Journal of Achievements in Materials and Manufacturing Engineering
VOLUME 49
ISSUE 2
December
2011

Virtual examinations of alloying elements influence on alloy structural steels mechanical properties

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: rafal.honysz@polsl.pl

Received 11.10.2011; published in revised form 01.12.2011

Analysis and modelling

ABSTRACT

Purpose: The paper introduces analysis results of selected alloying elements influence on mechanical properties of alloy structural steels for quenching and tempering.
Design/methodology/approach: Investigations were performed in virtual environment with use of materials science virtual laboratory. Virtual investigations results were verified in real investigative laboratory.
Findings: Materials researches performed with use of material science virtual laboratory in range of determining the mechanical properties are consistent with the results obtained during the real research in real laboratory.
Practical implications: 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.
Originality/value: Modelling of structural steels mechanical properties is valuable for steel designers and manufacturers, because it is associated with financial benefits, when expensive and time-consuming researches are reduced to necessary minimum.
Keywords: Computational material science; Materials science virtual laboratory; Structural steel; Virtual investigations

Reference to this paper should be given in the following way:
L.A. Dobrzański, R. Honysz , Virtual examinations of alloying elements influence on alloy structural steels mechanical properties, Journal of Achievements in Materials and Manufacturing Engineering 49/2 (2011) 251-258.

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 year, computer system based on artificial intelligence methods and used to predict the mechanical properties of steels.

Modelling of steels mechanical properties is also associated with financial benefits, because of expensive and time-consuming researches are reduced to necessary minimum. Necessary is the verification of computations. Research centres for materials science for several years are engaged in intensive activity to develop computational models applicable to determination of the mechanical properties [1-5].

The development of computational methods and computer simulations makes possible the replacement of the traditional laboratories in favour of the virtual laboratory. Development of virtual tools, simulating operation the research 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 [6-10].

2. Material

For materials investigation alloyed structural steels have been selected. They are used to manufacture steel construction in building industry and machinery or for manufacturing of installation parts of the typical purpose. Parts made of these steels are joined by welding, riveting or by screws.

Structural steels are the most often produced steel species in the Polish steel industry. They are delivered to the customer as the semi-manufactured or finished products in the form of rods, wires, sections, sheet metals and pipes. Examinations were focused only on the long products in the figure of rods with round, square and rectangular section to the dimension from 20mm to 220mm. These products are the most often produced shapes and in the largest dimension assortment [10]. Structural Steels are used in many applications, because they combining good mechanical properties with low price. There are produced in many grades. The uses are various including civil and industrial engineering.

Steels used to the building of constructions are not fine melts of the iron with the carbon. Except these two elements, steels contain also insignificant quantities of different elements. They are inserted to steel in the metallurgical process in the aim of better deoxidisation or desulphurisation, for improvement of mechanical proprieties, or they stay in the steel in insignificant quantities, because their total removal would be very expensive and unprofitable. However, that they are present in small quantities, they presence induce the essential influence on properties of steel. Some chemical elements gets to steel accidentally, the most often from the scrap-iron, different chemical elements are putted on purpose. In spite, that they the basic alloy element maintain carbon, which regulates the properties of steel and from which content depends the application of the steel [2-3].

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. It was developed using the artificial intelligence tools and virtual environment User can find manual instructions of simulated 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.

Materials science virtual laboratory [17] developed and implemented in Institute of Engineering Materials and Biomaterials, Gliwice, Poland, allows the mechanical properties prediction of non-alloy and alloy structural steel. It is an application virtual laboratory, in which based on 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 based on mechanical properties values is possible to determine steel's production conditions. The results of computational experiments are presented in an openly form in simulations or printed as the investigation protocol of the mechanical and technological properties in accordance with [18].

Relations between production conditions and mechanical properties are generated in the form of graphs. This laboratory allows modelling of structural steels with any chemical composition from the given ranges of thirteen elements concentration. Steel in the shape of rods with round, square or rectangle section can be quenched and tempered or normalised. Heat treatment is described by temperature, duration time and cooling medium. Material also can be rolled or forged. Prepared in this laboratory virtual samples files can be saved on computer’s hard disc for later use.

Described laboratory was created, to help the engineers, designers and students in extension of their skills and abilities on the investigations guidance subject from the field of material science, to acquaint them with the scientific tools build for the investigative work and to introduce the methodology of investigations performed with their usage [11-16].

4. Influence analysis of alloying elements on mechanical properties of selected structural steels

For investigations, structural steels to toughening produced according to [19-20] were selected. 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. Alloy additions in these steels are introduced to them by purpose in quantities, which exceeds the given minimum concentration. Steel signatures and the chemical composition of steels selected to examination are introduced in table 1. Material 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 forged round rods. The diameters of rods and heat treatment conditions are introduced in Table 2.

In aim of modelling and properties prediction, 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.

To verify modelling correctness, results obtained during virtual examinations were compared with the results of real material investigations performed on real steel samples in real laboratory. The mechanical properties prediction was conducted for all selected steel grades. Results are introduced in table 3. Results of modelling were marked as correct, because all five types were recognised correctly. Differences among measured and predicted values of mechanical properties are very small and the values of the neural networks tolerances were not exceeded. It can be concluded, that results obtained by analysis performed with use of materials science virtual laboratory are correct.

Virtual analysis was conducted to calculate how big the influence of the alloying elements concentration on steels mechanical properties is. Six alloying elements were selected - silicon, chrome, molybdenum, vanadium, aluminium and copper. Relationship graphs were generated with use of NeuroLab system among estimated mechanical properties and the concentration of chosen alloying additions. The ranges of concentration were selected above and below the base value. The aim of this was to show how strong the influence is by increasing or decreasing of selected addition chemical concentration on selected mechanical property of examined steels. Selected relationship graphs are presented on Figures 1-10. Full set of obtained results and generated influence graphs is presented in [1].

Table 1.
Chemical composition of selected alloy steels

Steel grade	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
24CrMo4	0.27	0.6	0.39	0.009	0.002	1.18	0.16	0,24	0	0.001	0.003	0	0.021
30CrMo5-2	0.33	0.55	0.32	0.014	0.006	2.072	1.24	0.23	0.001	0.02	0.003	0.11	0.026
34CrNiMo6	0.34	0.52	0.2	0.008	0.004	1.48	1.43	0.16	0	0.16	0.001	0.1	0.022
41Cr4	0.41	0.63	0.24	0.031	0.036	0.87	0.31	0.07	0.004	0.002	0.009	0.16	0.012
42CrMo4	0.4	0.72	0.24	0.014	0.001	0.99	0.09	0.17	0.001	0.003	0.005	0.13	0.04

Table 2.
Shape and heat treatment conditions of selected alloy steels

Steel grade	Quenching			Tempering			Diameter
	Temperature [°C]	Time [min]	Cooling medium	Temperature [°C]	Time [min]	Cooling medium	
24CrMo4	880	180	water	630	200	air	Φ150
30CrMo5-2	860	120	oil	630	240	air	Φ166
34CrNiMo6	860	150	polymer	550	240	air	Φ220
41Cr4	840	150	polymer	620	145	air	Φ120
42CrMo4	860	120	water	640	240	air	Φ182

Table 3.
Comparison between measured and predicted mechanical properties of selected alloy steels

Property	Measured	Predicted	Measured	Predicted	Measured	Predicted
Material	24CrMo4	24CrMo4	30CrMo5-2	30CrMo5-2	34CrNiMo6	34CrNiMo6
$R_{0,2}$ [MPa]	680	679	819	803	880	872
R_m [MPa]	791	778	1000	991	976	984
A_5 [%]	20.2	19,4	19.6	17.2	15.1	15.2
Z [%]	56.6	56,2	55.1	54.9	52.1	55.6
KCU2 [J/cm^2]	199-208	210-214	76-100	80-112	158-170	155-189
HB	222-268	220-245	277-292	281-289	310-325	316-332
Material			41Cr4	41Cr4	42CrMo4	42CrMo4
$R_{0,2}$ [MPa]			771	773	616	630
R_m [MPa]			912	909	825	851
A_5 [%]			17.6	17.6	18.6	18.6
Z [%]			55.0	54.9	55.0	55.1
KCU2 [J/cm^2]			164-199	165-189	95-130	103-144
HB			255-267	240-255	262-269	253-263

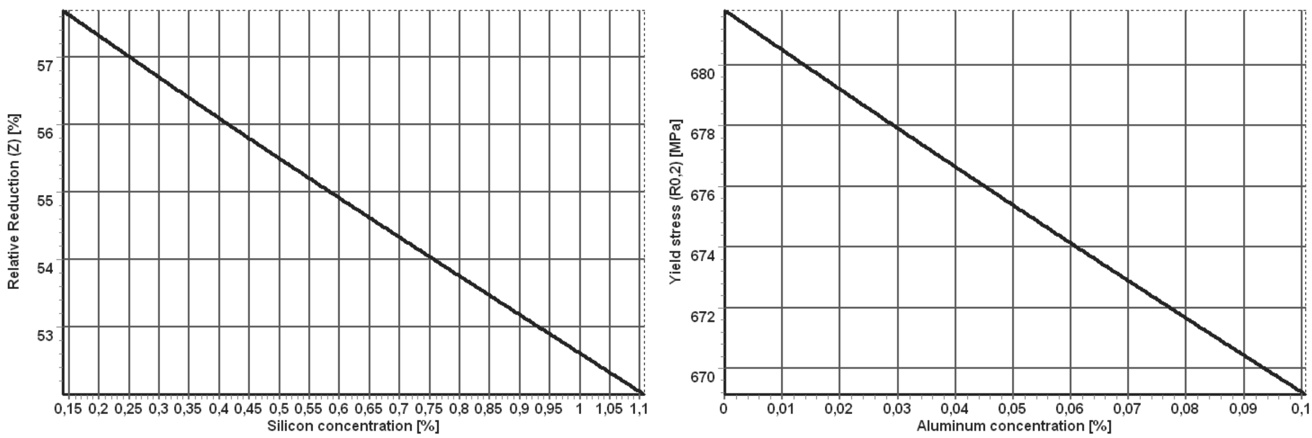

Fig. 1. Influence of silicon concentration on relative area reduction and aluminium concentration on yield stress based on 24CrMo4 steel

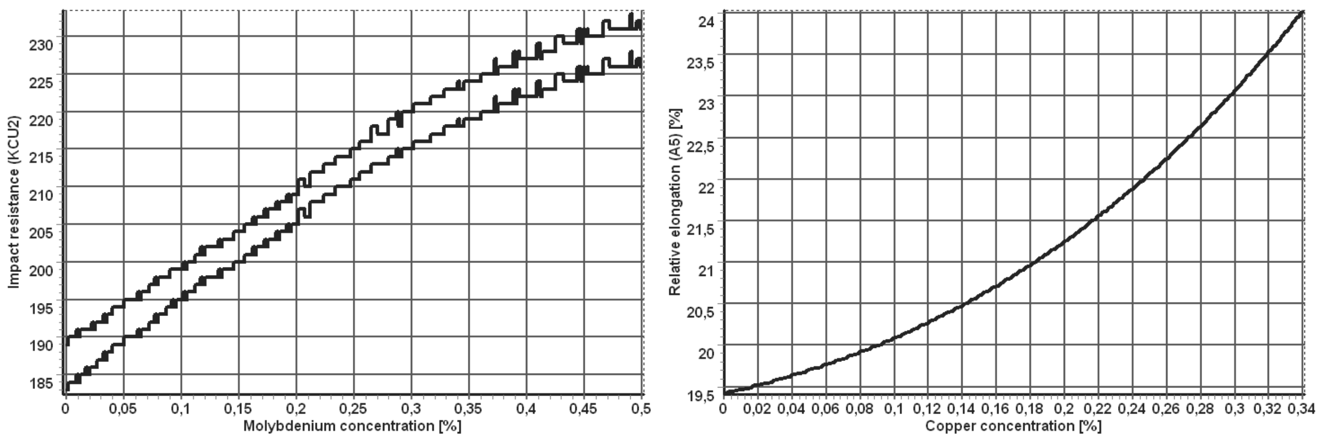

Fig. 2. Influence of molybdenum concentration on impact resistance and copper concentration on relative elongation based on 24CrMo4 steel

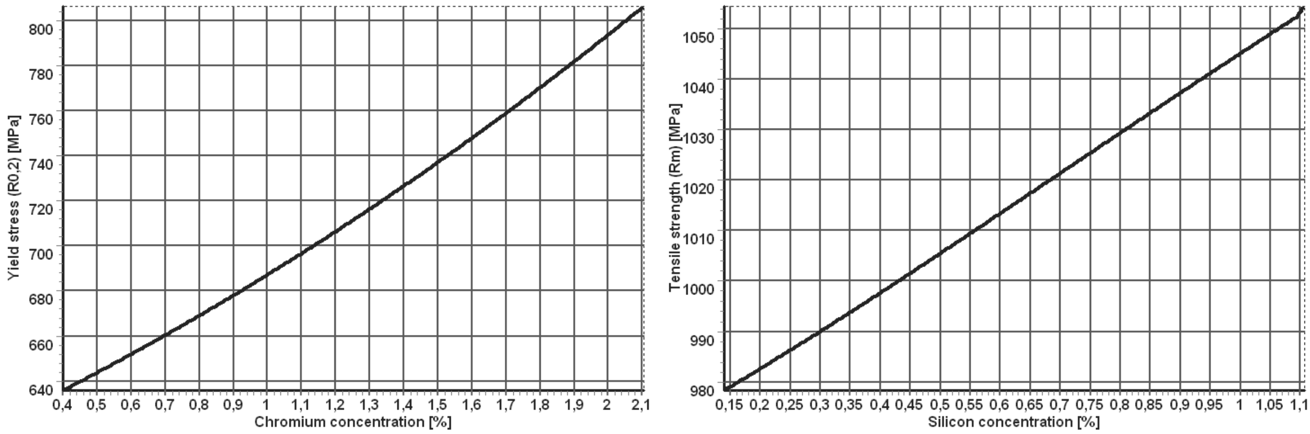

Fig. 3. Influence of chromium concentration on yield stress and silicon concentration on tensile strength based on 30CrMo5-2 steel

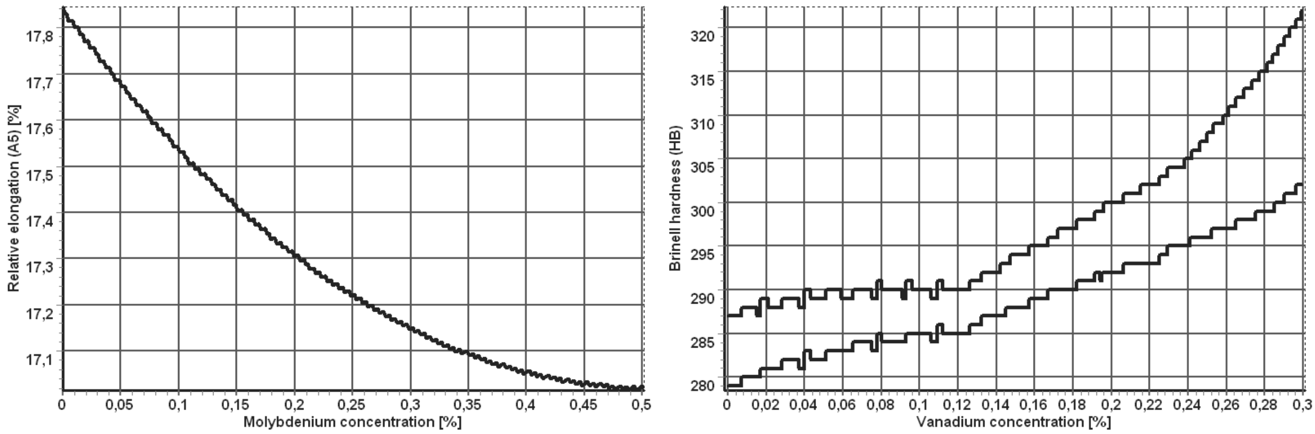

Fig. 4. Influence of molybdenum concentration relative elongation and vanadium concentration on Brinell hardness based on 30CrMo5-2 steel

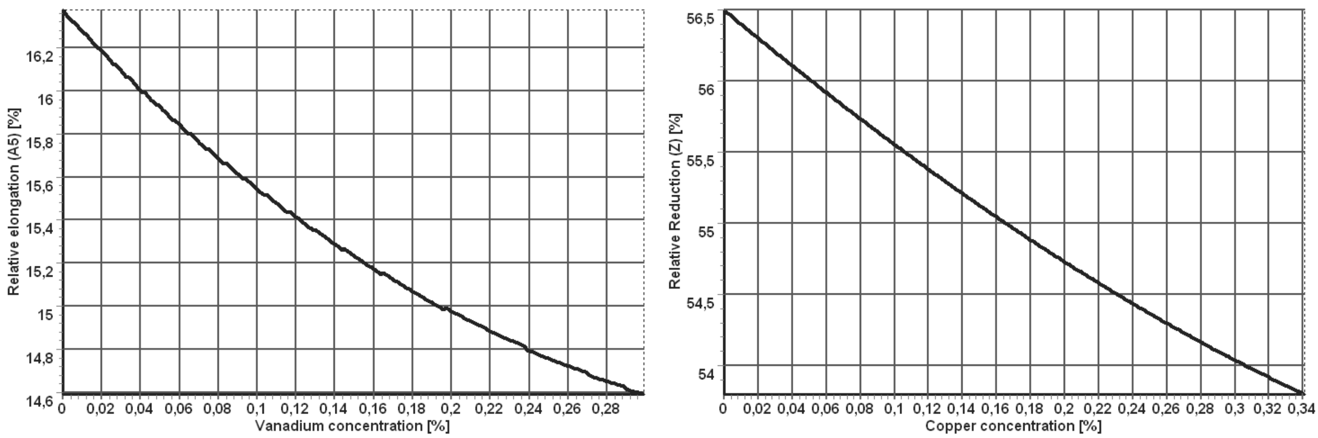

Fig. 5. Influence of vanadium concentration on relative elongation and copper concentration on relative area reduction based on 34CrNiMo6 steel

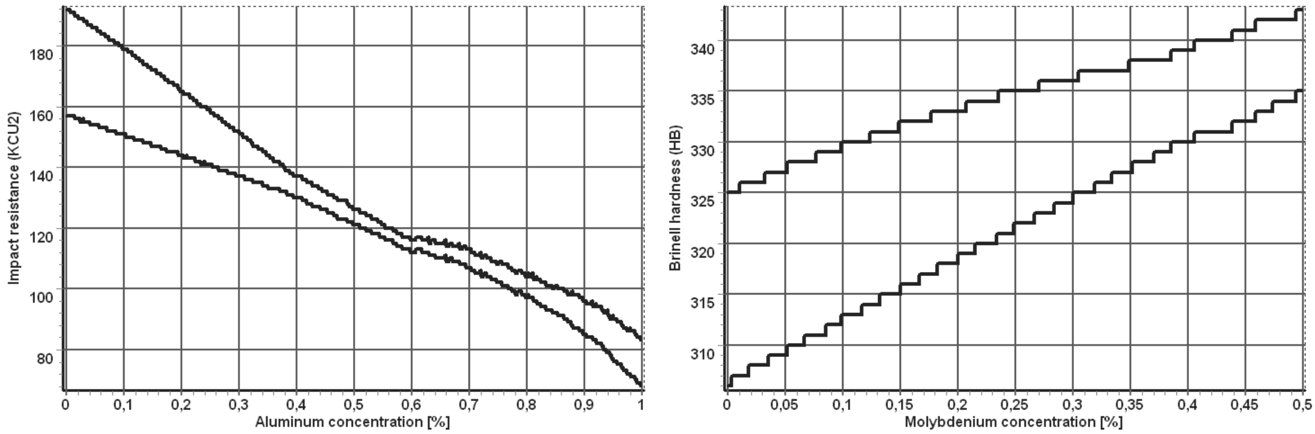

Fig. 6. Influence of aluminium concentration on impact resistance and molybdenum concentration on Brinell hardness based on 34CrNiMo6 steel

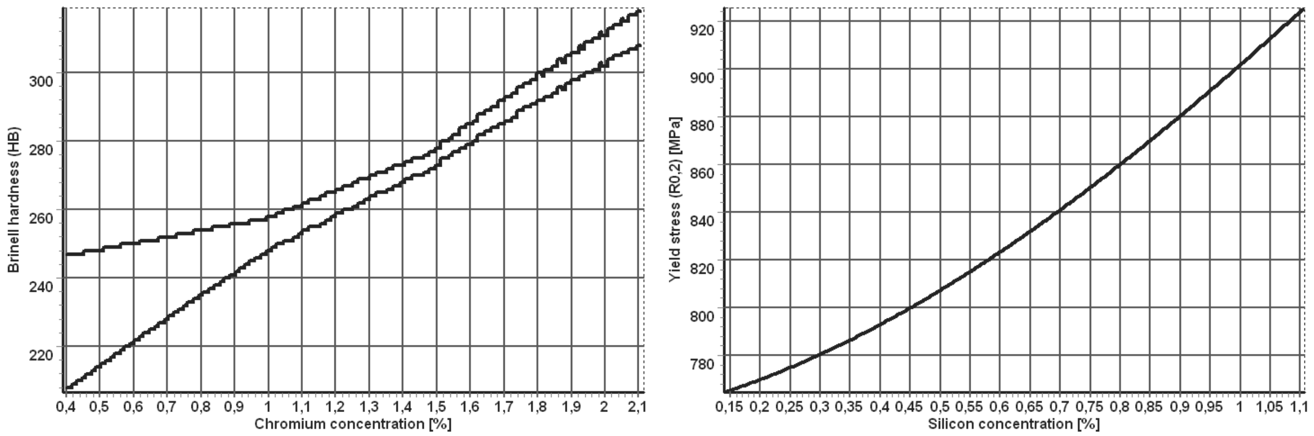

Fig. 7. Influence of chromium concentration on Brinell hardness and silicon concentration on yield stress based on 41Cr4 steel

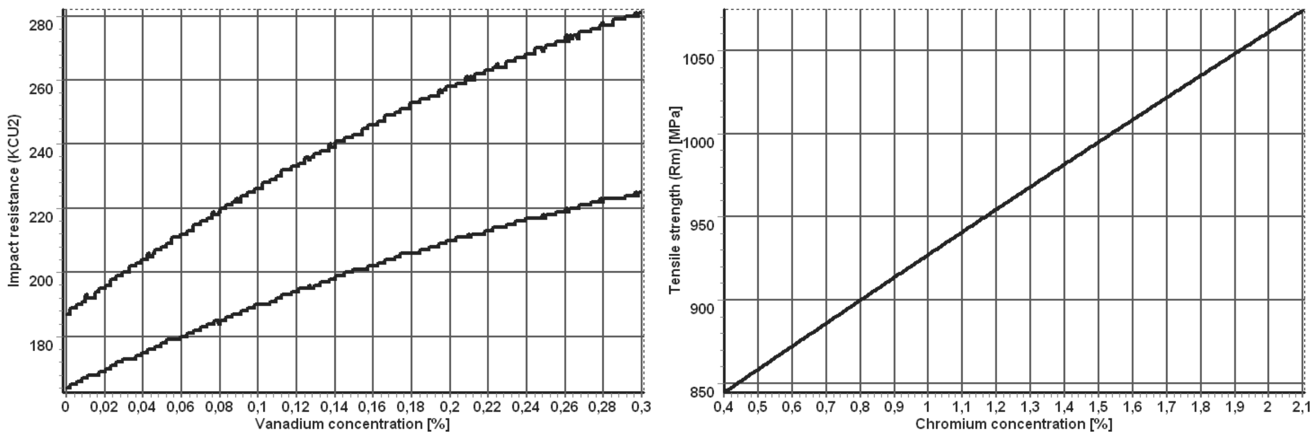

Fig. 8. Influence of vanadium concentration on impact resistance and chromium concentration on tensile strength based on 41Cr4 steel

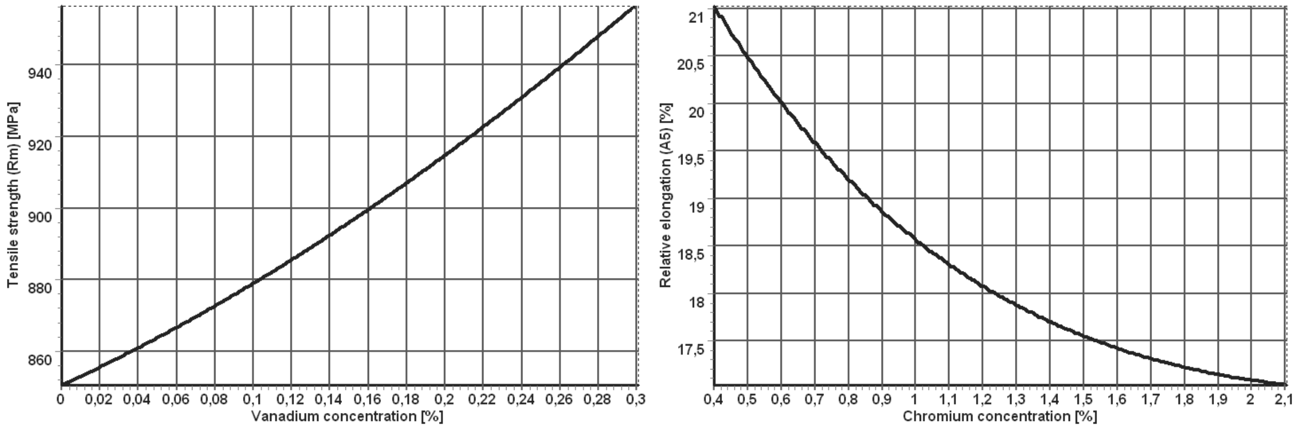

Fig. 9. Influence of vanadium concentration on tensile strength and chromium concentration on relative elongation based on 42CrMo4 steel

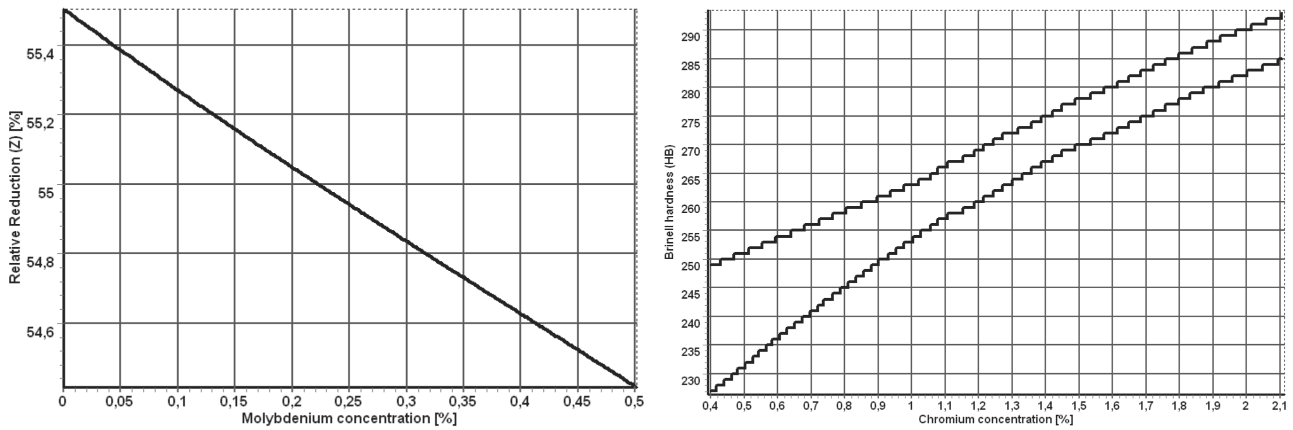

Fig. 10. Influence of molybdenium concentration on relative area reduction and chromium concentration on Brinell hardness based on 42CrMo4 steel

5. Conclusions

Materials researches performed in virtual environment with use of material science virtual laboratory in range of determining the mechanical properties of alloy structural steels are consistent with the results obtained during the real research in real investigative laboratory. Results 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 for quenching and tempering.

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.

Based on chemical elements concentration, parameters of heat and mechanical treatment, rod shape and geometrical dimensions with use of material science virtual laboratory it is possible to calculate the mechanical properties of any type of structural steel, with descriptors within the respective ranges. Results of virtual examinations can be presented as raw data or influence charts.

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, Descriptive physical metallurgy of iron alloys, Publishing House of the Silesian University of Technology, Gliwice, 2007 (in Polish).

[3] L.A. Dobrzański, Metal engineering materials, WNT, Warsaw, 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] 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.
[6] 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, Proceedings of the XXXVII Materials Science School, Cracow, 2009, 385-391.
[7] 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.
[8] L.A. Dobrzański, R. Honysz, Computer modelling system of the chemical composition and treatment parameters influence on mechanical properties of structural steels, Proceedings of the XXXVIII Materials Science School, Cracow, 2010, 368-373.
[9] L.A. Dobrzański, R. Honysz, Artificial intelligence and virtual environment application for materials design methodology, Journal of Machine Engineering 11/1-2 (2011) 102-119.
[10] R.L. Brockenbrough, F.S. Merritt, Structural steel designer's handbook, McGraw-Hill Professional, New York, 1999.
[11] 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.
[12] 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.
[13] 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.
[14] 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.
[15] 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.
[16] L.A. Dobrzański, R. Honysz, The idea of material science virtual laboratory, Journal of Achievements in Materials and Manufacturing Engineering 42/1-2 (2010) 196-203.
[17] http://www.vlab.imiib.polsl.pl.
[18] PN-EN 10204:2006.
[19] PN-EN 10083-1:2008.
[20] PN-EN 10083-3:2006.