction, impact strength and Brinell hardness. The input values for prediction process were chemical composition, type and parameters of heat and plastic treatment and element shape and size.

Results obtained from the given ranges of input data show the very good ability of artificial neural networks to predict mechanical properties of normalised steels. The Pearson correlation coefficient over 90% and low deviation ratio inform about the correct execution of the training and obtained small differences in the relation between computed and experimentally measured values. The uniform distribution of vectors in every set indicates about the good ability of the networks to results generalisation.

Peculiarity, on special attention deserves small differences among training and testing sets. A large divergence among these sets in the practice makes the network useless.

Received results also have confirmed the correctness of the artificial neural networks usage as the simulating tool possible for the application in the area of material engineering for the prediction of mechanical properties. Applied with success for normalised structural steels it gives the chance on the effective application for different steel grades or even for the different types of engineer materials.

The virtual samples of normalised steels, created with the use of described networks will be an immense aid in the Materials Science Virtual Laboratory for constructors and also for students, whose will experience this group of engineers materials [4,5].

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