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ANALYSIS OF ALLOYING ELEMENTS INFLUENCE ON PROPERTIES OF STRUCTURAL STEEL WITH USE OF MATERIALS SCIENCE VIRTUAL LABORATORY

ANALIZA WPŁYWU DODATKÓW STOPOWYCH NA WŁASNOŚCI STALI KONSTRUKCYJNYCH Z WYKORZYSTANIEM METODYKI WIRTUALNEGO LABORATORIUM INŻYNIERII MATERIAŁOWEJ

A b s t r a c t

The paper introduces analysis results of selected alloying elements influence on mechanical properties of alloy structural steels for quenching and tempering. Investigations were performed in virtual environment with use of materials science virtual laboratory. Virtual investigations results were verified in real investigative laboratory.

Keywords: *materials science virtual laboratory, structural steels, virtual investigations*

S t r e s z c z e n i e

W artykule przedstawiono przykładowe wyniki analizy wpływu wybranych pierwiastków stopowych na własności mechaniczne stopowych stali konstrukcyjnych do ulepszania cieplnego. Badania zostały wykonane w przestrzeni wirtualnej z wykorzystaniem wirtualnego laboratorium inżynierii materiałowej. Wyniki wirtualnych badań zweryfikowano w rzeczywistym laboratorium.

Słowa kluczowe: *wirtualne laboratorium inżynierii materiałowej, stal konstrukcyjna, wirtualne badania*

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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.

Modelling of steel 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. Material science research centres are engaged in intensive researches to develop computational models applicable to determination of the mechanical properties for several years [1–5].

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 performed 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 the tests 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 types 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 20 mm to 220 mm. 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 [12]. It was developed using the artificial intelligence tools and applied in 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 allows the mechanical properties prediction 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 results of computational experiments are presented in a openly form in simulations or printed as the investigation protocol of the mechanical and technological properties in accordance with [13]. 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 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 laboratory virtual sample files can be saved on computer hard disc for later use.

4. Influence analysis of alloying additions on mechanical propertiesof selected steels

For investigations, structural steels to toughening produced according to [14–15] were selected. 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 presented in table 1. Material was delivered as 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 the 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 types. Results are introduced in the table 3. Results of modelling are correct, because all three 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.

Influence analyses were conducted to calculate how big the influence of the alloy addiction concentration on steels mechanical properties is. Eight alloy addictions were selected - silicon, chrome, molybdenum, tungsten, vanadium, titanium, aluminium and copper. Dependence 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 procedure 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 influence graphs are presented on figures. 1-6. Full set of obtained results and generated influence graphs is presented in [1].

Table 1

Chemical composition of examined alloy steels

Steel sign.	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
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	0.024
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
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 examined alloy steels

Steel signature	Quenching			Tempering			Shape
	temp. [°C]	time [min]	medium	temp. [°C]	time [min]	medium	
30CrMo5-2	860	120	Oil	630	240	air	Φ166
34CrNiMo6	860	150	Polymer	550	240	air	Φ220
42CrMo4	860	120	Water	640	240	air	Φ182

Table 3

Comparison between measured and predicted mechanical properties of examined alloy structural steels

Property	measured	predicted	measured	predicted	measured	predicted
Material	30CrMo5-2		34CrNiMo6		42CrMo4	
$R_{0,2}$ [MPa]	819	803	880	872	616	630
R_m [MPa]	1000	991	976	984	825	851
A_5 [%]	19.6	17.2	15.1	15.2	18.6	18.6
Z [%]	55.1	54.9	52.1	55.6	55.0	55.1
KCU2 [J/cm^2]	76-100	80-112	158-170	155-189	95-130	103-144
HB	277-292	281-289	310-325	316-332	262-269	253-263

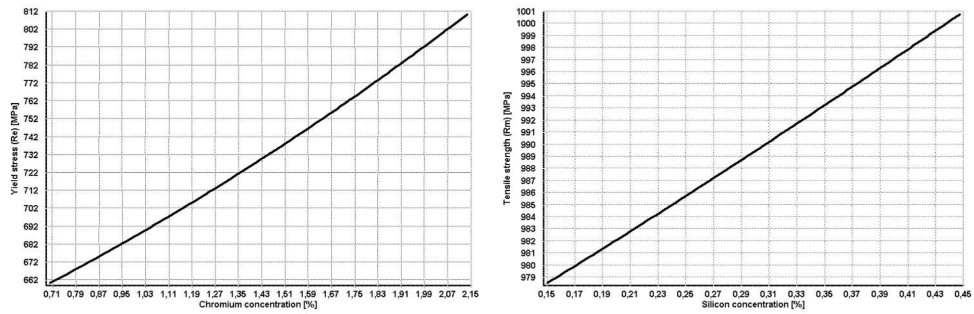

Fig. 1. Influence of chromium and silicon concentration on selected mechanical properties of 30CrMo5-2 steel

Rys. 1. Wpływ chromu i krzemu na wybrane własności mechaniczne stali 30CrMo5-2

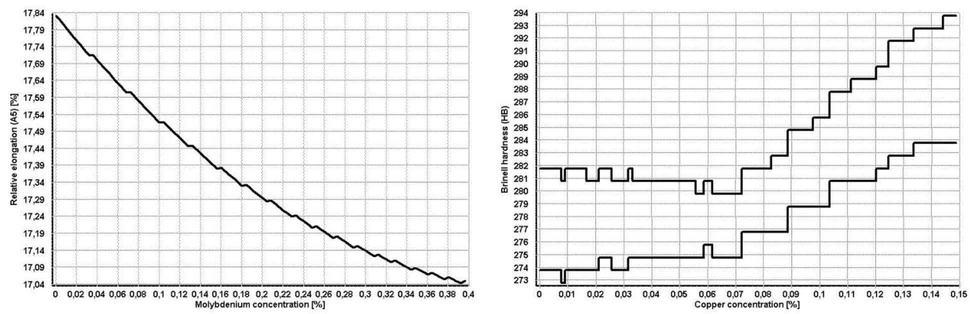

Fig. 2. Influence of molybdenum and copper concentration on selected mechanical properties of 30CrMo5-2 steel

Rys. 2. Wpływ molibdenu i miedzi na wybrane własności mechaniczne stali 30CrMo5-2

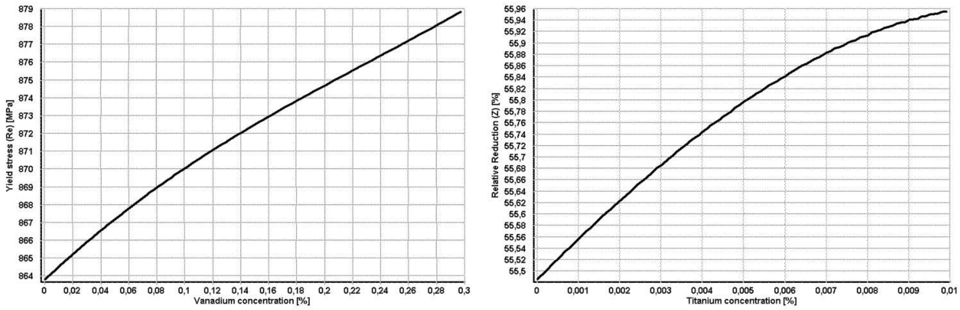

Fig. 3. Influence of vanadium and titanium concentration on selected mechanical properties of 34CrNiMo6 steel
Rys. 3. Wpływ wanadu i tytanu na wybrane własności mechaniczne stali 34CrNiMo6

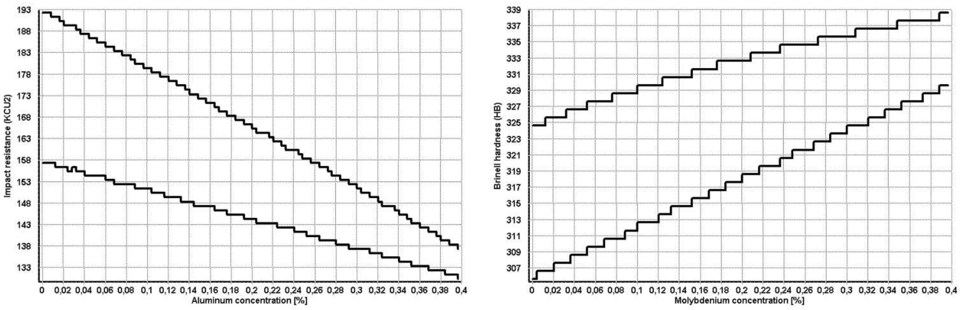

Fig. 4. Influence of aluminium and molybdenum concentration on selected mechanical properties of 34CrNiMo6 steel
Rys. 4. Wpływ aluminium i molibdenu na wybrane własności mechaniczne stali 34CrNiMo6

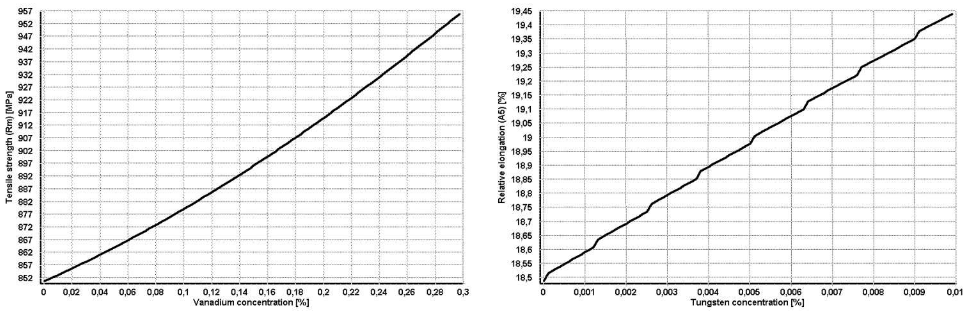

Fig. 5. Influence of vanadium and tungsten concentration on selected mechanical properties of 42CrMo4 steel
Rys. 5. Wpływ wanadu i tytanu na wybrane własności mechaniczne stali 42CrMo4

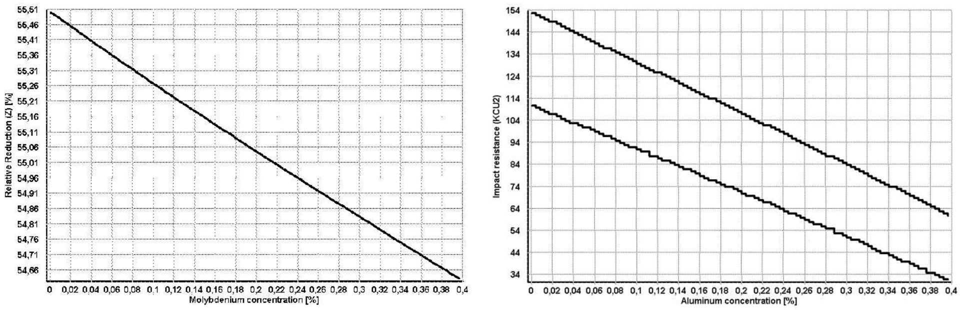

Fig. 6. Influence of molybdenum and aluminium concentration on selected mechanical properties of 42CrMo4 steel

Rys. 6. Wpływ molibdenu i aluminium na wybrane własności mechaniczne stali 42CrMo4

5. Conclusions

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. 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.

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