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Artificial intelligence and virtual environment application for materials design methodology

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ABSTRACT

Purpose: The purpose of this study is to develop a methodology for material design, enabling the selection of the chemical elements concentration, heat and plastic treatment conditions and geometrical dimensions to ensure the required mechanical properties of structural steels specified by the designer of machinery and equipment as the basis for the design of material components manufactured from these steels, by using a computational model developed with use of artificial intelligence methods and virtual environment. The model is designed to provide impact examinations of these factors on the mechanical properties of steel only in the computing environment.

Design/methodology/approach: A virtual research environment built with use of computational model describing relationships between chemical composition, heat and plastic treatment conditions, product geometric dimensions and mechanical properties of the examined group of steels was developed and practical applied. This model enables the design of new structural steel by setting the values of mechanical properties based on material production descriptors and allows the selection of production descriptors on the basis of the mechanical properties without the need for additional tests or experimental studies in reality.

Findings: Virtual computing environment allows full usage of the developed intelligent model of non-alloy and alloy structural steel properties and provides an easy, intuitive and user-friendly way to designate manufacturing descriptors and mechanical properties for products.

Research limitations/implications: The proposed solutions allow the usage of developed virtual environment as a new medium in both, the scientific work performed remotely, as well as in education during classes.

Practical implications: The new material design methodology has practical application in the development of materials and modelling of steel descriptors in aim to improve the mechanical properties and specific applications in the production of steel. Presented examples of computer aid in structural steel production showing a potential application possibility of this methodology to support the production of any group of engineering materials.

Originality/value: The prediction possibility of the material mechanical properties is valuable for manufacturers and constructors. It ensures the customers quality requirements and brings also measurable financial advantages.

Keywords: Materials science virtual laboratory; Artificial intelligence methods; Computational material science and mechanics; Iron alloys metallurgy

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METHODS OF ANALYSIS AND MODELLING

1. Introduction

The increasing consumer demands about better quality of steel products forcing on manufacturers the usage of more precise manufacturing processes, which are based on the rigorous standards. To stay on the market, it is necessary to use computer systems supporting steel production or project managing on each stage of manufacturing. Increase in computing power, observed in recent years, favours the development of modern tools used for improving of product quality or for lowering its price. On special attention deserves, developed for several years, computer systems based on artificial intelligence methods and used to predict the mechanical properties of manufactured material. These systems absolving manufacturers from the multiple repetitions of expensive and long-term laboratory researches. The ability of structural steels mechanical properties obtainment is extremely valuable for manufacturers and designers, which are manufacturing or using steel elements. This allows fulfilling all customers' requirements regarding the quality of supplied products. Modelling of steels mechanical properties is also associated with financial benefits, when expensive and time-consuming researches are reduced to necessary minimum. Necessary to conduct is only the verification of computations [1-4].

This situation forced to develop a new computational model covering a wide range of input values, such as the high number of chemical elements, treatment conditions and geometrical dimensions, and relate them with the greatest possible number of mechanical properties. Suitable tools developed for modelling facilitation of these properties will enable more effective selection of steel production descriptors. It will also enable manufacturing of higher quality product, which are cheaper and are more optimized for customer needs. The development of computational methods and computer simulations resulted in replacement of the traditional laboratory in favour of the virtual laboratory. Development of virtual tools, which are simulating the investigative equipment and simulating the research methodology, can serve as a basis for combining aspects of laboratory research, simulation, measurement, and education. Application of these tools will allow the transfer of research and teaching procedures from real laboratory to virtual environment. This will increase the number of experiments conducted in virtual environment and thus, it will increase the efficiency of such researches. This will also allows the training of more professionals. This is not the work on real hardware. This is work with use of suitably designed simulators, namely those, in which the real research methodology is faithfully reproduces. Such simulators are very helpful, not only in industrial applications, but also in engineering education. Such researches were already preformed in the Department of Materials Processing Technology, Management and Information Technology in Materials Institute of Engineering Materials and Biomaterials, but this was not an integrated and comprehensive approach. Presented in this paper the new approach allows the methodical use of all available computational techniques, including the artificial intelligence tools and virtual environment [4-6].

2. A literature review

2.1. The usage of IT tools in the design of material products

The aim of new engineering materials design is to optimize their functional properties in technological, economic and environmental aspect. This usually applies to products made from these materials, which meet the strict usage requirements. Such design, usually computer aided, must be based on a thorough knowledge of relations (theoretical and empirical) between the chemical composition of the material, its structure, treatment conditions and mechanical properties. The main benefit is the ability to design a suitable material selection (or manufacturing) methodology for various industrial applications [7-9]. The idea of modelling is shown in Figure 1.

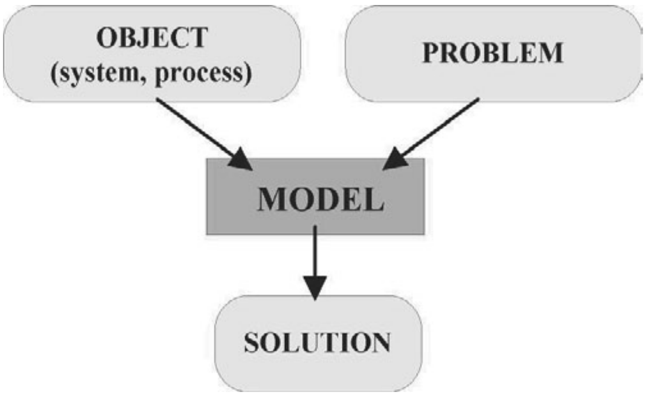

Fig. 1. The idea of modelling

Models shall be construed as a reflection of the system with use of logical relationships between variables describing them. Manipulation of these variables allows the analysis, how the model behaves in certain conditions [10]. Computational model is a simplified description of the relation between steels mechanical properties and conditions of its production. It ignores certain dependencies occurring in reality (considered by model developers to be less important) [8, 11-13].

Evaluation of simulation results obtained with use of developed computational model is based on comparison of all relevant variables model with the measured data [14-15]. It is recommended when developing a model to obtain a comparable level of the representation accuracy for most variables than the unusually precise terms of one variable (although important), and poorly to others [16-19].

Computational material models are collections of information on their properties and descriptors, expressed as a mathematical equation. Modelling is thus formalizing the description methodology of the given property, limited to set of properties shown by the physical model with use of formulas and mathematical relationships. This means that the physical model determines the form of a mathematical model. The mathematical model should clearly correspond to the physical model [20-23].

2.2. Numerical and mathematical models of structural steels

There are many techniques of mathematical modelling using several different algorithms described in available literature. They are used among others to modelling the steels mechanical properties. Equally large is collection of articles and books related to properties' modelling, from the simple dependence equations, through statistical analyses and on the methods of artificial intelligence finishing. However, there is no universal method of mechanical properties prediction. Developed and described in the literature models can be applied in very limited range of the chemical elements concentration or even for single steel grade with very narrow manufacturing conditions. Some part of all models does not take into consideration important conditions as e.g. the production focusing exclusively on the chemical composition on maximum four alloy additions [20-23].

2.3. Virtual laboratories methodology in scientific researches and education

Virtual laboratory is, located in virtual environment, set of simulators and trainers, whose main objective is to simulate the research methodology of investigative equipment located in real scientific laboratory. Additionally, user can find manual instructions of equipment usage, real and virtual experiments descriptions, training exercises possible to perform and many other materials supporting the cognitive processes of research methodology. Virtual laboratory is among other, training environment for staff and students who have just started work with the given device type. They can acquire basic skills and abilities to operate the device without worrying about damaging expensive equipment or causing danger to life or health of their own and other peoples present in the lab. Improper handling of simulated device ends only on the simulated malfunction or damages, visible only on the monitor screen. Then, user simply needs to reset the simulation to the initial state and repeat the experiment with the introduced correct parameters. Researches conducted in academic centres indicate that the ability to perform the experiment at home without supervisor has a positive effect on the student. He don't feel helpless and he doesn't make as many mistakes as a student familiar only with the theoretical descriptions of machines and having a first contact with the real device only in the classroom under the supervision of an instructor leading the subject [24-34].

3. Course and range of own work

3.1. Research scope

In order to develop a computer-aided method of steel mechanical properties modeling with use of artificial inteligence tools and virtual environment, materials research were carried out in order to build a database of experimental results, which was then used in the training process of artificial neural networks. This database was used to build a computational dependences model based on structural steels. To take full advantage of the developed computational model a materials science virtual laboratory was designed, developed and then used to predict the mechanical properties of the structural steels and to visualization of modelling results. It is placed in virtual reality an open science, research, simulation and teaching environment, which enable researches on selected mechanical properties of structural steels. Verification researches were performed to confirm the efficiency of virtual environment application for the purpose of modelling, simulation and prediction of mechanical properties of engineering materials on the example of structural steel on the basis of descriptors such as chemical composition, heat and plastic treatment conditions and shape and dimensions of the product. Developed software and obtained experimental results were used to work on the modelling of production conditions of non-alloy and alloy structural steel meeting the requirements specified by the designers of machinery and equipment. Possible are also classes on science research methodology and operation of research equipment for students and young engineers carried out by use of traditional and e-learning methods.

3.2. Material and research methodology of structural steels mechanical properties

Non-alloyed and alloyed structural steels were selected for examinations as example material. As the main criterion for selection of steel types was the carbon concentration, which for structural steel does not exceed 0.6% [35-36]. Further criteria for minimal and maximal chemical elements concentration, conditions of heat and plastic treatment were taken from [49] and [50]. The selection of mechanical properties, which were examinated was based on [51] and on analysis of the steel markets [41-45] and study the literature [7, 12, 37-40].

For the description of structural steel, six mechanical properties present in the metallurgical certificate have been selected. To describe the above properties set of descriptors characterizing steel in manufacturing process has been developed. It consists of chemical composition described by concentration of thirteen of the most common elements in steels, two technologies of heat treatment used in manufacturing, two technologies of plastic treatment and the geometric dimensions of the final product. Steel was manufactured in electric arc furnaces with devices for steel vacuum degassing (VAD). The material was supplied in the form of heat and plastic treated long rods.

3.3. Description of own work methodology for prediction and modelling of examined structural steels mechanical properties

Developed artificial neural networks were used to build the computational dependency model in structural steel. To build such model forty-nine artificial neural networks were trained. This model was built to verify the correctness of networks' training process and to enable the effective usage of artificial neural networks for prediction and modelling of structural steels properties. The model describes the relationships, which exist between the conditions of steel production and its mechanical properties after manufacturing. After passing into models' inputs the input parameters, which are:

- in case of straight modelling - chemical composition, head and plastic treatment conditions and geometrical dimensions,
- in case of reversed modelling - mechanical properties.

These values are transferred into active block in the computation model. There, these values are distributed simultaneously on all artificial neural networks. Complete results, namely:

- in case of straight modelling - values or ranges of materials properties,
- in case of reversed modelling - concentrations of chemical elements, conditions of heat and plastic treatment or geometric dimensions,

are transferred outside of the model through the user interface. This model was, in the next step, used to build a materials science virtual laboratory. In application part of the laboratory, developed model is used in direct determination of the descriptors or properties of examined steels. In the network part on the basis of achieved results, the virtual sample file is generated. This file is a representation of real material sample in virtual environment. To obtain the results from this file it should be examined with the use of investigative equipment simulators, like a real material sample.

In order of experimental verification of the developed computational dependency model, a dozen types of non-alloy and alloy structural steels for different purposes were selected for examinations. Comparative studies were conducted using the material science virtual laboratory and real laboratory of the Institute of Engineering Materials And Biomaterials. A set of files describing the conditions of production and mechanical properties of selected species and corresponding to them real, material samples taken from the ready-made steel rods were developed. At model inputs, the production conditions of steel were inputted. Obtained computational results were compared with those obtained by real examinations of real samples of steel material.

The results obtained during examination of real steel were introduced into the material science virtual laboratory. Results obtained in virtual environment were compared with results obtained in real investigations. Computations were conducted independently for all tested steel types.

Based on the simulation data graphs showing the impact of the steel descriptor on the selected mechanical property of steel was developed. In the appropriate panel of NeuroLab application, production conditions among with the steels property with an appropriate range of variability were inputted.

Operations performed in order to design new type of steel were made. Designed new steel should fulfil all strict requirements given by the customer in terms of production conditions and mechanical properties. New steel types were developed with use of material science virtual laboratory as material sample files, which are describing new types of steel meeting all requirements in virtual environment. In order to verify the correctness of performed simulations new steel types were manufactured in real world. The results obtained by modelling and simulation were compared with results obtained experimentally.

Materials descriptors and mechanical properties values, which were used in the verification of the model in design of new steel types and in the researches of mechanical properties of structural steels, were produced by another production company. This data was not used at any stage in the process of building the model.

4. Analysis of own work results

4.1. Results of own work for mechanical properties examination of non alloy and alloy structural steels

The total number of examined melts was 37970. Accepted ranges of investigated steels chemical elements are shown graphically in Fig. 2a. Ranges of heat and plastic treatment conditions of examined structural steels are presented in chart Fig. 2b for quenched and tempered steel and in Fig. 2c for normalized steel. Materials researches have been partially realised in the laboratories of the Department of Materials Processing Technology, Management and Information Technology in Institute of Engineering Materials and Biomaterials, and partly in a research laboratories "Batory" in Chorzów, Poland [46].

Static steel tensile examinations has been done to determine the yield strength ($R_{0.2}$), tensile strength (R_m), relative elongation (A_5) and relative area reduction (Z). Standard round sample with diameter φ10 mm and length 50 mm were used. The results were divided according to the type of heat and plastic treatment (Fig. 3).

4.2. The results of own work for development of structural steel integrated computational model using artificial neural networks

In order to build the model, set of vectors are divided into four subsets. It was decided, that for each individual property, whose value should be estimated, to create a separate neural networks. For properties whose values in steel certificates are given in a range, two networks were trained to provide the estimation for the minimum and maximum values separately. The best results were obtained with artificial neural networks of multilayer perceptron structure with one or two hidden layers. Network types for each property along with the numbers of neurons and the parameters used in quality assessment for a set of test are shown in Table 1. In all cases, trained artificial neural network reached a value of the correlation coefficient above 0.9 and the relatively low values of deviation ratio. That is a very good representation of the state space. On special attention deserves networks providing prediction of the yield strength ($R_{0.2}$) and the tensile strength (R_m). The correlation coefficient above 0.98 and the deviation ratio of less than 0.2 indicate a very good network quality.

The developed artificial neural networks were the basis for developing a computational model of structural steel dependences. Forty-eight of the developed artificial neural networks are grouped in four blocks with twelve networks each for steels after quenching and tempering, normalising, forging and rolling. Appropriate block is activated depending on the type of heat and plastic treatment. Each block contains a set of artificial neural networks necessary to carry out the prediction of mechanical properties. A separate network is responsible for steel's type classifications. The examined steel's concentrations of chemical elements are compared with the chemical concentration of base steels and as a result, a base steel type, which the chemical composition is most similar to examined steel's chemical composition, is given.

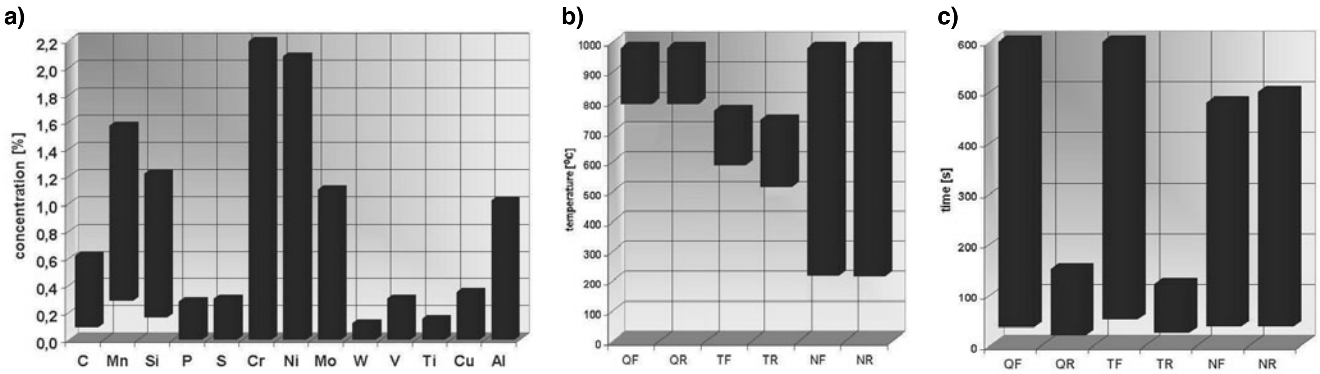

Fig. 2. Ranges of a) chemical elements concentration, b) temperature of heat treatment, c) time of heat treatment in investigated structural steels

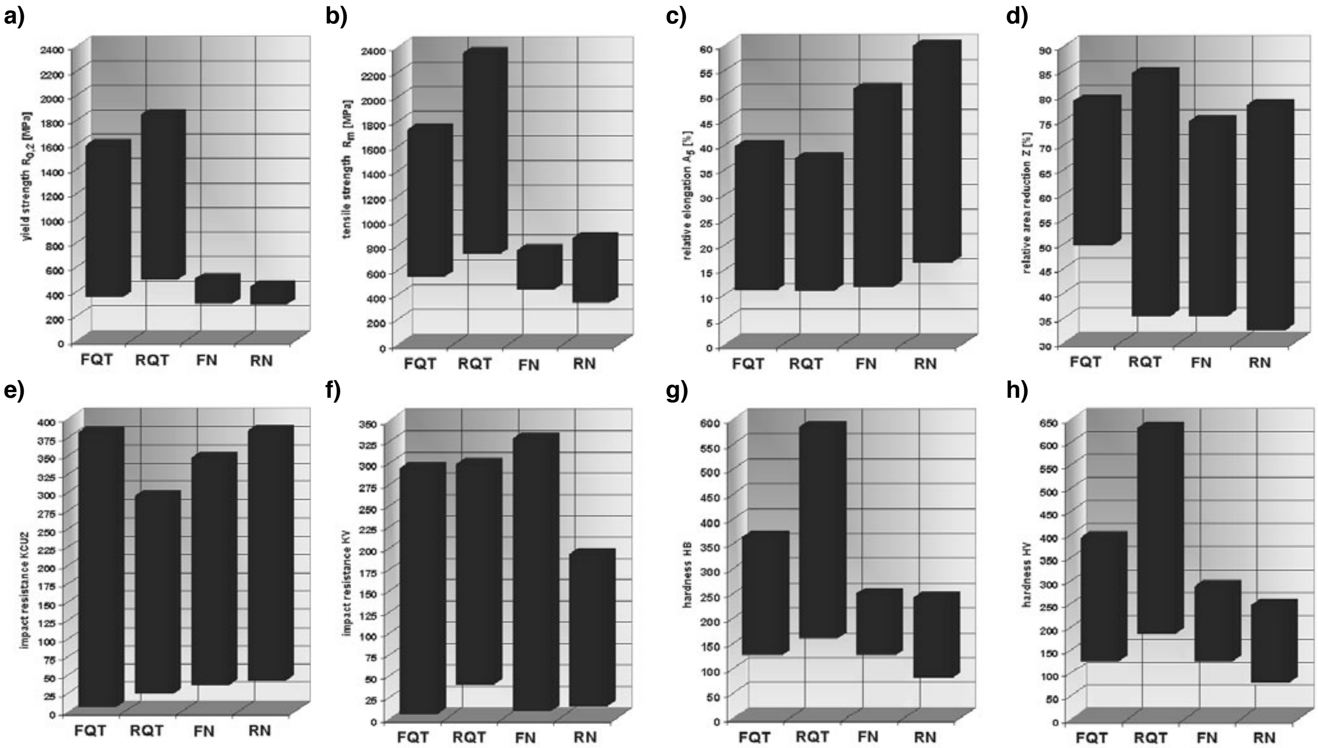

Fig. 3. The ranges of obtained test results: a) yield strength $R_{0,2}$, b) tensile strength R_m, c) relative elongation A_5, d) relative area reduction Z, e) impact strength (KV), f) impact strength (KCU2) g) Brinell hardness HB, h) Vickers hardness HV

4.3. The results of own work for development of software for integrated modelling and prediction of mechanical properties

The training of artificial neural networks itself does not make possible the effective prediction of structural steels mechanical parameters. Statistica Neural Network is superb application for training of such networks. However, it is difficult to apply this system as effective environment applicable for properties modelling Necessary becomes the creation of new system, which will:

- 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 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 enable the beginning of the work to the user and facilitating her guidance.

Table 1.
Parameters of computed neural networks for steels after quenching, tempering, normalising, rolling and forging processes

properties of forged steel		quenched and tempered				normalised			
		network architecture	average absolute error	standard deviation ratio	Pearson corellation	network architecture	average absolute error	standard deviation ratio	Pearson corellation
yield strength ($R_{0.2}$)		22:29-9-1:1	26.44	0.20	0.98	18:18-5-1:1	18.14	0.18	0.98
tensile strength (R_m)		22:26-16-13-1:1	23.60	0.19	0.98	18:18-4-1:1	16.02	0.19	0.98
relative elongation (A_5)		17:19-7-1:1	1.26	0.36	0.93	14:14-6-1:1	1.32	0.36	0.93
relative area reduction (Z)		22:26-13-10-1:1	1.7	0.33	0.94	16:16-10-1:1	1.89	0.30	0.95
impact strength (KV)	(min)	16:20-8-1:1	16.42	0.34	0.93	15:15-6-1:1	15.91	0.35	0.93
impact strength (KV)	(max)	24:28-14-1:1	16.64	0.35	0.93	18:18-8-1:1	19.45	0.34	0.93
impact strength (KCU2)	(min)	12:14-7-1:1	10.65	0.35	0.93	14:14-9-1:1	14.62	0.30	0.95
impact strength (KCU2)	(max)	15:17-9-1:1	16.72	0.35	0.93	13:13-8-1:1	14.07	0.24	0.97
hardness (HB)	(min)	18:22-7-1:1	9.80	0.27	0.96	11:11-5-1:1	4.74	0.29	0.95
hardness (HB)	(max)	12:16-8-1:1	11.77	0.31	0.94	15:15-6-1:1	6.03	0.33	0.94
hardness (HV)	(min)	24:28-8-1:1	8.71	0.24	0.97	17:17-7-1:1	6.50	0.32	0.94
hardness (HV)	(max)	15:19-8-1:1	9.17	0.22	0.97	16:16-4-1:1	6.23	0.33	0.93
properties of rolled steel		quenched and tempered				normalised			
		network architecture	average absolute error	standard deviation ratio	Pearson corellation	network architecture	average absolute error	standard deviation ratio	Pearson corellation
yield strength ($R_{0.2}$)		21:23-26-13-1:1	35.11	0.18	0.98	17:17-9-5-1:1	7.13	0.20	0.98
tensile strength (R_m)		21:23-7-7:1	25.48	0.16	0.98	17:17-12-6-1:1	13.15	0.18	0.98
relative elongation (A_5)		19:21-17-11-1:1	0.97	0.38	0.92	14:14-6-1:1	1.05	0.30	0.95
relative area reduction (Z)		17:19-13-1:1	1.41	0.35	0.93	13:13-4-1:1	1.19	0.31	0.95
impact strength (KV)	(min)	9:9-6-1:1	8.86	0.38	0.92	10:10-5-1:1	20.47	0.41	0.91
impact strength (KV)	(max)	19:21-7-1:1	8.48	0.33	0.94	16:16-6-1:1	19.08	0.37	0.92
impact strength (KCU2)	(min)	17:19-9-1:1	4.91	0.20	0.97	14:14-8-1:1	10.39	0.35	0.93
impact strength (KCU2)	(max)	18:20-8-1:1	6.57	0.26	0.96	16:16-11-1:1	12.16	0.38	0.92
hardness (HB)	(min)	13:13-8-1:1	8.29	0.29	0.98	8:8-5-1:1	5.84	0.33	0.94
hardness (HB)	(max)	10:12-6-1:1	8.95	0.22	0.97	12:12-8-1:1	4.76	0.28	0.92
hardness (HV)	(min)	16:18-12-4-1:1	12.40	0.21	0.97	18:18-8-1:1	5.52	0.33	0.94
hardness (HV)	(max)	19:19-12-8-1:1	13.94	0.27	0.96	10:10-9-1:1	6.01	0.31	0.94

To fulfil all requirements a material science virtual laboratory has been developed. It is located in the virtual reality an open, academic, research, simulation and teaching environment, which makes possible researches on selected mechanical properties of structural steels.

5. The materials science virtual laboratory project

5.1. The application part of the material science virtual laboratory

The laboratory was divided into two parts with different functionality. The first one is application "NeuroLab" which use artificial intelligence algorithms to predict the mechanical properties of non-alloy and alloy structural steel. It is an application virtual laboratory, in which on the basis of the input steels manufacturing conditions is possible to determine its mechanical properties without the need for real examinations. Also possible is the reversed inference, namely on the basis of mechanical properties values is possible to determine steel's production conditions. The application interface consists of four cards. Input parameters card (Fig. 4a) is used for data input about investigated steel. Predicted results card (Fig. 4b) is used for computation results presentation. Relation chart card (Fig. 4c) is used to generate dependency graphs between the mechanical properties of steel and the production conditions used for their estimation. It is possible to examine the influence of any condition present in input parameters card onto any mechanical property present in predicted results card, when the rest of descriptors remains unchanged. Neural network description card (Fig. 4d) presents information about the neural networks that were used for the construction of the structural steel dependency model. This model is applied in this software.

The results of computational experiments are presented in a openly form in the application window or printed as the investigation protocol of the mechanical and technological properties as print the test protocol of mechanical and technological in accordance with [51]. Relations between production conditions and mechanical properties are generated in the form of graphs in a separate window.

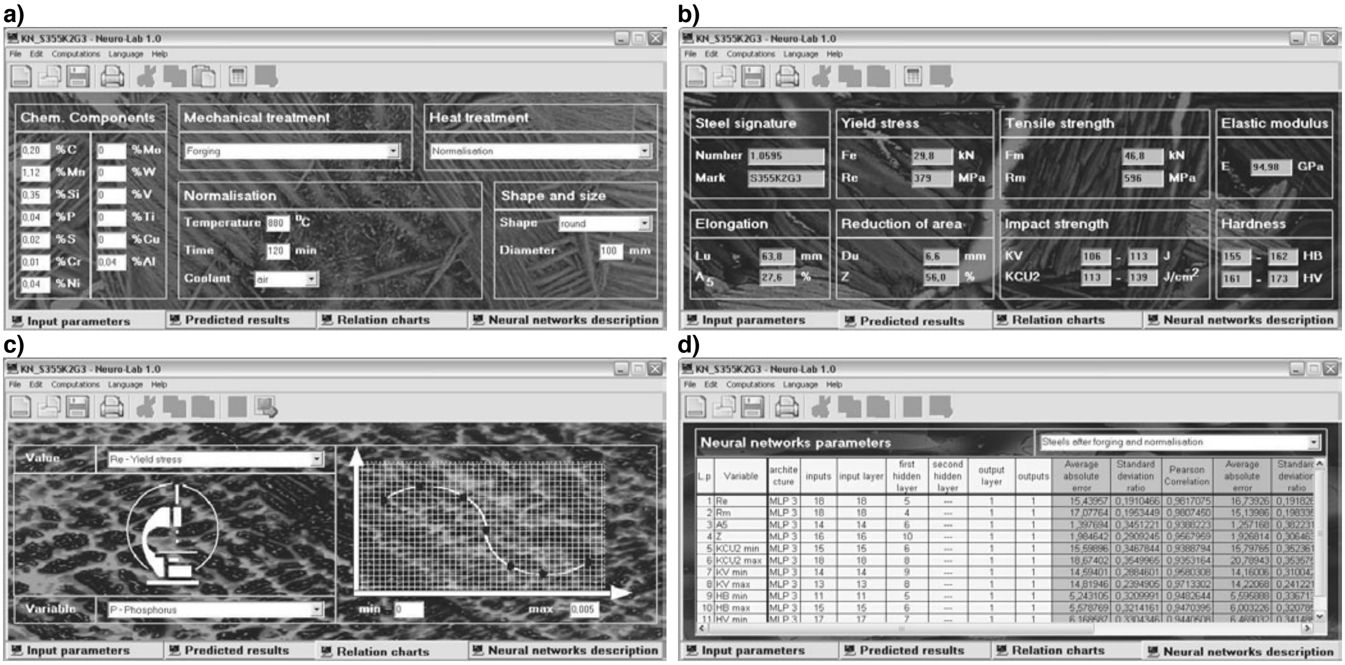

Fig. 4. Application materials science virtual laboratory - NeuroLab 1.1 a) input parameters card, b) predicted results card, c) relation charts card, d) neural networks description card

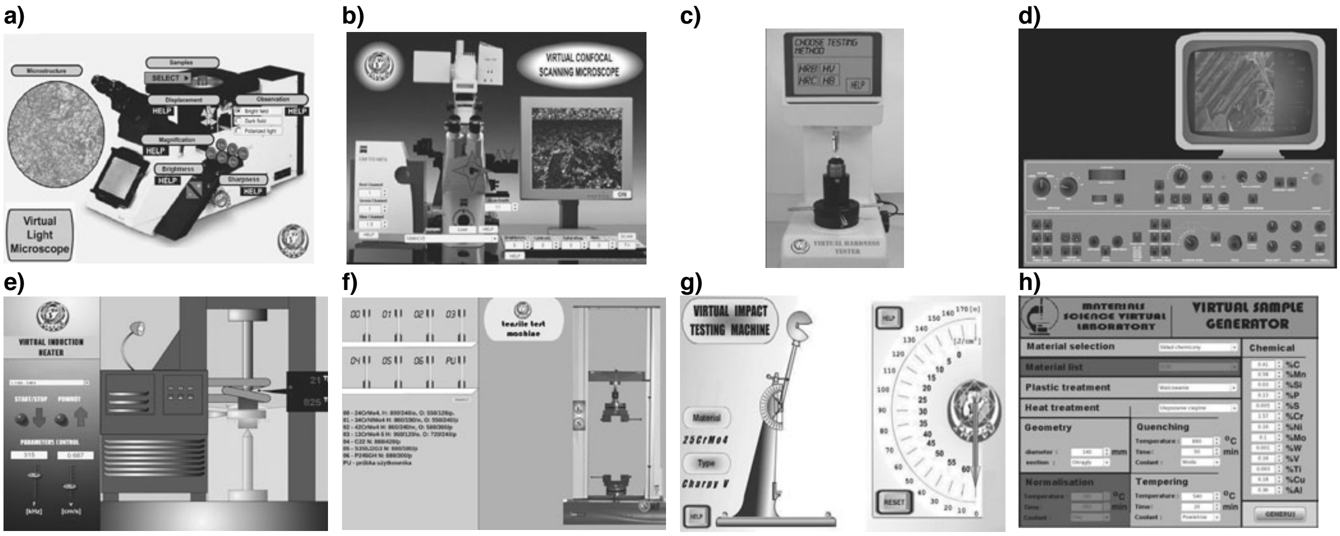

Fig. 5. Simulation of laboratory equipment installed in network material science virtual laboratory, a) light microscopy, b) laser scanning confocal microscope, c) universal hardness tester, d) scanning electron microscope, e) surface heater, f) tensile machine, g) Charpy pendulum machine, h) samples file generation panel

5.2. The network part of the material science virtual laboratory

Network part of materials science virtual laboratory [47-48] is a tool with extended functionality in relation to the NeuroLab application. This is a network laboratory placed in the Internet on e-Learning Platform of the Institute of Engineering Materials and Biomaterials. This same computational model of structural steel's dependencies is applied in network part, so it is possible to perform the same examination range, which can be performed using the application part of virtual laboratory. However, there are differences in examination methodology. Opposite to the application part of the laboratory, in network part user do not receive the results of examinations in the open form. The modelling results are stored in a file, which is a virtual representation of real steel sample in virtual world. In order to obtain the results this file should be placed in machine simulators.

Examination of created material model mechanical properties and material structures consists of exact research equipment representation with an exact reproduction of the device's research methodology. Only after the examination performed in the virtual environment, user gets the property examination result (or an error message when the examination failed because of an error). Figure 5 presents simulations of the investigative equipment available in the laboratory along with the panel for generating files representing material samples.

The research methodology with use of simulations is exactly the same as the real device. All the manipulators, such as buttons or knobs are placed in the simulation at the appropriate places, like in a real machine. The functionality of the real machine is mapped in the simulations without any changes and modifications.

6. The verification of experimental and virtual influence examinations of chemical concentration and conditions of heat and plastic treatment on the mechanical properties of structural steels performed with use of materials science virtual laboratory

In order to experimental verification of computational model successively three aspects has been emerged. The first describes the experimental verifications aimed in the correctness verification of the computational model developed in order to answer the question whether it is possible to perform virtual material examinations exclusively in the virtual environment. This was followed by virtual materials researches aimed to determine the influence, which the structural steel's mechanical properties have on steels descriptors, such as the concentration of chemical elements, the conditions of heat and plastic treatment and geometrical dimensions. The last of these activities was to design a chemical composition and heat treatment conditions of two hypothetical structural steels to meet the client's requirements about values of mechanical properties.

For verification purposes, an experimental set of vectors describing the material descriptors and steel's mechanical properties has been developed. These vectors describe each of the 135 types of examined steel. To exclude the possibility of adjusting the artificial neural network only to the products of one manufacturer's material vectors, verification samples were collected from a different manufacturer. Samples, produced from these types of steel, were examined in order to obtain verification vectors. To minimize differences between training and validation data, material researches has been performed in the same way and using the same equipment, that were used in the main researches. In addition, the vectors used for comparative researches were constructed in the same way as the vectors used for training of artificial neural network used in the calculation model of dependences in to structural steel. Vectors, in which values of material descriptors or mechanical properties went beyond the accepted ranges for the vectors used for construction of artificial neural networks, were rejected. The results obtained by virtual examination have been compared with those obtained experimentally in a real laboratory.

As example, the influence analysis of the admixtures concentration on the mechanical properties was conducted. Three types of steel were selected for investigations. There are non-alloy structural steels for general use described in [52]. Steel signatures and chemical compositions are introduced in Table 2. The material was delivered as forged, normalised round rods. Material descriptors, such as chemical composition, heat treatment, plastic treatment and geometric parameters were inputted to material science virtual laboratory. All data were saved in files, which are representation for real material samples in the virtual world.

The mechanical properties estimation was performed for every single virtual sample. Results obtained with use of this method were compared with results obtained by use of real material investigations. All are introduced in Table 3. It was found, that all estimated results are correct for all examined steel samples, because all three steel species were recognised correctly, and differences among predicted and measured values of mechanical properties are very small and predicted results did not exceed the neural network tolerance values for corresponding property.

The next stage of investigative work was the analysis how big is the influence of the admixtures concentration on steels mechanical properties. The influence graphs were generated with use of NeuroLab among estimated properties and the concentration of admixtures. Influence graphs are presented in Figs. 6-11.

Table 2.
Chemical composition of examined non-alloy steels

steel signature	chemical elements concentration								normalising parameters			shape
	C	Mn	Si	P	S	Cr	Ni	Al	temp. [°C]	time [min]	cooling medium	
S235J2G3	0.16	0.81	0.22	0.01	0.02	0.13	0.09	0.04	880	60	air	Φ100
S275JR	0.18	0.7	0.31	0.01	0.01	0.11	0.13	0.02	880	60	air	Φ100
S355K2G3	0.20	1.12	0.35	0.04	0.02	0.01	0.04	0.04	880	60	air	Φ100

Table 3.
Comparison between measured and predicted mechanical properties of examined non-alloy steels

property	measured	predicted	measured	predicted	measured	predicted
Material	S235J2G3	S235J2G3	S275JR	S275JR	S355K2G3	S355K2G3
$R_{0.2}$ [MPa]	307	306	302	304	362	379
R_m [MPa]	461	467	506	502	573	596
A_5 [%]	33.8	34.0	35.5	33.8	31.0	27.6
Z [%]	64.1	65.7	59.9	62.3	52.0	56.0
KV [J]	137-143	108-143	124-142	111-126	102-139	106-113
HB	112-129	124-134	143-146	138-146	149-159	155-162

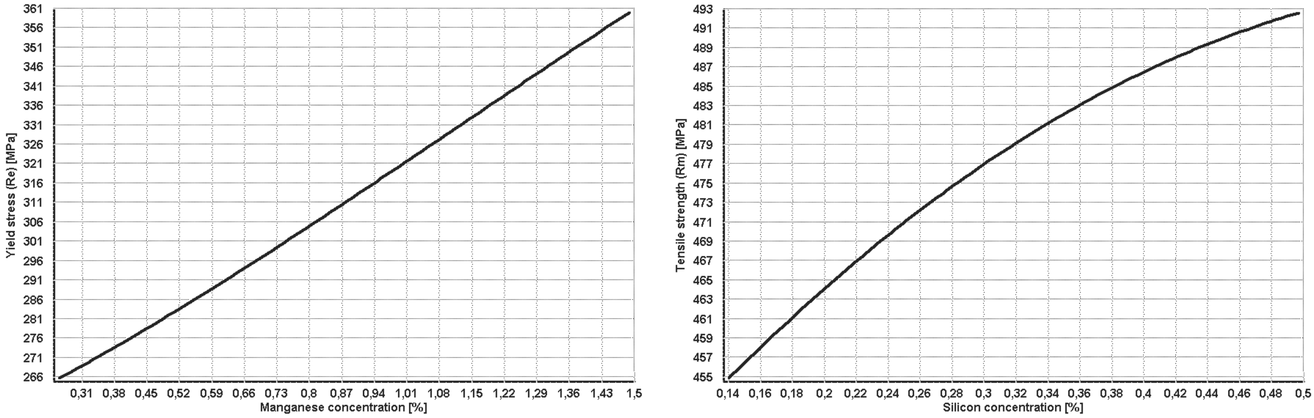

Fig. 6. Influence of manganese and silicon concentration on selected mechanical properties of S235J2G3 steel

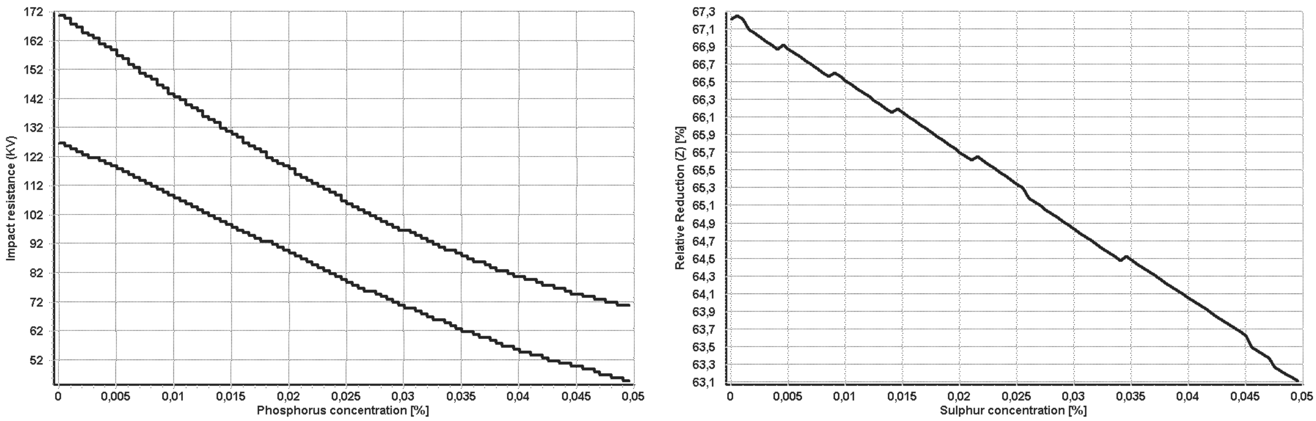

Fig. 7. Influence of phosphorus and sulphur concentration on selected mechanical properties of S235J2G3 steel

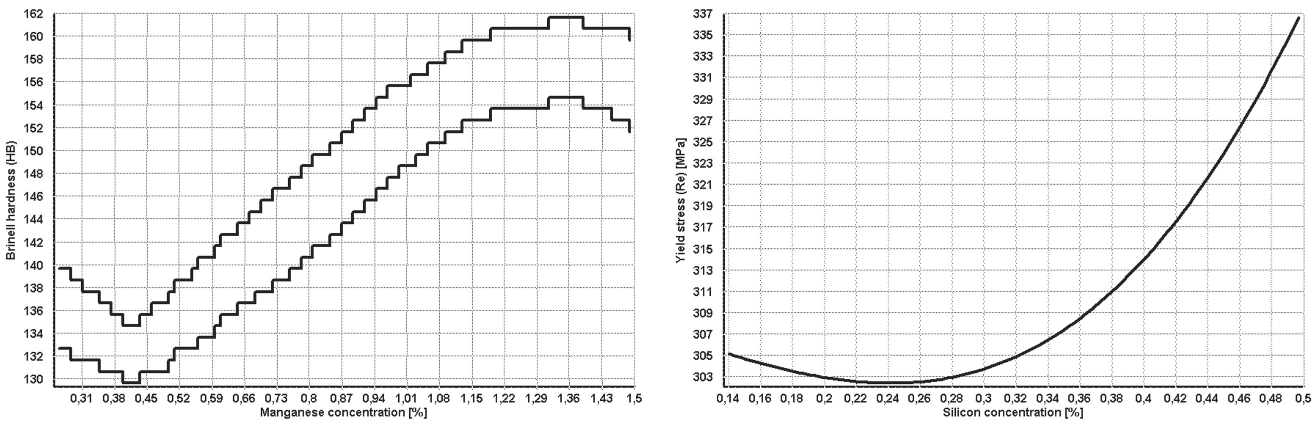

Fig. 8. Influence of manganese and silicon concentration on selected mechanical properties of S275JR steel

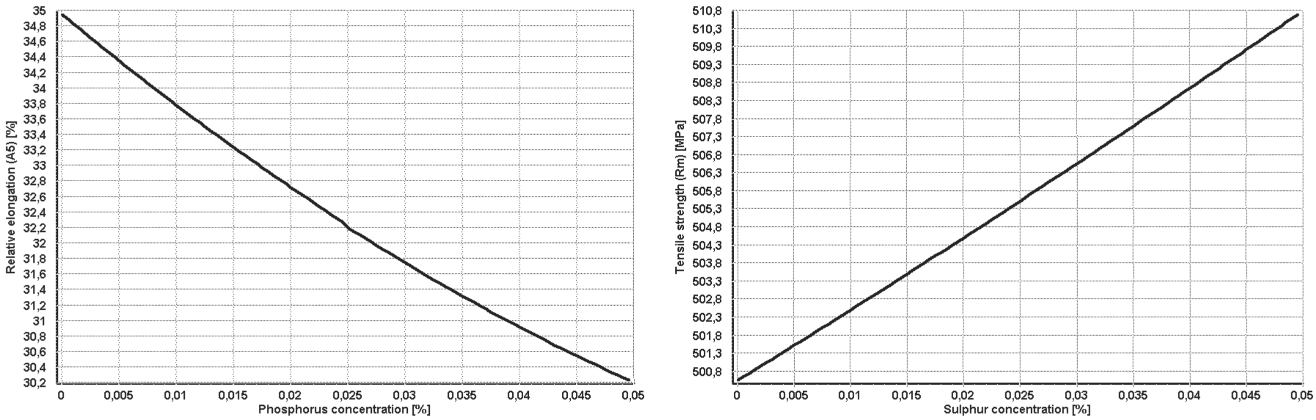

Fig. 9. Influence of phosphorus and sulphur concentration on selected mechanical properties of S275JR steel

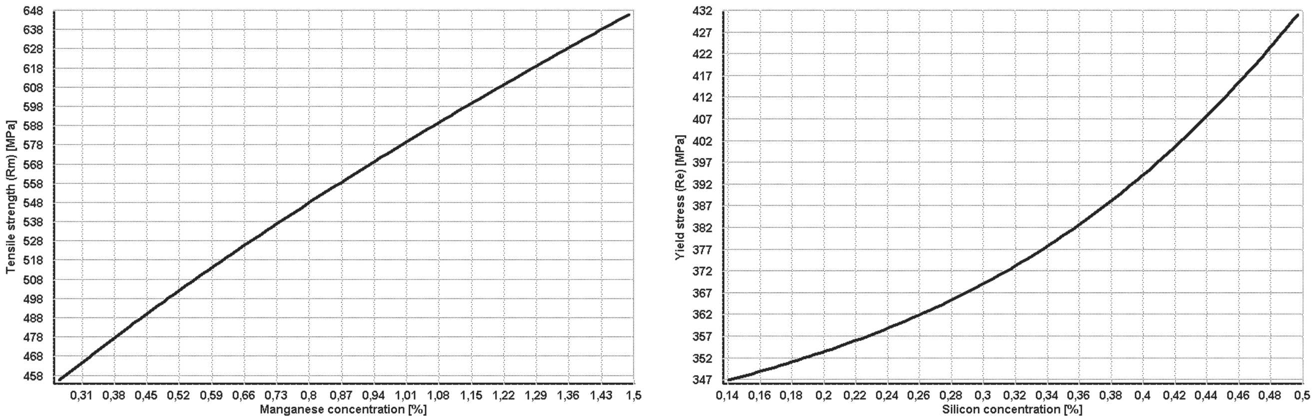

Fig. 10. Influence of manganese and silicon concentration on selected mechanical properties of S355K2G3 steel

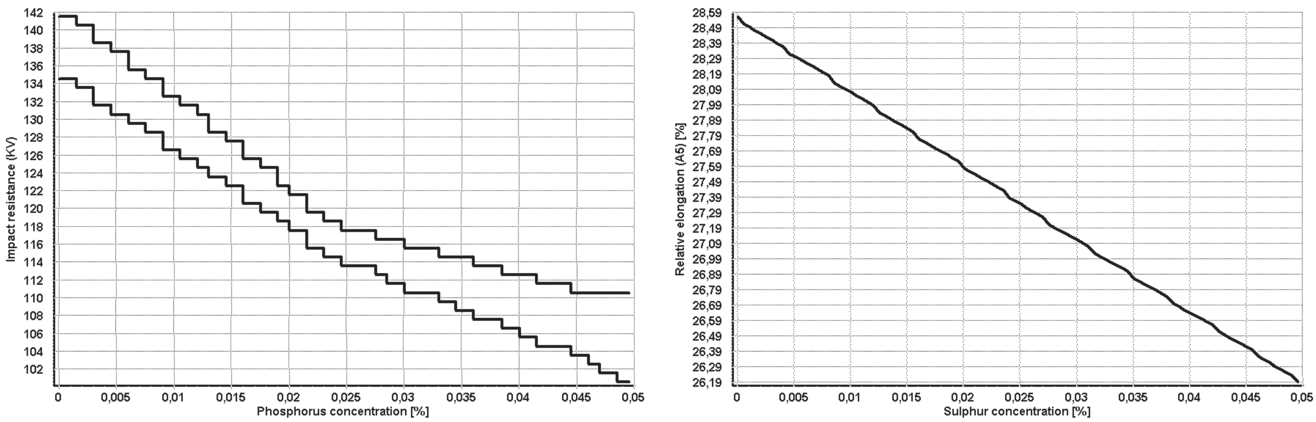

Fig. 11. Influence of phosphorus and sulphur concentration on selected mechanical properties of S355K2G3 steel

7. Summary

On the basis of experimental results obtained in the virtual and real examinations of structural steels mechanical properties it has been proved, that the selection of chemical composition, heat and plastic treatment conditions and geometrical dimensions of structural steels, to ensure the required mechanical properties specified by the designer of machinery and equipment, as the basis for the design of the material elements manufactured from these steels, can be obtain by using a computational model developed using the artificial intelligence tools and virtual environment providing the impact study of these factors on the mechanical properties of steel only in computing environment. Results, obtained during virtual experiments, indicates on very good compatibility of the model with the data obtained experimentally in real laboratory and demonstrate the effectiveness of the model application for the prediction, simulation and modelling of the steel properties and also the design of chemical composition, heat and plastic treatment and geometrical of newly designed steels.

The model calculation correctness has been fully verified by experiment. Materials researches performed in the virtual environment, both, in range of determining the mechanical properties and in the field of chemical composition and treatment conditions design, are consistent with the results obtained during the real research in real laboratory. Consistency was observed in the whole range of steel descriptor variation: of concentrations of chemical elements, heat and mechanical treatment conditions and mechanical properties of examined structural steels. Developed virtual environment enables the modelling of new, non-standard types of steel. Through the determination of relations between selected mechanical properties and the steel descriptors at specified range, it is possible to obtain data on the hypothetical and the newly designed materials, which have not been produced yet and existing only in virtual environment. Possibility of designing new materials with unique properties strictly adjusted to actual customer needs is crucial in achieving of the market success. The presented examples of computer aid in structural steel production showing a potential application possibilities of this methodology to support the production of any group of engineering materials.

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References

[1] R. Honysz, Materials design methodology with use of materials science virtual laboratory, PhD thesis, Institute Of Engineering Materials and Biomaterials, 2010.

[2] L.A. Dobrzański, The descriptive metallography of iron alloys, Silesian University Publishing, Gliwice, 2007 (in Polish).

[3] L.A. Dobrzański, Metal Engineering materials, WNT, Warsaw-Gliwice, 2004 (in Polish).

[4] L.A. Dobrzański, M. Kowalski, J. Madejski, Methodology of the mechanical properties prediction for the metallurgical products from the engineering steels using the artificial intelligence methods, Journal of Materials Processing Technology 164-165 (2005) 1500-1509.

[5] L.A. Dobrzański, R. Honysz, Analysis system of the influence of chemical compositions, the parameters of the heat and plastic treatment on mechanical properties of structural steels, Proceednigs of the XXXVII Materials Science School, Kraków, 2009, 385-391.

[6] L.A. Dobrzański, R. Honysz, Application of materials science virtual laboratory in traditional and distance learning, Proceedings of the 5th Polish-Ukrainian Young Scientists Conference, Bukowina Tatrzańska, 2007.

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

[8] L.A. Dobrzański. Fundamentals of material design methodology, Silesian University of Technology Publishing, Gliwice, 2009 (in Polish).

[9] L.A. Dobrzański, Introduction to material science, Silesian University of Technology Publishing, Gliwice, 2007 (in Polish).

[10] T. Bednarski, Mechanics of plastic flow in the outline, PWN, Warsaw, 1995.

[11] J. Adamczyk, Theoretical metallurgy part 1: structure of metals and alloys, Silesian University of Technology Publishing, Gliwice, 2007 (in Polish).

[12] E. Krzemień, Material science, Silesian University of Technology Publishing, Gliwice, 2007 (in Polish).

[13] M. Hetmańczyk, Fundamentals of material science, Silesian University of Technology Publishing, Gliwice, 2007 (in Polish).

[14] M.F. Ashby, Materials selection in engineering design, WNT, Warsaw, 1998.

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

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[16] A.J. Rokach, Schaum's outline of theory and problems of structural steel design: load and resistance factor method, McGraw-Hill Professional, New York, 1990.
[17] A.R. Tamboli, Handbook of structural steel connection design and details, McGraw-Hill Professional, New York, 1990.
[18] G.E. Totten, Steel heat treatment: metallurgy and technologies, CRC Press, New York, 2006.
[19] R.L. Brockenbrough, F.S. Merritt, Structural steel designer's handbook, McGraw-Hill Professional, New York, 1999.
[20] L.A. Dobrzański, 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.
[21] L.A. Dobrzański, R. Honysz, Application of artificial neural networks in modelling of quenched and tempered structural steels mechanical properties, Journal of Achievements in Materials and Manufacturing Engineering 40/1 (2010) 50-57.
[22] J. Gutenbaum, Mathematical systems' modeling, Exit, Gliwice, 2003.
[23] D. Szeliga, J. Gawąd, T. Kondek, M. Pietrzyk, Identification of material models parameters based on inverse analysis, Computational Methods and Systems 3 (2003) 761-766.
[24] K. Stec, Computer simulation as an aid tool in the theoretical electrical engineering laboratory. Computer Application in Electrical Engineering, Poznań/Kiekrz, 1996, 398-399.
[25] A. Mucha, Virtual machines, Engineering Design and Construction 5/8 (2008) 34-38.
[26] L.A. Dobrzański, R. Honysz, Building methodology of virtual laboratory posts for materials science virtual laboratory purposes, Archives of Materials Science and Engineering 28/1 (2007) 695-700.
[27] L.A. Dobrzański, R. Honysz, Computer modelling system of the chemical composition and treatment parameters influence on mechanical properties of structural steels, Journal of Achievements in Materials and Manufacturing Engineering 36/2 (2009) 119-126.
[28] L.A. Dobrzański, R. Honysz, S. Fassois, On the identification of composite beam dynamics based upon experimental data, Journal of Achievements in Materials and Manufacturing Engineering 16 (2006) 429-432.
[29] L.A. Dobrzański, R. Honysz, Development of the virtual light microscope for a material science virtual laboratory, Journal of Achievements in Materials and Manufacturing Engineering 20 (2007) 571-574.
[30] L.A. Dobrzański, R. Honysz, Materials science virtual laboratory - innovatory didactic tool in the teaching of material engineering performed by traditional and e-learning methods, Acta Mechanica et Automatica 2/4 (2008) 5-10.
[31] 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.
[32] L.A. Dobrzanski, R. Honysz, On the implementation of virtual machines in computer aided education, Journal of Materials Education 31/1-2 (2009) 131-140.
[33] L.A. Dobrzański, R. Honysz, The idea of material science virtual laboratory, Journal of Achievements in Materials and Manufacturing Engineering 42 (2010) 196-203.
[34] L.A. Dobrzanski, A. Jagiełło, R. Honysz, Virtual tensile test machine as an example of material science virtual laboratory post, Journal of Achievements in Materials and Manufacturing Engineering 27/2 (2008) 207-210.
[35] L.A. Dobrzański, Engineering materials and materials design. Fundamentals of materials science and physical metallurgy, WNT, Warsaw-Gliwice, 2006 (in Polish).
[36] W. Jasiński, Material science: lectures, Kielce University of Technology, Kielce, 2003.
[37] J. Adamczyk, Theoretical Metallurgy, part 1: structure of metals and alloys, Silesian University of Technology Publishing, Gliwice, 1999 (in Polish).
[38] J. Adamczyk, Theoretical Metallurgy, part 2: plastic deformation, strengthening and cracking, Silesian University of Technology Publishing, Gliwice, 1999 (in Polish).
[39] M.W. Grabski, The essence of engineering materials, Warsaw University of Technology Publishing, Warsaw, 2006 (in Polish).
[40] M.W. Blicharski, Introduction to material science, WNT, Warsaw, 1998.
[41] http://www.steel.keytometals.com/
[42] http://www.steelconstruction.org/
[43] http://www.steelframingalliance.org/
[44] http://www.worldsteel.org/
[45] http://www.metallograf.de/
[46] http://www.hutabatory.com.pl/
[47] http://www.platforma.imiib.polsl.pl/
[48] http://www.vlab.imiib.polsl.pl/
[49] PN-EN 10020:2003, Definition and Classification of Grades of Steel.
[50] PN-EN 10250-3:2001, Open die steel forgings for general engineering purposes - Part 3: Alloy special steels.
[51] PN-EN 10204:2006, Metallic materials. Types of inspection documents.
[52] PN-EN 10250-1:2001, Open die steel forgings for general engineering purposes - Part 1: General requirements.