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Application of artificial neural networks in modelling of quenched and tempered 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 structuralal steels after quenching and tempering processes.
Design/methodology/approach: On the basis of input parameters, which are chemical composition, parameters of mechanical and heat treatment and dimensions of elements, steels' mechanical properties : yield stress, tensile strength stress, elongation, area reduction, impact strength and hardness are predicted.
Findings: Results obtained in the given ranges of input parameters indicates on very good ability of artificial neural networks to values prediction of described mechanical properties for steels after quenching and tempering processes. The uniform distribution of descriptive vectors in all, training, validation and testing sets, indicates on good ability of the networks to results generalisation.
Practical implications: Artificial neural networks, created during modelling, allows easy prediction of steels properties and allows the better selection of both chemical composition and the processing parameters of investigated materials. It's possible to obtain steels, which are qualitatively better, cheaper and more optimised under customers needs.
Originality/value: The prediction possibility of the material mechanical properties is valuable for manufacturers and constructors. It allows the preservation of customers quality requirements and brings also measurable financial advantages
Keywords: Artificial intelligence methods; Computational material science and mechanics; Artificial neural networks; Mechanical properties

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1. Introduction

The material mechanical properties prediction possibility is valuable for manufacturers and design engineers. That is why over one year ago, in [1] modelling results of normalised structural steels mechanical properties with use of artificial neural networks were published. Now authors would like to present the continuation of modelling investigation. This paper describes the investigation results of quenched and tempered structural steels mechanical properties. To preserve the possibility of results comparison the applied modelling methodology was identical with the methodology used in [1].

2. Investigated material

Structural non-alloy and alloy steels were chosen for investigations. They are used in manufacturing of steel constructions, devices and machines elements of the typical destination. Mechanical properties of over 135 various structural non-alloy and alloy steel species were examined. Examples of those steels are showed in Table 1. Examined material was delivered in a form of round and square rods. Steels were manufactured as quenched and tempered wish various processing parameters. Ranges of chemical elements, temperatures, times, kinds of coolants for heat treatment and geometrical parameters are presented in Table 2.

3. Modelling methodology

For properties simulation of structural steels after quenching and tempering processes, the data set, consisting of over 17000 vectors was used. This data was obtained during investigation of steel produced in the „Batory" steel plant in Chorzów, Poland [23] 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 net was created.

Predicted mechanical parameters were: [1-9,16,17,19]

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

Input values, which are used for parameter prediction are:

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

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

The set of all descriptive vectors was spited on three subsets. The first set, which was containing the half of all vectors was used for modification of neurons weights in training stage (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 examination of prediction correctness, when the training process was finished.

Networks were trained with use of the back propagation and conjugate gradient methods [13,15,18].

For the verification of networks usability in the aim of parameters prediction the following quality valuation parameters were used:

- average absolute error – difference between measured and predicted output values of the output variable
- standard deviation ratio – standard deviation of errors for the output variable.
- 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, which means, that 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: [7,9,11-13,21]

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

All computations were made which 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 [24].

4. Modelling results

To make all results comparable with results of investigation results presented in [1] the modelling methodology was identical. Separate neural networks for every parameter, whose value has to be predicted were build. As in [1] the best results were obtained for multi-layer perceptrons with one or two hidden neuron layers. The types of the neural network for individual properties among with the numbers of used neurons and the parameters of the quality valuation for all three sets are introduced in the Table 3 and Table 4.

For all trained neural networks the Pearson correlation coefficient has reached the value above 90% and comparatively low values of the standard deviation ratio. This indicates very good representation of modelled mechanical properties. Neural network parameters and modelling results obtained for quenched and tempered structural steels are similar to results coming from modelling of normalised steels [1].

For graphical representation of networks quality comparative graphs among predicted and measured values obtained for testing set are shown on Figures 1-2. For every estimated parameter the vectors distribution is comparable for all three subsets. This 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.

To analyse the influence of individual input parameters on estimated parameter surfaces graphs were prepared. Examples are introduced on Figures 3-8. Figure 9 shows two architectures of artificial neural networks obtained during investigation.

Table 1.
Examples of steels selected for examination

Non-alloy steels			Alloy steels			
Steels to general purposes [25]	Steels to toughening [26]	Steels on pressure devices [27]	Steels to toughening [28]	Spring steels [29]	Steels to nitrogenising [30]	Steels with elevated properties [31]
C45	C22E	P265GH	21CrMoV5-11	45SiCrV6	30NiCr11	20Mn5
C55	C35R	P295GH	25CrMo4	46Mn7	31CrMoV9	21Mn6
C60	C40E	P310GH	30NiCrMo9-5	52CrMoV4	34CrAlMo5	21CrMoV5-7
S235JRG2	C45C	P275N	34Cr4	54SiCr6	34CrAlNi7	34CrMo4
S355J2G3	C50R	P355NH	40NiCrMo2-2	58CrV4	40NiCr6	40Mn4
20Mn5	C60E	P460N	50CrMo4	64Mn3	41CrAlMo7	40NiCrMo6

Table 2.
Ranges of chemical elements, temperature, time, 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	20	- round - square - rectangle	0.07	0.26	0.14	0	0	0	0	0	0	0	0	0	0	- rolling - forging
max	220		0.60	1.57	1.20	0.28	0.30	2.19	2.08	1.10	0.12	0.30	0.15	0.35	1.02	

range	Quenching			Tempering		
	Temperature [°C]	Time [min]	Cooling medium	Temperature [°C]	Time [min]	Cooling medium
min	760	30	- oil - polymer - water	480	12	- air - oil - water
max	980	150		740	120	

Table 3.
Parameters of computed neural networks for steels after quenching, tempering and forging processes

Variable	Network architecture	Training set			Validation set			Testing set		
		Average absolute error	Standard deviation ratio	Pearson correla-tion	Average absolute error	Standard deviation ratio	Pearson correla-tion	Average absolute error	Standard deviation ratio	Pearson correla-tion
Re	MLP 22:29-9-1:1	28.872	0.1991	0.9800	30.623	0.1999	0.9801	26.443	0.2011	0.9801
Rm	MLP 22:26-16-13-1:1	23.718	0.1968	0.9804	23.523	0.1983	0.9802	23.608	0.1996	0.9800
A5	MLP 17:19-7-1:1	1.278	0.3636	0.9317	1.324	0.3477	0.9377	1.265	0.3674	0.9301
Z	MLP 22:26-13-10-1:1	1.572	0.3270	0.9452	1.677	0.3417	0.9401	1.704	0.3307	0.9442
KV	MLP 12:14-7-1:1	11.387	0.3572	0.9340	10.014	0.3885	0.9215	10.653	0.3552	0.9358
HB	MLP 18:22-7-1:1	9.476	0.2780	0.9606	8.283	0.2796	0.9609	9.806	0.2785	0.9605

Table 4.
Parameters of computed neural networks for steels after quenching, tempering and rolling processes

Variable	Network architecture	Training set			Validation set			Testing set		
		Average absolute error	Standard deviation ratio	Pearson correla-tion	Average absolute error	Standard deviation ratio	Pearson correla-tion	Average absolute error	Standard deviation ratio	Pearson correla-tion
Re	MLP 21:23-26-13-1:1	30.275	0.1918	0.9814	35.240	0.1959	0.9806	35.114	0.1841	0.9829
Rm	MLP 21:23-7-1:1	23.238	0.1632	0.9865	26.718	0.1546	0.9879	25.483	0.1693	0.9855
A5	MLP 19:21-17-11-1:1	0.946	0.3809	0.9245	1.029	0.3890	0.9212	0.976	0.3894	0.9215
Z	MLP 17:19-13-1:1	1.511	0.3486	0.9372	1.641	0.3841	0.9237	1.415	0.3544	0.9351
KV	MLP 17:19-9-1:1	4.542	0.2006	0.9797	4.062	0.2285	0.9773	4.915	0.2071	0.9783
HB	MLP 13:13-8-1:1	7.032	0.2085	0.9781	8.840	0.1924	0.9813	8.293	0.1956	0.9806

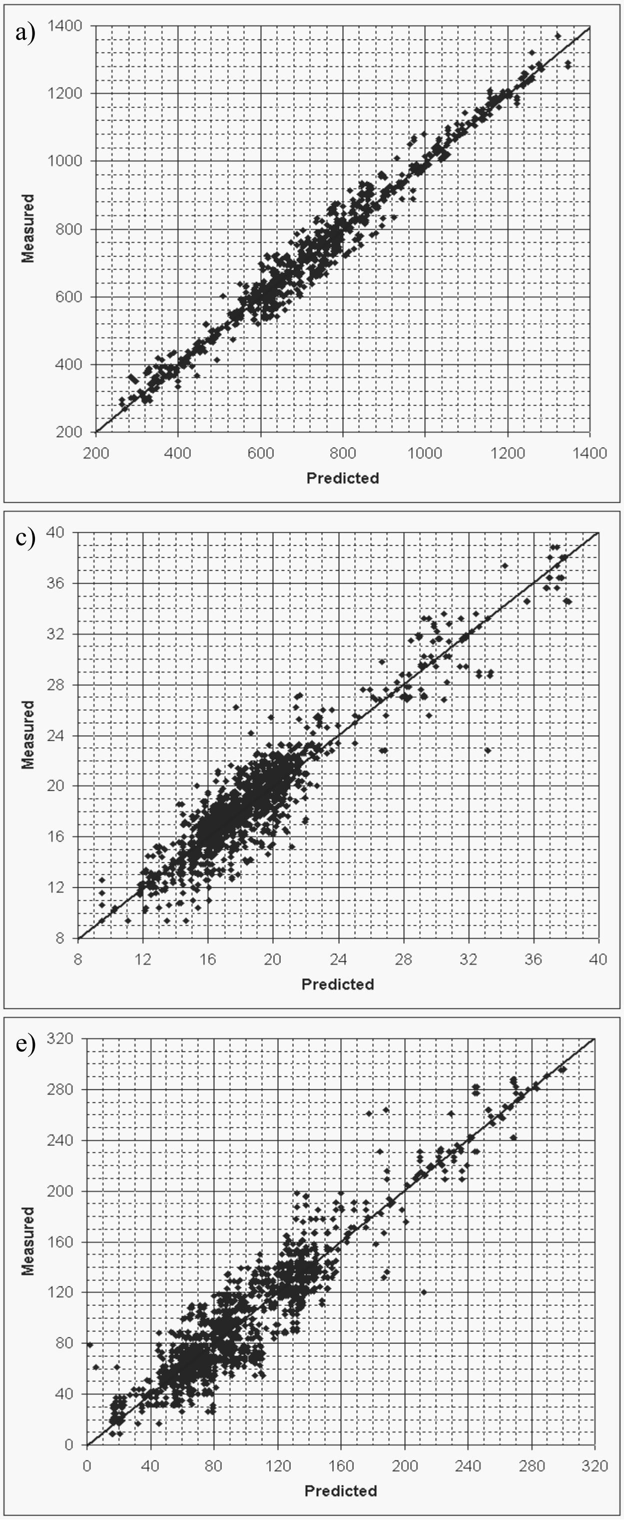

Fig. 1. Comparative graph of a) yield stress R_e, b) tensile strength R_m, c) relative elongation A_5, d) relative area reduction Z, e) impact strength KV, f) Brinell hardness HB, calculated with use of artificial neural networks (testing set) and determined experimentally for steels after quenching, tempering and forging processes

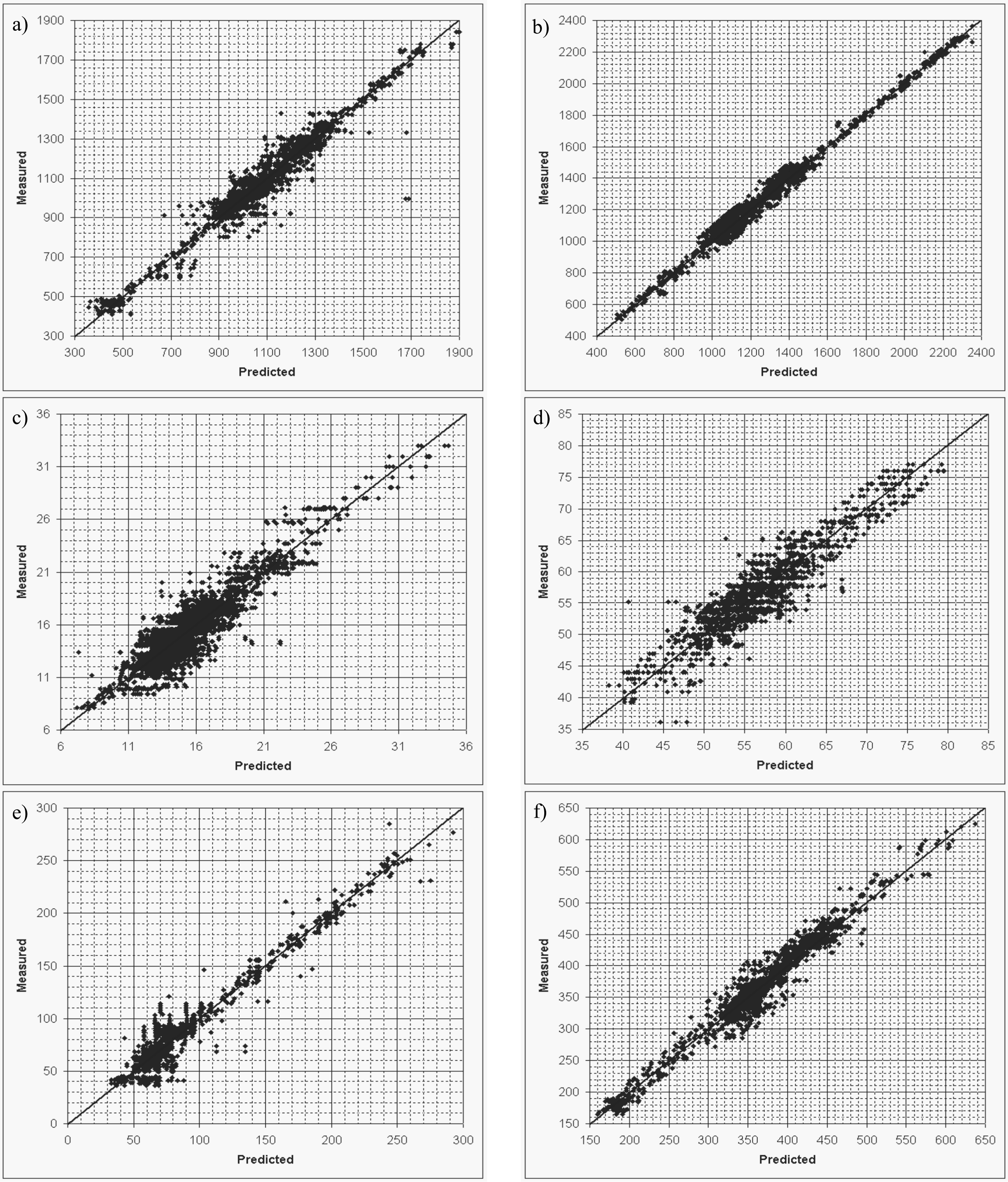

Fig. 2. Comparative graph of a) yield stress R_e, b) tensile strength R_m, c) relative elongation A_5, d) relative area reduction Z, e) impact strength KV, f) Brinell hardness HB, calculated with use of artificial neural networks (testing set) and determined experimentally for steels after quenching,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

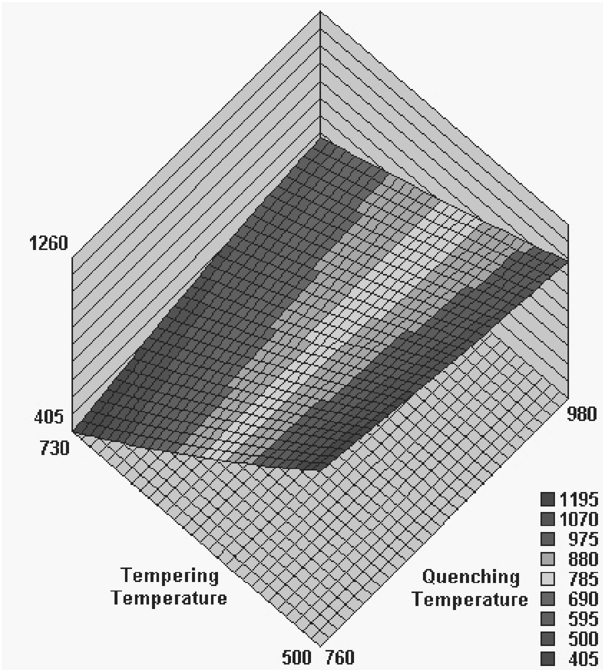

Fig. 3. Influence of quenching and tempering temperatures on yield stress Re, (shape:square, size: 115mm, quenching parameters: 120min/oil, tempering parameters: 90min/air, 0.42%C, 0.76%Mn, 0.26%Si, 0.005%P, 0.009%S, 1.01%Cr, 0,17%Ni, 0.17%Mo, 0%W, 0.006%V, 0%Ti, 0.16%Cu, 0%Al)

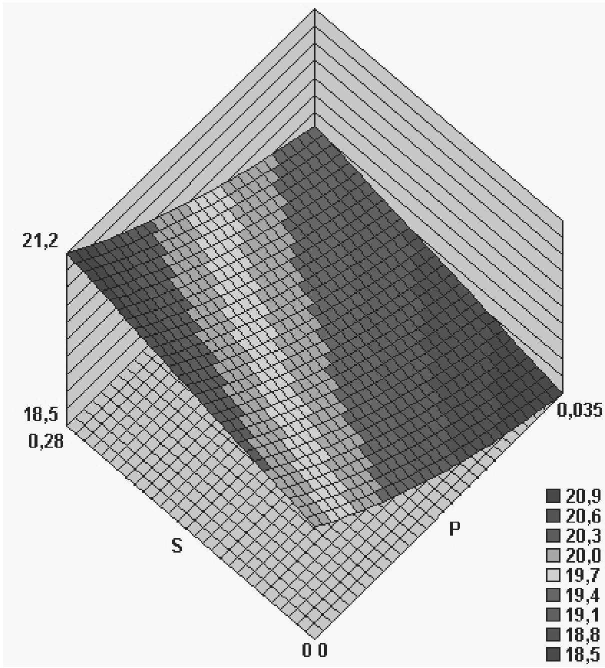

Fig. 5. Influence of sulphur and phosphorus concentration on relative elongation A_5, (shape:round, diameter:160mm, quenching parameters: 890°C/150min/water, tempering parameters: 610°C/210min/air, 036%C, 0.56%Mn 0.22%Si, 0.97%Cr, 0.94Ni, 0.17%Mo, 0%W, 0%V, 0.011%Ti, 0.17%Cu, 0.024%Al)

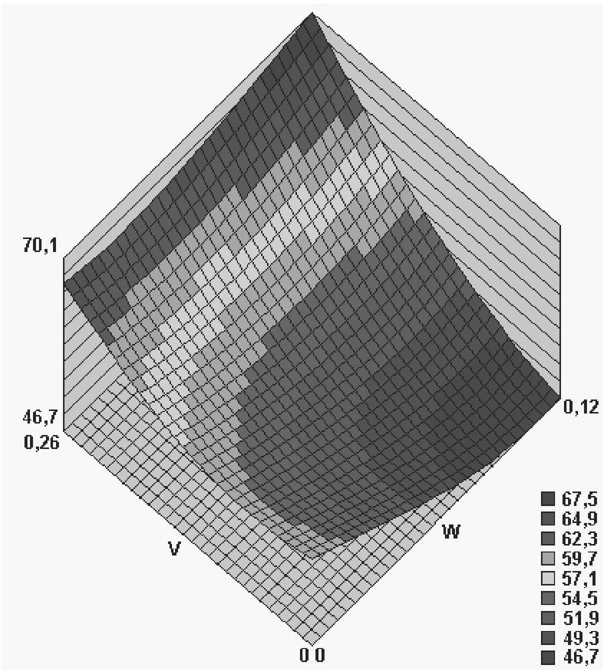

Fig. 4. Influence of vanadium and tungsten concentration on relative area reduction Z, (shape:round, size: 40mm, quenching parameters: 880°C/30min/oil, tempering parameters: 550°C/45min/air, 0.44%C, 0.6%Mn, 0.24%Si, 0.01%P, 0.001%S, 0.92%Cr, 1.37%Ni, 0.23%Mo, 0%Ti, 0.19%Cu, 0.05%Al)

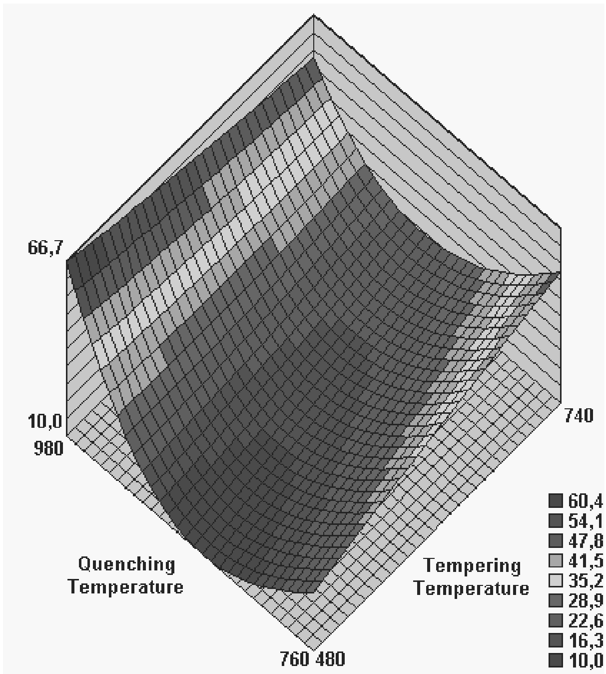

Fig. 6. Influence of quenching and tempering temperatures on impact resistance, (shape:round, diameter: 130mm, quenching parameters: 50min/water, tempering parameters: 14min/oil, 0.39%C, 0.41%Mn, 0.31%Si, 0.015%P, 0.011%S, 0.72%Cr, 1.46%Ni, 0.39%Mo, 0.01%W, 0.002%V, 0.03%Ti, 0.13%Cu, 0.07%Al)

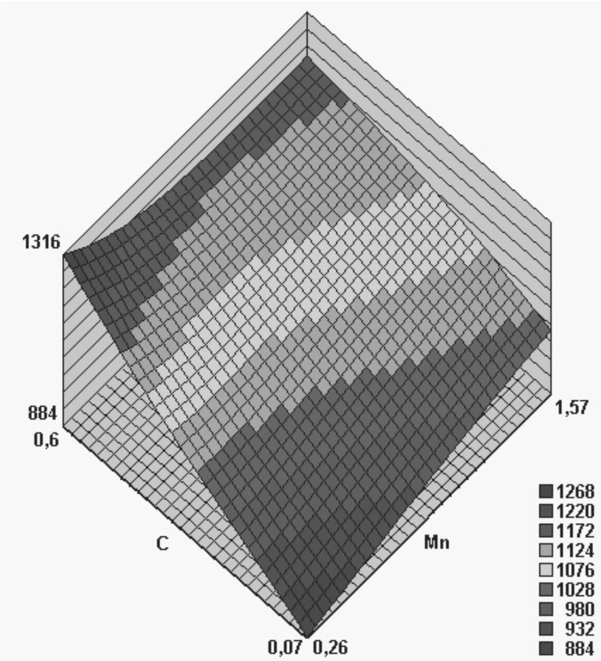

Fig. 7. Influence of carbon and manganese concentration on strength stress Rm, (shape:round, diameter: 60mm, quenching parameters: 900°C/50min/water, tempering parameters: 630°C/ 14min/oil, 0.17%Si, 0.01%P, 0.01%S, 1.38%Cr, 0.09Ni, 0.02%Mo, 0.001%W, 0.01%V, 0.04%Ti, 0.21%Cu, 0.04%Al)

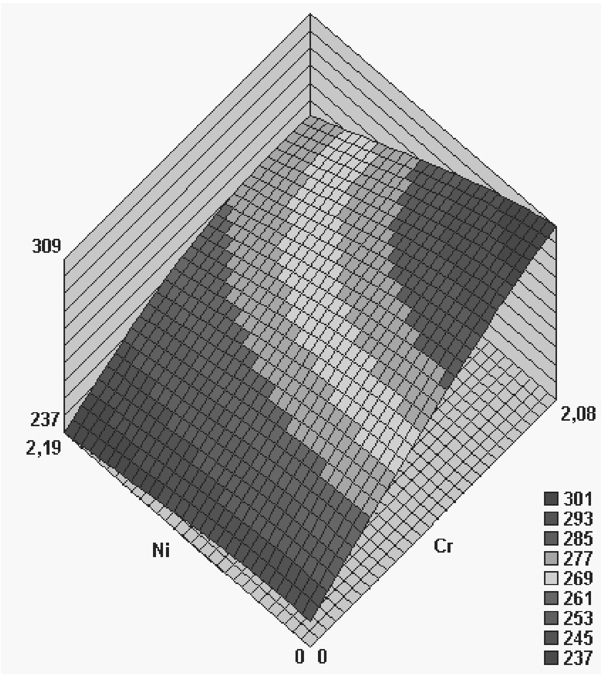

Fig. 8. Influence of nickel and chromium concentration on Brinell hardness HB, (shape:round, diameter: 110mm, quenching parameters: 840°C/120min/water, tempering parameters: 630°C/ 180min/air, 0.48%C, 0.53%Ni, 0.22%Si, 0.018%P, 0.011%S, 0.18%Mo, 0%W, 0%V, 0%Ti, 0.19%Cu, 0.01%Al)

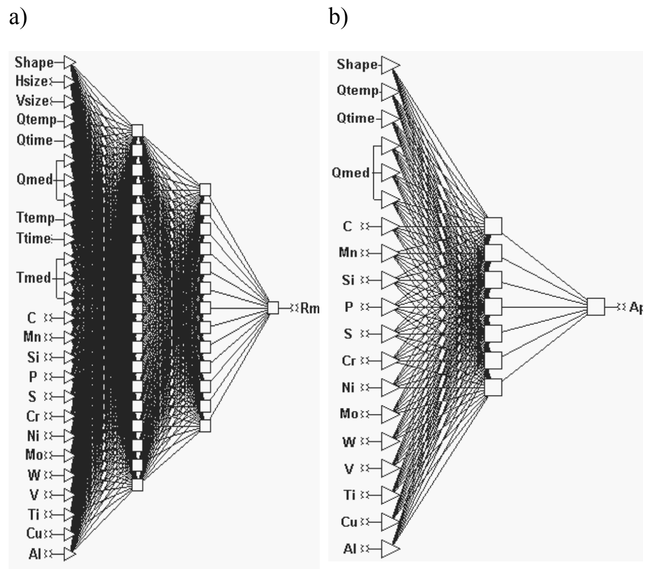

Fig. 9. Architectures of artificial neural networks developed for prediction of steels mechanical parameters a) tensile strength KV, four-layer perceptron 22:26-16-13-1:1, b) relative elongation A_5, three-layer perceptron 17:19-7-1:1

5. Conclusions

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

On special attention deserving small differences among values obtained in training and testing sets. A large divergence among these sets in the practice will made the network useless

Results obtained for quenched and tempered structural steels are comparable with results obtained for normalised steels. Comparable values of quality valuation parameters confirm the ability of correct properties prediction for both types of heat treatment.

Obtained results have confirmed the correctness of the artificial neural networks usage as the simulating tool. It makes possible to apply this networks in the area of material engineering for the prediction of structural steel mechanical properties. Applied with success for quenched and tempered, as well as for normalised constructional steels gives the chance on the effective usage for several steel grades or even for different types of engineer materials.

The virtual samples of quenched/tempered and normalised steels, created with use of described networks will be an immense aid in the Materials Science Virtual Laboratory developed for design engineers and also for students, whose will investigate and discover this group of engineers materials [1,5-7].

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