Computer modelling system of the chemical composition and treatment parameters influence on mechanical properties of structural steels

L.A. Dobrzański*, R. Honysz

Division of Materials Processing Technology, Management, and Computer Techniques
in Materials Science, Institute of Engineering Materials and Biomaterials,
Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland
* Corresponding author: E-mail address: leszek.dobrzanski@polsl.pl

Analysis and modelling

ABSTRACT

Purpose: This paper presents Neuro-Lab. It is an authorship programme, which use algorithms of artificial intelligence for structural steels mechanical properties estimation.

Design/methodology/approach: On the basis of chemical composition, parameters of heat and mechanical treatment and elements of geometrical shape and size this programme has the ability to calculate the mechanical properties of examined steel and introduce them as raw numeric data or in graphic as influence charts. Possible is also to examine the dependence among the selected steel property and chosen input parameters, which describes this property.

Findings: There is no necessity of carrying out any additional material tests. The results correlations between calculated and measured values are very good and achieve even the level of 98%.

Practical implications: Presented programme can be an effective replace of the real experimental methods of properties determination in laboratory examinations. It can be applied as the enlargement of experimental work. Possible is also the investigation of models coming from new steel species, that wasn't produced yet.

Originality/value: The ability of the mechanical properties estimation of the ready, or foreseen to the use, material is unusually valuable for manufacturers and constructors. This signifies the fulfilment of customer's quality requirements as well as measurable financial advantages for material manufacturers.

Keywords: Computational material science and mechanics; Numerical techniques; Artificial intelligence methods; Structural steels

1. Introduction

The continuousp growth of personal computers processing speed aids the development of modern computer tools, which are used for improvement of products quality and to lowering market prises.

To hold the place on the market, for manufacturers necessary becomes the use of computer systems for support the production on every stage. Constructors and manufacturers are using advisory systems in the selection of materials or as the decision consultant in the field of material properties selection or of the production parameters optimisation.

On the special attention deserved developed from several years' systems, which are based on the artificial intelligence algorithms. They are serving for prediction of the production parameters, releasing also manufacturers from expensive and long-term real investigations.

Aims of computational materials science are to enhance the relations between experimental materials research and computational work on both existing and new, advanced materials and their applications

That is why the effective tools, which will fulfil as these aims are indispensable. Such systems should be easy in the service for material engineers, which they often doesn't have the informative education [1-4].

2. System assumptions

The training of artificial neural networks itself does not make possible the effective prediction of structural steels mechanical parameters. Statistica Neural Network [16] is superb application for training of such networks but she did not come true as the effective environment applicable to the aims of properties modelling Necessary appeared the creation of new system, which will: [4-8]
- use of intuitive graphic user interface,
- protect the user form processing of incorrect data
- use several neural networks simultaneously in the modelling process ,
- make possible the graphic representation of computed results as figures or graphs,
- export the modelling results out of the as raw data or as report
- allow to save all data as the file on the disc for later use
- make accessible the necessary documentation, which will enabling the beginning of the work to the user and facilitating her guidance

virtual laboratory

3. Neuro-Lab system

3.1. System description

Neuro-Lab (Fig. 1.) is an authorship programme written in C++ that use algorithms of artificial intelligence for prediction of the structural steels mechanical properties. On the basis of

chemical composition, parameters of heat and mechanical treatment and elements geometrical shape and size this programme has the ability to calculate the mechanical properties, such as
- yield stress (R_e),
- tensile strength (R_m),
- relative elongation (A_5),
- relative area reduction (Z),
- impact strength (KV and KCU2) and
- hardness (HB and HV).
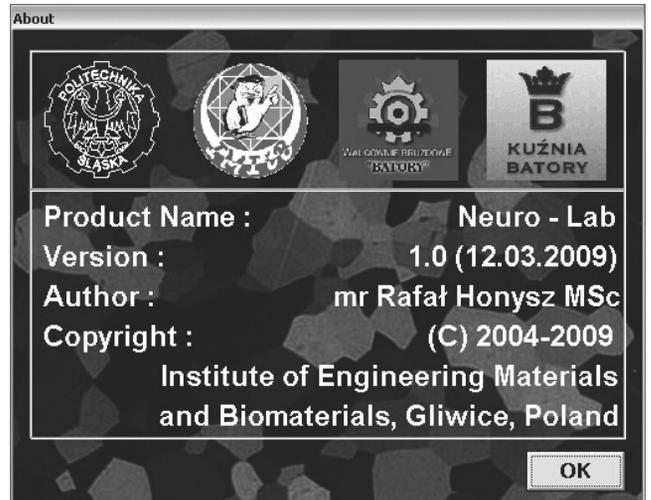
Fig. 1. Neuro-Lab 1.0 – Information window

There is no necessity of carrying out any additional material tests. The results correlation between calculated and measured values is very good and achieves for yield stress and tensile strength even the level of 98% [11].

Presented programme can easily replace the real experimental methods of properties determination in laboratory examinations. It can be applied as the supplement of experimental work. Possible is also the investigation of models coming from new steel species, that wasn't produced yet.
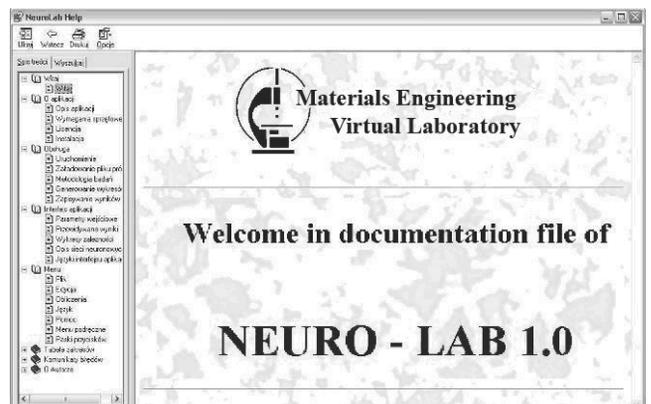
Fig. 2. Neuro-Lab 1.0 – Documentation
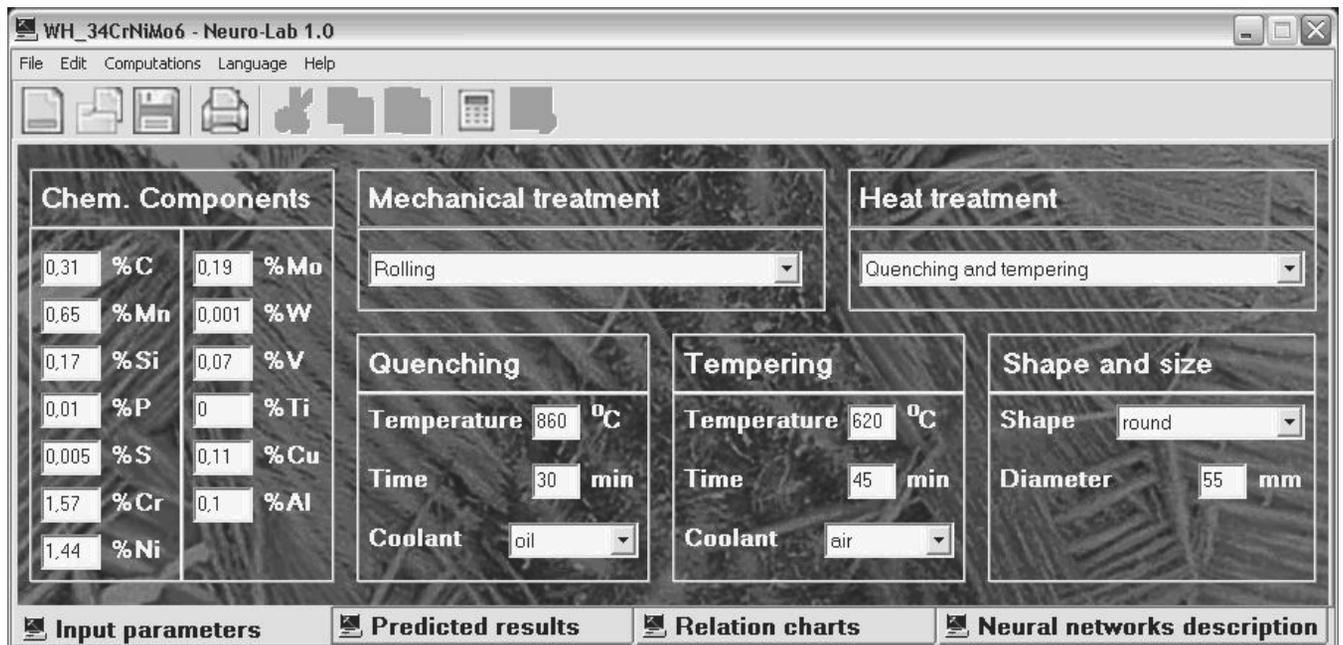
Fig. 3. Neuro-Lab 1.0 – Input parameters card

Table. 1.
Ranges of input data for steels sample generator

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	0.32	0.26	0.15	0.35	1.02	- forging

Range	Quenching			Tempering			Normalizing		
	Temperature [°C]	Time [min]	Cooling medium	Temperature [°C]	Time [min]	Cooling medium	Temperature [°C]	Time [min]	Cooling medium
min	760	30	- oil - polymer - water	550	45	- air - oil - water	180	30	- air
max	980	630		750	600		980	500	

The ability of the mechanical properties estimation of the ready, or foreseen to the use, material is unusually valuable for manufacturers and constructors. This signifies the fulfilment of customer's quality requirements as well as measurable financial advantages for material manufacturers.

To the application building created artificial neural networks were used. Training data set is coming from the investigations of structural steel manufactured in the foundry "Batory" in Chorzów, Poland [15]. In total, the properties of 135 steel species gives over fourteen thousand training vectors.

Trough the use of artificial neuronal networks to the prediction of mechanical properties, presented application makes possible the analysis execution of the mechanical properties changes in dependence from the change of one or more input parameters. Neural networks possess the ability of

knowledge generalising, which consist in solving cases not formulated in the process of training. In example it is possible to calculate the influence of steels' chemical composition on tensile strength with unchanged parameters of the mechanical and heat treatment [10-15].

The interface of presented programme was written as user-friendly. The interface is intuitive in the service and should not inflict any problems in the service. To communicate the user can use both the mouse (clicking on suitable icons), as well as the keyboard (using the operation). All functions assigned to them are described in the programme documentation accessible form the programme (Fig. 2) [9].

On every stage of the work with this programme the user have access to programme documentation. A help file can be enabled through the help menu or pressing F1 key. In this file user can
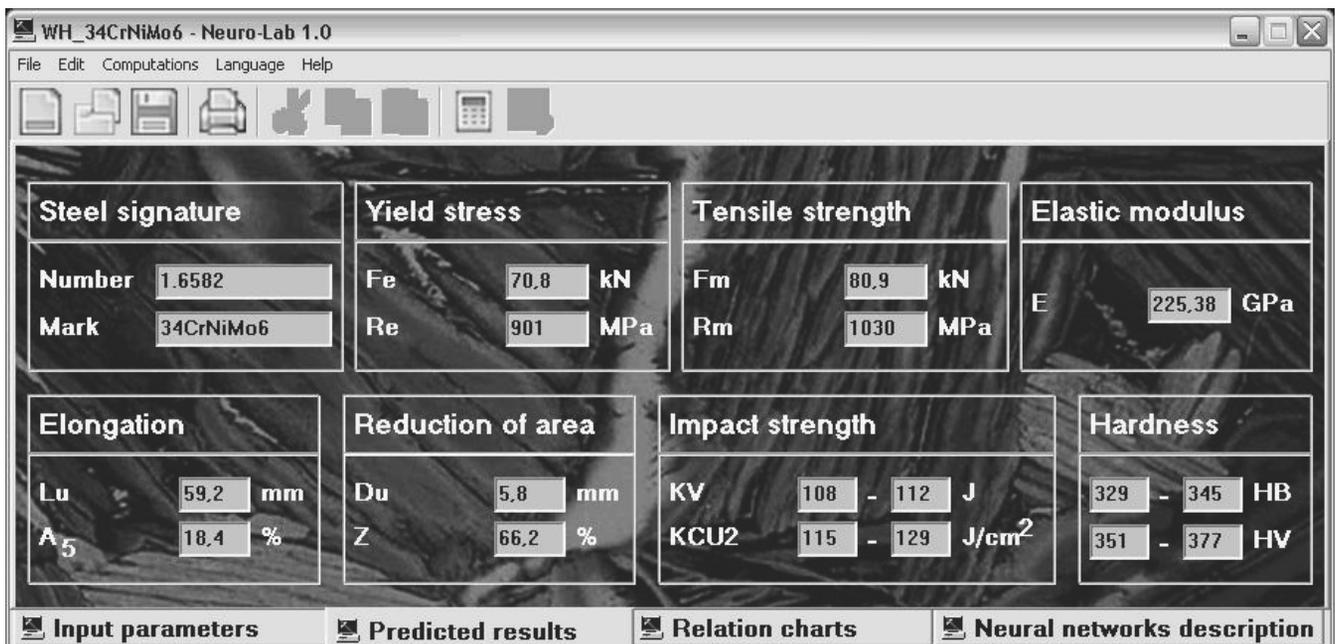
Fig. 4. Neuro-Lab 1.0 – Predicted results card

find all indispensable information required for effective work with the system, such as parameters description, modelling methodology, manual instructions, keyboard shortcuts and many more.

Security mechanisms built-in in the programme are protecting the user from the possibility of the incorrect data processing. Suitable announcement including information in which field the inappropriate value is inputted and how to correct it are shown when any error occurs. The list of all errors together with their description and the handling procedures is described in the programme documentation [9].

3.2. System requirements

To begin the work with the application necessary is [9]:
- PC class personal computer with 300 MHz processor (or better)
- Colour graphic card with resolution min. 1024x768 pixels
- 64MB RAM memory
- Operational system with graphic user interface
  - Windows - 2000/XP/Vista
  - Linux/Unix (kernel 2.6.22 or better, KDE, Gnome or XFCE graphical environment and Wine 1.1 package are required)
- 15MB of hard disc space

4. Graphic User Interface

The programme is communicating with users with the use of the operating system graphic user interface. After the installation and starting the programme the welcoming window

appears with short information on its subject. The main working window of the programme is activated directly after.

The application possesses the interface in Polish, English and German language. The choice of which language should be used can be achieved in pull-down menu Language.

Every command, which can be used by use of button or from pull-down menus, possesses an information plate with the prompt informing to what the given function serves [9].

It consists of the menu bar, the buttons bar and the main window divided on four cards: Input parameters, Predicted results, Relation graphs and Neural network description.

The cards are called out by clicking on them or by choosing from the keyboard accordingly F5, F6, F7 and F8

As example of modelling results, the sample of 34CrNiMo6 steel after rolling, quenching and tempering is introduced below. More information about modelling methodology and system usage can be found in [11] and [12].

4.1. Input parameters card

The „Input parameters" card (Fig. 3) is used for data introducing of studied steel. This card is divided on sections:
- Chemical components – this section contains the input fields in which the user should pass proportional concentrations of thirteen chemical elements, admixtures and alloy components: carbon, molybdenum, silicon, phosphorus, sulphur, chrome, nickel, molybdenum, tungsten, vanadium, titanium, copper and aluminium. The admissible ranges of concentrations are introduced in Table 1.
- Mechanical treatment – user should choose from the list the kind of the mechanical processing of which the studied steel was subjected. There are two options: Rolling and Forging
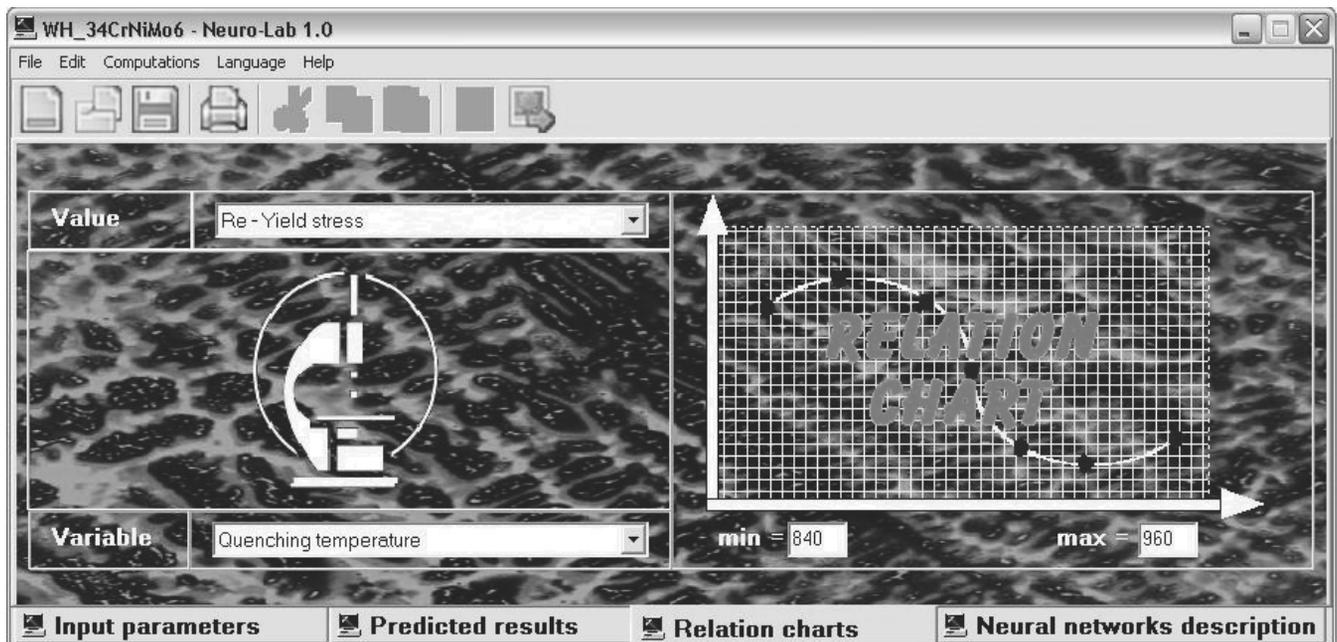
Fig. 5. Neuro-Lab 1.0 – Relation charts card
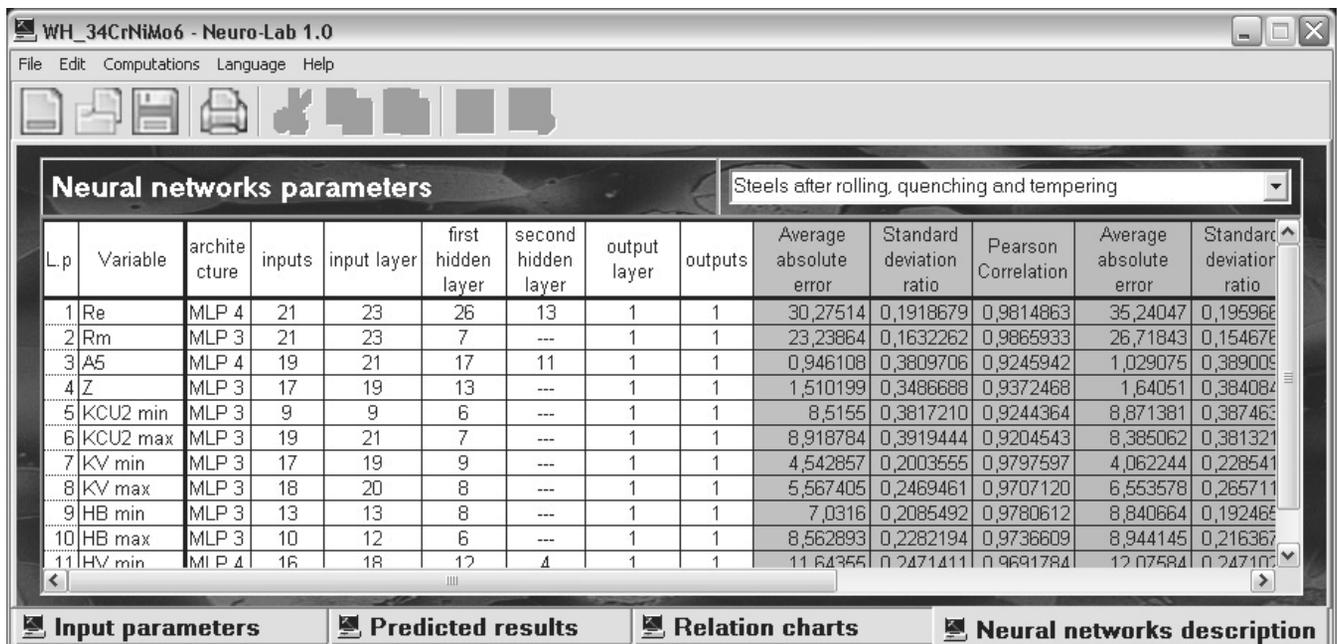
Fig. 6. Neuro-Lab 1.0 – Neural networks description card

- Heat treatment - user should choose from the list of the heat treatment of the studied steel. There are two options: the first is quenching and tempering, the second is normalisation. In dependence of this sections for passing the parameters of choosed treatment will be activated. The heat treatment parameters are temperature, time and coolant for each of selected treatment. The admissible ranges of the parameters and kinds of used coolants are described in Table 1.

- Shape and size - The geometrical dimension of product delivered by manufacturers in the figure of rods with round, square or rectangular section were considered. User should give or the diameter or the lengths of the sides of the rod in dependence from the chosen shape.

4.2. Predicted results card

The „Predicted results" card (Fig. 4) presents the output parameters calculated with use of neural networks on the basis of given input values. The sections of this card are:
- Steel signature - the chemical composition of the given sample is compared with hundred thirty-five steel species which were examined during the programme creation. As the result the number and the mark of the species with the biggest convergence is shown in corresponding fields on this card.
- Yield stress – computed is the value of yield stress (R_e) and the value of related force (F_e) for the standardised sample φ10x5
- Tensile strength - computed is the value of tensile strength (R_m) and the value of related force (F_m) for the standardised sample φ10x5
- Elastic modulus – The Young elastic modulus (E) is calculated as stress divided by the corresponding strain inside the proportional deformation range (below the value of yield stress
- Elongation – predicted are the relative elongation (A_5) and the ruthless length of the sample (L_u) after test execution.
- Reduction of area – predicted are the relative reduction (Z) and the ruthless diameter (D_u) of the sample after test execution.
- Impact strength – calculated are the minimum and maximum values for Charpy type samples with V notch (KV) and with U notch (KCU2).
- Hardness – calculated are the minimum and maximum values of measurements performed by Brinell method (HB) and by Vickers method (HV).

4.3. Relation charts card

The „Relation Charts" card (Fig. 5.) serves to relation graphs generation between the mechanical properties of steel and parameters used to their estimation. Possible is the examination of the influence of any parameter from the Input parameters card on the value of any mechanical properties from the card of Predicted results, when the rest of parameters remain unchanged.

Possible is for example the examination the influence of chemical elements on the steels' with unchanged parameters of the thermal processing. User should choose the described mechanical property (section „value"), and the parameter, which describes this property (section „variable"). It is necessary to define the minimum and maximum values. These values define the range, in which the examined property will be estimated. The values should not exceed the limits described in Table 1

4.4. Neural network description card

The card „Neural networks description" (Fig 6) presents all necessary information about the neural networks, which were trained on the needs of the programme. For every estimated property four independent single multilayer perceptron was created. The division was executed with the regard of mechanical and heat treatment type. Separate networks were trained for impact strength and hardness for minimum and maximum values.

Introduced in four tables information are about the architecture of the given network, the number of inputs and outputs, the quantity of neurons in every layers and the training algorithm. As the parameters of the quality of the network, the average absolute error, standard deviation ratio and Pearson R correlation are calculated separately for every network in the training set (grey colour), validation set (red colour) and test set (blue colour).

In total, 49 neural networks were trained and used to programme building [11].

5. Modelling methodology

After the installation process the programme can be activated in two ways:
- by choose of the programme icon from the Menu Start of the operational system,
- by clicking on the sample file. Material samples have the *.smp extension.

User can input the data into the application on three ways. First of them is fulfilment of all fields placed in the „Input parameters" card. Second one is to read in the data from the sample file with use of Open command placed in the menu „File". The last way is to click on the sample file. The application will start and the data will be read in from the chosen sample automatically.
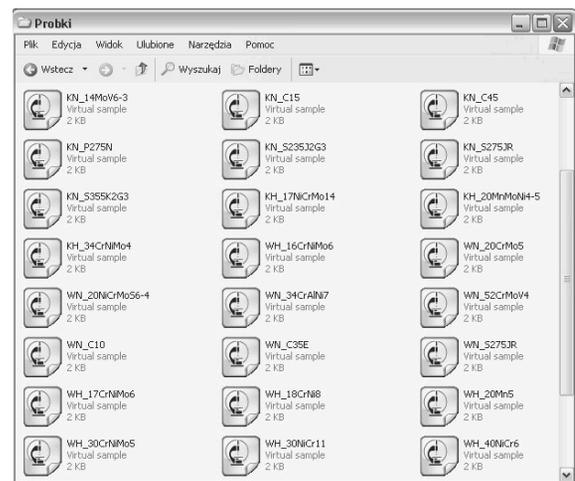
Fig. 7. Steel sample files

To get aquatinted with the possibilities of the programme the set of sixty samples representing several steel species manufactured in the various way was prepared. Installed together with the system are placed in the user documents catalogue on hard disc. The samples are directly ready to use (Fig.7).

If the user wants to create the new sample file he can do this by choosing New command from File menu. The system will be cleaned up from all data, which were read into the memory with the last sample. The Input parameters card will be also called out. System is now ready to collect the new data.

Fig. 8. Neuro-Lab 1.0 – The investigations protocol of mechanical and technological properties
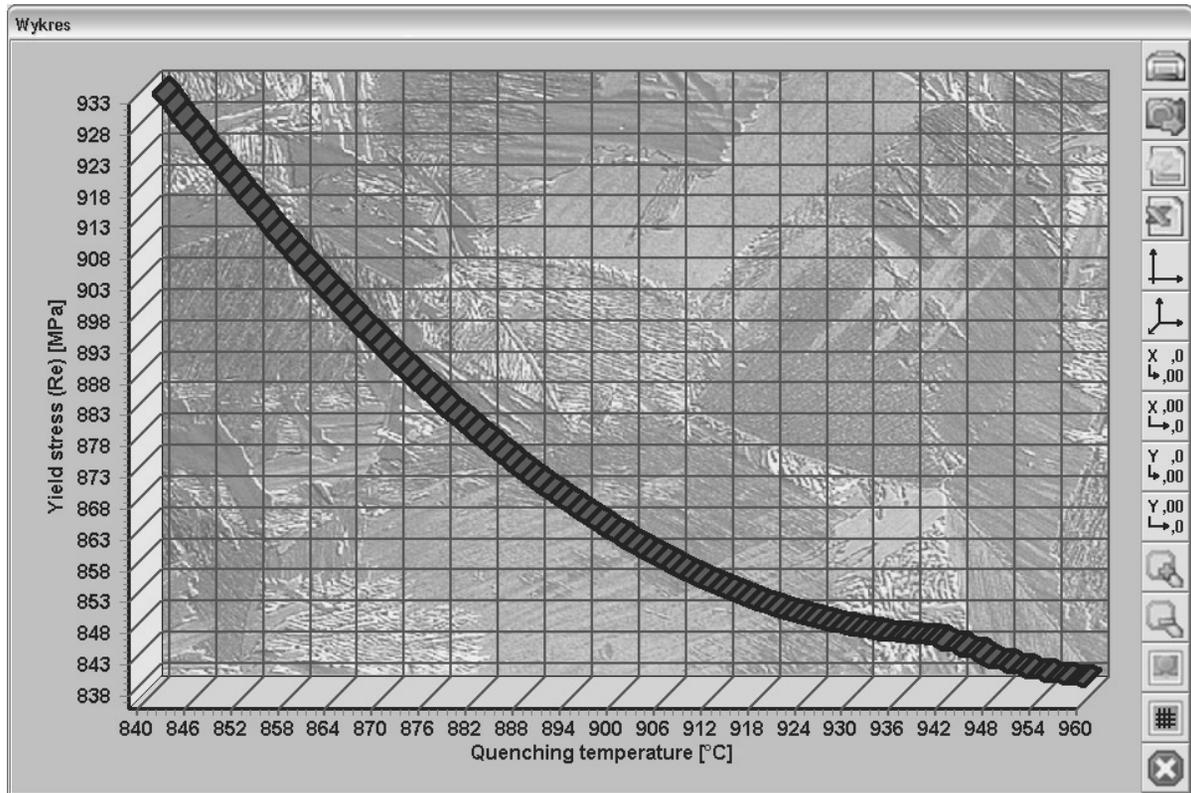
Fig. 9. Neuro-Lab 1.0 – Graph window presenting the influence of quenching temperature on yield stress for 34CrNiMo6. Other parameters shown in Fig.1

To begin the investigations, that is to predict mechanical properties of the given steel species user should fulfil all the fields in the Input Parameters card, or to load the data from the saved file. As soon as all data was introduced, user should choose the Compute Parameters from the Calculation menu. This same effect can be achieved by clicking the calculation button, which are representing calculator on the buttons bar of the application.

If all inputted data are correct the Predicted Parameters card will be called out with all calculated, with use of neural networks, material properties. If some of the data are incorrect an error is reported. If will happened so, user should return to input card make necessary corrections.

The computation results can be transferred to printer as the investigations protocol of mechanical and technological properties (Fig. 8). Print command is placed in File menu and on buttons bar (printer button).

Possible is the influence examination of chosen input parameter on selected steel property. This can be done with use of Relation chart card.

To generate the influence chart user should call the Relation Chart card and choose the described mechanical property (Value), and input parameter, which is describing this property (Variable).

After that, user should input the minimum and maximum value of the variable from the range, in which he want to examine this influence on the chosen mechanical property. Admissible ranges of variables are described in Table 1.Ranges of predicted mechanical properties are set automatically.

The graph window (Fig 9) is the effect of the work in the panel. The example shows the influence of the quenching temperature on yield stress of 34CrNiMo6 hardened and tempered.
Dragging the mouse pointer over the graph area will result in marking and increasing of the selected fragment. Clicking with the right mouse button in the area of the graph will "catch" the graphs plot window and the possibility of graph movement will activate. The graph window has a button bar placed on its right side. The precise description of the buttons functionality is placed in the help file.

The application makes possible saving of the data in various formats in dependence from the type of the data.

It is possible to save the data as sample file from the main window of the application. User should choose the Save or Save as command from the menu File, or to click the floppy disk button on the buttons bar. The results of calculations can be also saved as report on the printer.

The created graph can be saved as bitmap picture or as raw numeric data. Suitable command buttons are placed in the b window's button bar.

6. Conclusions

Presented in this paper Neuro-Lab. is an authorship programme, which use algorithms of artificial intelligence for structural steels mechanical properties estimation.

On the basis of chemical composition, parameters of heat and mechanical treatment and elements geometrical shape and size this programme has the ability to calculate the mechanical properties of examined steel and introduce them as raw data or influence charts.

Possible is also to examine the dependence among the selected steel property and chosen input parameters, which describes this property. Examination with use of user-friendly graphical interface is easy and intuitive.

Neuro-Lab is a very effective tool possible to application in material industry.

References

[1] L.A. Dobrzański, R. Honysz, The significance of multimedia didactic aids in the informative society, Archives of Materials Science and Engineering32/2 (2008) 117-120.

[2] J. Cecil, A. Kanchanapiboon, Virtual engineering approaches in product and process design, The International Journal of Advanced Manufacturing Technology 31 (2007) 846-856.

[3] J. Chromiec, E. Strzemieczna, Artificial intelligence. The Methodology of construction and the analysis of advisory systems, PLJ, Warsaw, 1994.

[4] G.J. Myers, Reliable software projecting, WNT, Warsaw, 1980 (in Polish).

[5] I. Sommerville, Software engineering, WNT, Warsaw, 2003 (in Polish).

[6] D.W. MacVittie, L.A. MacVittie, Object oriented programming – New thinking method, Cardinal Business Media Inc., Warsaw, 1996.

[7] W.B. Lee, C.F. Cheung, J.G. Li, Applications of virtual manufacturing in materials processing, Journal of Materials Processing Technology 113 (2001) 416-423.

[8] R. Tadeusiewicz, Elementary introduction for neural networks techniques with sample applications, Academic Publishing House PLJ, Warsaw, 1998 (in Polish).

[9] NeuroLab 1.0 – programme documentation.

[10] L.A. Dobrzański, Engineering Materials and materials design. Fundamentals of materials science and physical metallurgy, WNT, Warsaw-Gliwice, 2006 (in Polish).

[11] L.A. Dobrzanski, R. Honysz, Application of artificial neural networks in modelling of normalised structural steels mechanical properties, Journal of Achievements in Materials and Manufacturing Engineering 32/1 (2009) 37-45.

[12] L.A. Dobrzanski, R. Honysz, Influence of common additions on mechanical properties of non-alloy structural steels, Journal of Achievements in Materials and Manufacturing Engineering (in print).

[13] L.A. Dobrzański, R. Honysz, The significance of multimedia didactic aids in the informative society, Archives of Materials Science and Engineering 32/2 (2008) 117-120.

[14] L.A. Dobrzański, R. Honysz, Materials science virtual laboratory as an aid of the computer aid in materials engineering, Journal of Achievements in Materials and Manufacturing Engineering 24/2 (2007) 219-222.

[15] L.A. Dobrzański, R. Honysz, On the implementation of virtual machines in computer aided education, Journal of materials Education 1-2 (2009) (in print).

[16] http://hutabatory.com.pl/.

[17] http://www.statsoft.pl/.