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Optimization of chemical composition and heat treatment condition of structural steel

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ABSTRACT

Purpose: This paper presents the methodology and results of virtual research project involving the optimization of the chemical composition and heat treatment conditions of structural steels. Investigations were performed in virtual environment with use of materials science virtual laboratory.

Design/methodology/approach: The first task was to search for such a range of chosen element concentration while keeping the concentration of other elements unchanged in order to satisfy all the conditions for steel mechanical properties defined by a virtual client. Second task of virtual research project consisted in searching for such ranges of temperature and time for hardening and tempering , to ensure that all the conditions for steel properties defined by a virtual client has been met without making changes in the chemical composition of steel.

Findings: Virtual investigations results were verified in real investigative laboratory. Results of virtual examinations are presented as raw data and influence charts.

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 shows 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: Computational material science; Materials science virtual laboratory; Structural steel; Virtual investigations

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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. Material science research centres for several years are engaged in intensive researches to develop computational models applicable to determination of the mechanical properties. Such model, with are providing a comprehensive modelling of the steels mechanical properties, has not been developed yet. There are many computational models described in the literature, which can be used for predicting the mechanical properties of different materials, but their usage in industry is limited because of narrow ranges of chemical composition or specific production conditions [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 were already developed in the Department of Materials Processing Technology, Management and Information Technology in Materials Institute of Engineering Materials and Biomaterials. Presented in this paper the new approach allows the methodical use of all available computational techniques, including the artificial intelligence tools and virtual environment [4-14].

2. Material

For materials investigation two non-alloy and alloy 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 section. 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 [10].

3. Results of the virtual designing of new, non-standard steel types

The aim of these researches was to design new hypothetical structural steels. Chemical composition and heat treatment conditions will be investigated and modified to meet the client's requirements about values of mechanical properties.

3.1. Chemical composition optimisation

The first design task for the virtual science virtual laboratory was to design a steel type, which fulfils the strict delivery conditions for concentrations of chemical elements. Demanded by the virtual client steel chemical composition is presented in Table 1. This is the 34CrNiMo6 steel produced in accordance with [15]. Steel has been heat and plastic treated to appropriate size. Processing conditions and geometric dimensions of the product are introduced in Table 2. Virtual client's demand was that steels chemical composition must be adapted to fulfil strictly defined conditions for the yield strength, tensile strength, relative elongation, impact strength and hardness with unchanged treatment conditions. All given assumptions are summarized in Table 3. For the chemical composition analysis eight chemical elements was selected – carbon, manganese, silicon, chromium, nickel, molybdenum, vanadium and titanium. Virtual research project in first task consisted in finding such a range of concentrations of given elements, while keeping the other concentrations and treatment conditions unchanged in order to fulfil all conditions for steel properties defined by a virtual client. The results of the analysis are performed in Table 4. Table 5 shows the results of properties modelling of 34CrNiMo6 steel before and after the modification of chemical composition.

Table 1.
Chemical composition of examined base steels

steel signature	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
34CrNiMo6	0.32	0.52	0.16	0.009	0.011	1.48	1.43	0.15	0	0	0	0.19	0
C45R	0.47	0.61	0.39	0.021	0.018	0.31	0.24	0.005	0.002	0.013	0	0.03	0.035

Table 2.
Shape and head treatment conditions of examined base steels

steel signature	quenching			tempering			rod shape
	temperature	time	coolant	temperature	time	coolant	
	°C	min		°C	min		
34CrNiMo6	860	180	oil	580	270	air	∅210
C45R	880	60	oil	690	60	air	□100

Table 3.
The required mechanical properties of structural steels for quenching and tempering

base steel	34CrNiMo6	C45R
$R_{0.2}$	min 680 MPa	750-850 MPa
R_m	880-1080 MPa	1200-1320 MPa
A_5	min 13%	min15%
KV	min 40 J	min. 40 J
HB	277-285	290-300

Table 4.
Results of chemical composition modelling of alloy structural steel for quenching and tempering 34CrNiMo6

Property	%C	%Mn	%Si	%Cr	%Ni	%Mo	%V	%Ti
$R_{0.2}$	0.34-0.47	1.01-1.58*	0.31-0.93	1.68-2.19*	1.97-2.08*	0.21-0.89	0.02-0.198	—
R_m	0.35-0.48	0.68-1.47	0.57-1.12*	1.25-2.19*	1.86-2.08*	0.29-1.09*	0.092-0.296	0-0.082
KV_{min}	0.32-0.44	0.26-1.36	0.43-1.20*	1.24-2.19*	0-2.01	0-0.53*	0-0.3*	0-0.008
KV_{max}	0.34-0.6*	0.52-1.58*	0.14-1.20*	1.78-2.19*	0-2.01	0.03-0.49	0.06-0.3*	0-0.124
HB_{min}	0.38-0.49	1.05-1.48	0.45-0.74	1.86-2.18	— **	0.55-1.09	0.16-0.3*	0.026-0.084
HB_{max}	0.36-0.40	0.92-1.28	0.36-0.54	1.75-2.02	— **	0.42-0.66	0.094-0.272	0.006-0.012
Range	0.38-0.40	1.05-1.28	—	1.86-2.04	—	—	0.16-0.198	—

* – range of property variability partially exceeded the permissible range of chemical element concentration.
** – range of property variability entirely exceeded the permissible range of chemical element concentration

Table 5.
Verification of the mechanical properties of 34CrNiMo6 steel before and after chemical modification

element	not	modified C		modified Mn		modified Cr		modified V	
property	modified	minimum	maximum	minimum	maximum	minimum	maximum	minimum	maximum
$R_{0.2}$	660	741	770	684	717	696	712	836	880
R_m	910	978	1001	1014	1060	960	981	965	981
A_5	17.5	16.8	16.6	16.8	16.6	17.7	16.8	16.7	16.5
Z	54.7	54.0	53.8	54.1	54	54.7	54.8	54.8	54.9
KV	96-104	78-95	72-92	86-91	85-91	90-99	87-97	82-93	80-91
HB	261-266	278-285	283-292	278-284	285-292	278-285	284-292	278-281	280-284

3.2. Heat treatment conditions optimisation

The second task was to design virtual steel, which meets strict delivery conditions by modifying only the conditions of heat treatment. Chemical composition of base steel supplied by the client (C45R according to [16]) is given in Table 1. Treatment conditions and geometric dimensions of the product are introduced in Table 2. This time, the virtual client's demand was matching of steel's heat treatment condition. Strictly defined conditions for the yield strength, tensile strength, relative elongation, impact strength and hardness with unchanged chemical composition should be achieved. All assumptions are summarized in Table 3. Virtual research project in the second task included the search for such ranges of temperature and time of quenching and tempering. All conditions for steel properties defined by a virtual client should be fulfilled without changes in the steel's chemical composition. Table 6 and Table 7 shows the results of properties modelling of C45R steel before and after the modification of heat treatment conditions. The relative elongation was not included in examinations, because this condition was already fulfilled the base steel.

3.3. Laboratory verification

To verify, if the projecting operations were performed correctly, steels with revisited descriptors have been manufactured in a factory. Steels from both tasks were marked with symbols PR1 and PR2. A modified chemical composition of steel is summarized in Table 8, the modified heat treatment conditions of steel PR2 are summarized in Table 9. Produced steels after heat and plastic treatment were examined in real laboratory. Obtained results are presented together with the results of the virtual examinations performed with use of material science virtual laboratory in Table 10. Real examinations results are comparable with results of virtual examinations, which means, that the projecting operations were performed correctly.

Comparison charts describing the range of variability of the chemical elements, temperature, and time ranges for defined mechanical properties were developed. Selected influence graphs for modified chemical composition are presented in Figs. 1-4. Selected influence graphs for modified heat treatment conditions are presented in Figs. 5-7. Complete set of results is presented in [1].

Table 6.
Results of heat treatment temperature and time modelling of non-alloy structural steel for quenching and tempering C45R

property	quenching temperature	quenching time	tempering temperature	tempering time
$R_{0.2}$	818-877	10-150*	592-671	61-85
R_m	844-887	77-150*	486-660	86-121
KV_{min}	760-858	63-150*	480-740*	12-120*
KV_{max}	762-888	41-89	480-740*	12-120*
HB_{min}	838-856	10-102*	589-628	68-76
HB_{max}	848-872	68-150	618-660	62-72
Range	848-856	77-89	658-662	—

* – range of property variability partially exceeded the permissible range of heat treatment temperature or time

Table 7.
Verification of the mechanical properties of C45R steel before and after heat treatment conditions modification

element	not modified	modified quenching temperature		modified quenching time		modified tempering temperature	
property		minimum	maximum	minimum	maximum	minimum	maximum
$R_{0.2}$	746	792	779	763	761	817	805
R_m	1154	1211	1201	1200	1216	1224	1218
A_5	21.0	18.5	19.1	19.6	19.4	18.1	18.4
Z	42.7	42.6	42.6	42.7	42.7	41.7	41.7
KV	33-44	43-62	40-58	49-79	58-99	70-92	71-93
HB	279-284	294-300	290-297	292-295	291-294	292-300	290-298

Table 8.
Chemical composition of examined newly designed steels

steel signature	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
PR_1	0.38	0.53	0.17	0.008	0.012	1.49	1.43	0.15	0	0	0	0.19	0.01
PR_2	0.45	0.64	0.39	0.017	0.016	0.3	0.24	0.005	0.002	0.012	0	0.03	0.031

Table 9.
Shape and head treatment conditions of examined newly designed steels

steel signature	quenching			tempering			rod shape
	temperature	time	coolant	temperature	time	coolant	
	°C	min		°C	min		
PR_1	860	180	oil	580	270	air	∅210
PR_2	880	60	oil	660	60	air	□100

Table 10.
Comparison between measured and predicted mechanical properties of newly designed steels

Property	predicted	measured	predicted	measured
Material	PR_1		PR_2	
$R_{0.2}$	744	748	797	800
R_m	980	977	1216	1218
A_5	16.8	16.3	16.7	16.3
Z	54.2	55.1	37.7	36.9
KV	77-94	78-103	96-102	88-113
HB	277-286	280-284	289-296	291-303

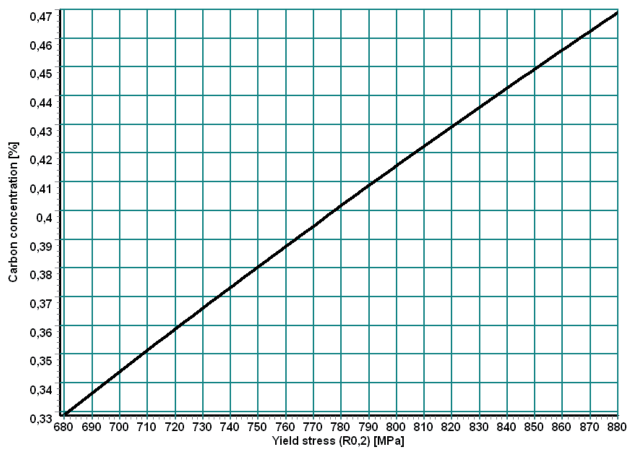

Fig. 1. Influence of yield stress on carbon concentration of 34CrNiMo6 steel

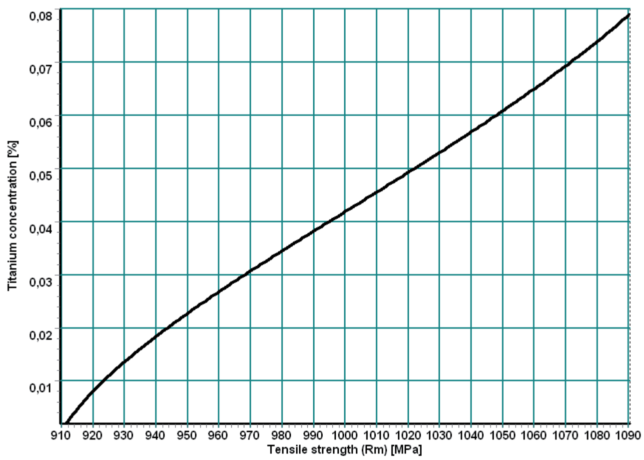

Fig. 2. Influence of tensile strength on titanium concentration of 34CrNiMo6 steel

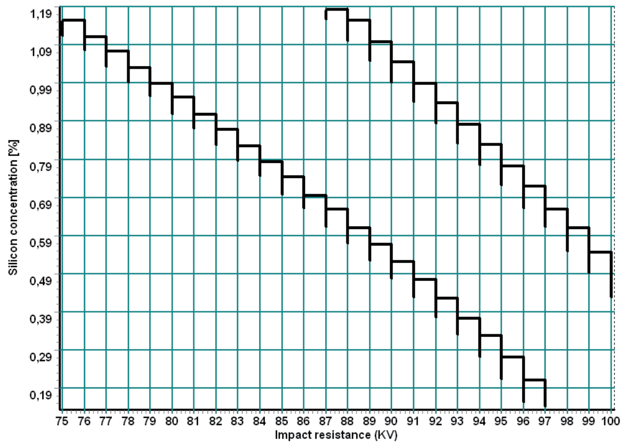

Fig. 3. Influence of impact resistance on silicon concentration of 34CrNiMo6 steel

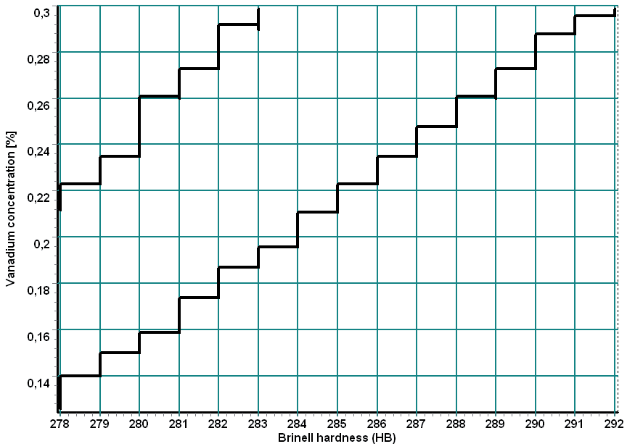

Fig. 4. Influence of Brinell hardness on vanadium concentration of 34CrNiMo6 steel

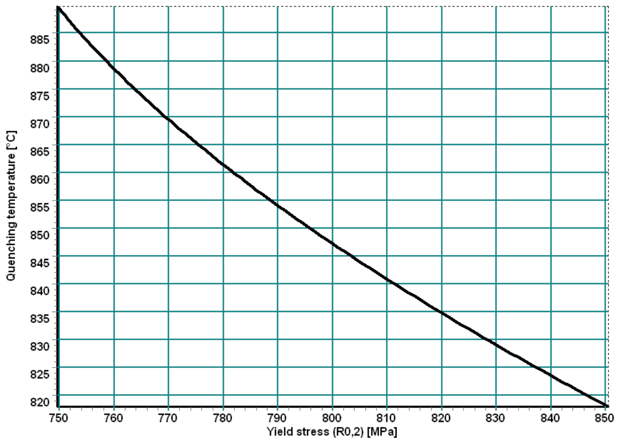

Fig. 5. Influence of yield stress on quenching temperature of C45R steel

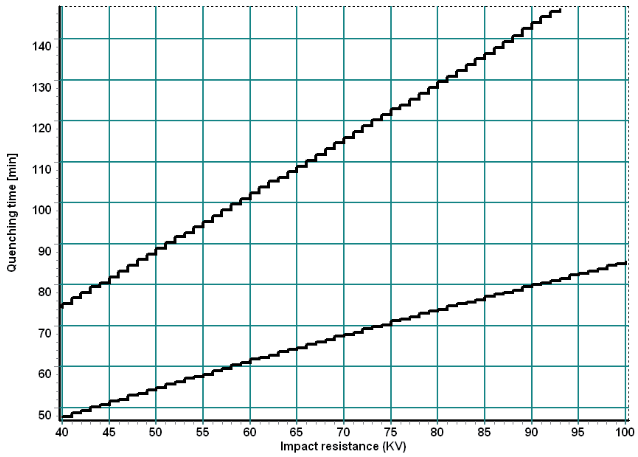

Fig. 6. Influence of impact resistance on quenching time of C45R steel

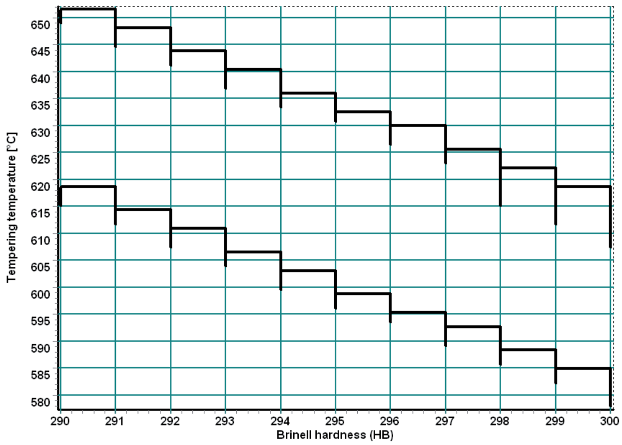

Fig. 7. Influence of Brinell hardnes on tempering temperature of C45R steel

4. Conclusions

Materials researches performed in virtual environment with use of material science virtual laboratory in range of chemical composition and heat treatment condition of structural steel optimisation 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. Performed verification investigations presented in this paper on selected mechanical properties modelling examples of structural steels confirm the possibility of its use in the industrial production, both to predict the properties, as well as to design new types of steel.

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