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Influence analysis of admixtures on mechanical properties of non-alloy structural steels

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

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1. Introduction

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 of 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 [1].

Modelling of steels mechanical properties is also associated with financial benefits, because expensive and time-consuming researches obtained in the real laboratory are reduced to necessary minimum. Necessary is the verification of computations [2-6].

Presented in this paper the new approach of steel investigation performed with use of materials science virtual laboratory allows the methodical use of all available computational techniques, including the artificial intelligence tools and virtual environment [7-13].

2. Material and investigation methodology

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. Structural Steels are used in many applications, because they combining good mechanical properties with low price. The uses are various including civil and industrial engineering [14].

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 the basic alloy element maintains carbon, which regulates the properties of steel and from which content depends the application of the steel [15-17].

All investigations were performed in NeuroLab system. This is authorship software, which use artificial intelligence algorithms to predict the mechanical properties of non-alloy and alloy structural steel. This 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 on the basis of mechanical properties values is possible to determine steel's production conditions. The results of computational experiments are presented in an openly form in the application window or printed as the investigation protocol of the mechanical and technological properties [18-23].

Investigations were performed with use of samples made from non-alloy structural steels for general use described in Polish and European standard [24]. Designation and chemical composition are presented in Table 1. 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. 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 and rolled round and square rods. Dimensions of rods and heat treatment conditions are presented in Table 2.

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

The influence analysis of the admixtures concentration on mechanical properties was conducted. Five types of steel grades were selected for investigations. 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.

NeuroLab system has the ability to generate relation graphs between the mechanical properties of steel and parameters used to their estimation. Possible is the examination of the influence of any parameter from the input parameters on the value of any mechanical properties from the predicted results, when the rest of parameters remain unchanged.

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. The chemical concentration ranges are:

- Mn to 1.5%,
- Si to 0.5%,
- P to 0.05%,
- S to 0.05%.

Influence graphs are presented in Figs. 1-10. Due to the limited space of the article, only selected graphs are presented. Complete result set obtained during this analysis is presented in [1]. Calculated values of yield stress $R_{0.2}$, tensile strength R_m, relative elongation A_5 and relative area reduction Z presented on graphs are marked with a single line. The value ranges of impact resistance KV and hardness HB are marked between two lines indicating the minimum and maximum value.

Table 1.
Chemical composition of examined non-alloy steels

Steel signature	C	Mn	Si	P	S	Cr	Ni	Cu	Al
S235J2G3	0.16	0.81	0.22	0.01	0.02	0.13	0.09	0.08	0.04
S235JR	0.14	0.73	0.34	0.01	0.01	0.13	0.15	0.11	0.03
S275JR	0.18	0.7	0.31	0.01	0.01	0.11	0.13	0.17	0.02
S355K2G3	0.20	1.12	0.35	0.04	0.02	0.01	0.04	0	0.04
S355J2G3C	0.29	1.52	0.89	0.01	0.007	0.14	0.07	0.004	0.23

Table 2.
Shape and heat treatment conditions of examined non-alloy steels

Steel signature	Normalising			plastic treatment	shape
	temperature [°C]	time [min]	cooling medium		
S235J2G3	880	60	air	rolling	Φ100
S235JR	880	120	air	forging	Φ120
S275JR	880	60	air	forging	Φ100
S355K2G3	880	60	air	forging	Φ100
S355J2G3C	900	90	air	rolling	Φ170

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

Property	Measured	Predicted	Measured	Predicted	Measured	Predicted
Material	S235J2G3	S235J2G3	S235JR	S235JR	S275JR	S275JR
$R_{0,2}$ [MPa]	307	306	304	305	302	304
R_m [MPa]	461	467	480	482	506	502
A_5 [%]	33.8	34.0	35.4	35.5	35.5	33.8
Z [%]	64.1	65.7	65.9	65.9	59.9	62.3
KV [J]	137-143	108-143	144-150	146-154	124-142	111-126
HB	112-129	124-134	135-142	137-143	143-146	138-146
Property			Measured	Predicted	Measured	Predicted
Material			S355K2G3	S355K2G3	S355J2G3C	S355J2G3C
R0,2 [MPa]			362	379	322	325
Rm [MPa]			573	596	588	595
A5 [%]			31.0	27.6	28.8	29.9
Z [%]			52.0	56.0	69.2	68.2
KV [J]			102-139	106-113	111-144	63-144
HB			149-159	155-162	155-156	155-160

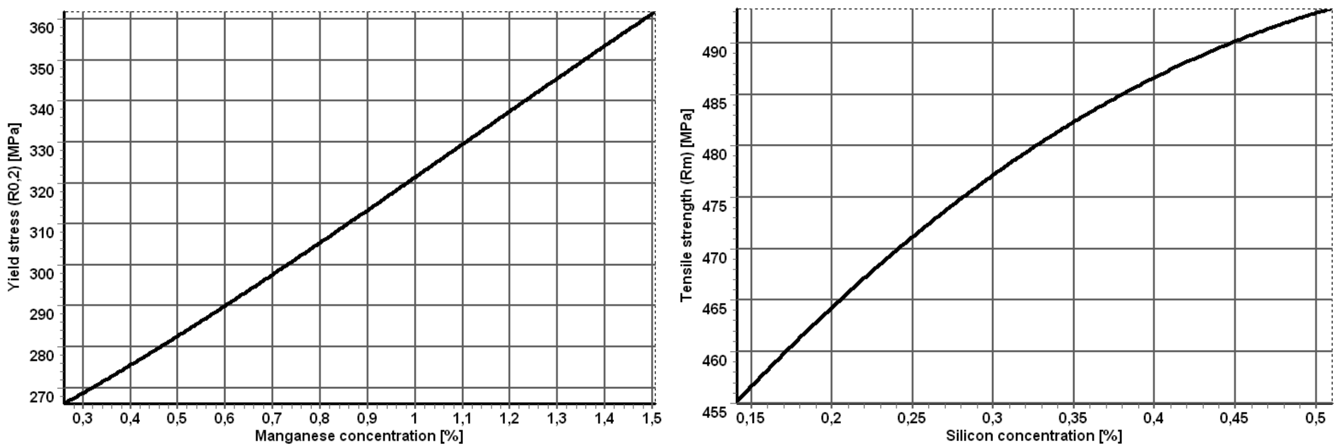

Fig. 1. Influence of manganese concentration on yield stress and silicon concentration on tensile strength of S235J2G3 steel

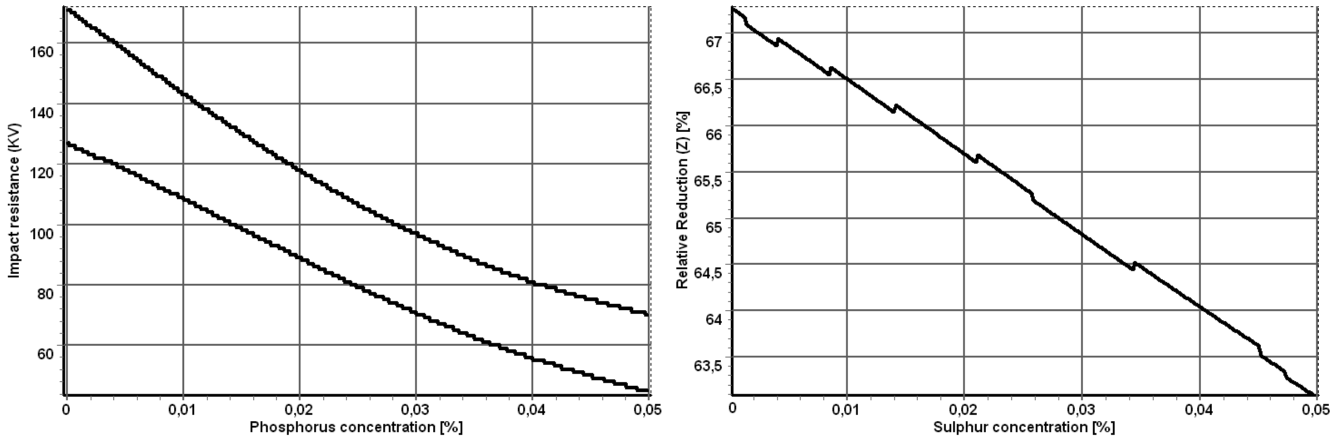

Fig. 2. Influence of phosphorus concentration on impact resistance and sulphur concentration on relative reduction of S235J2G3 steel

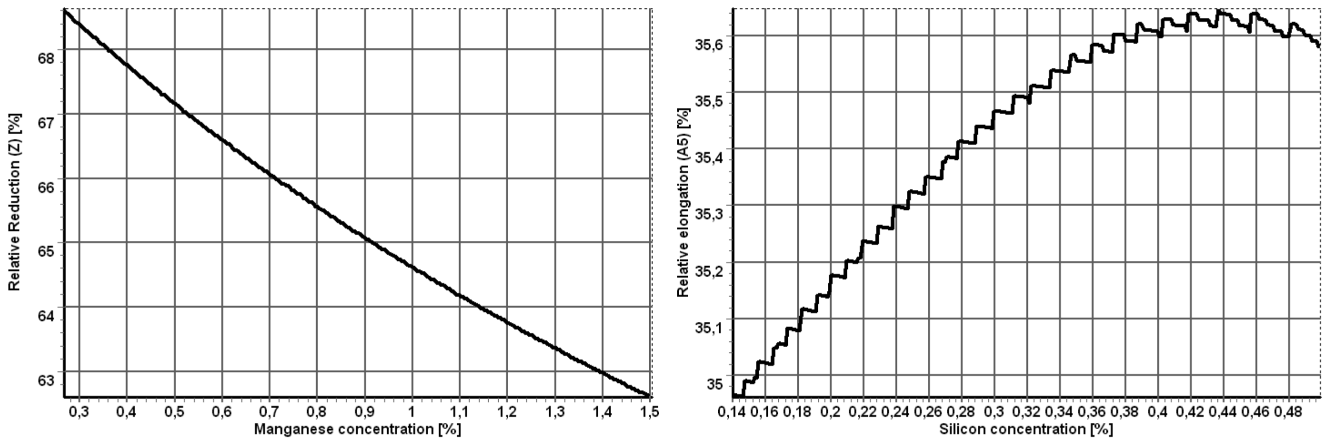

Fig. 3. Influence of manganese concentration on relative reduction and silicon concentration on relative elongation of S235JR steel

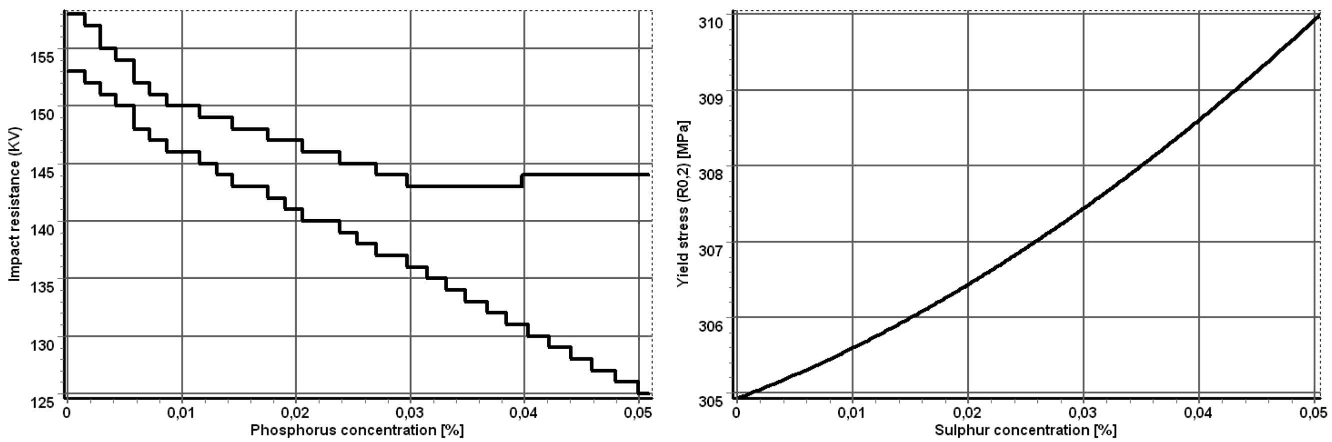

Fig. 4. Influence of phosphorus concentration on impact resistance and sulphur concentration on yield stress of S235JR steel

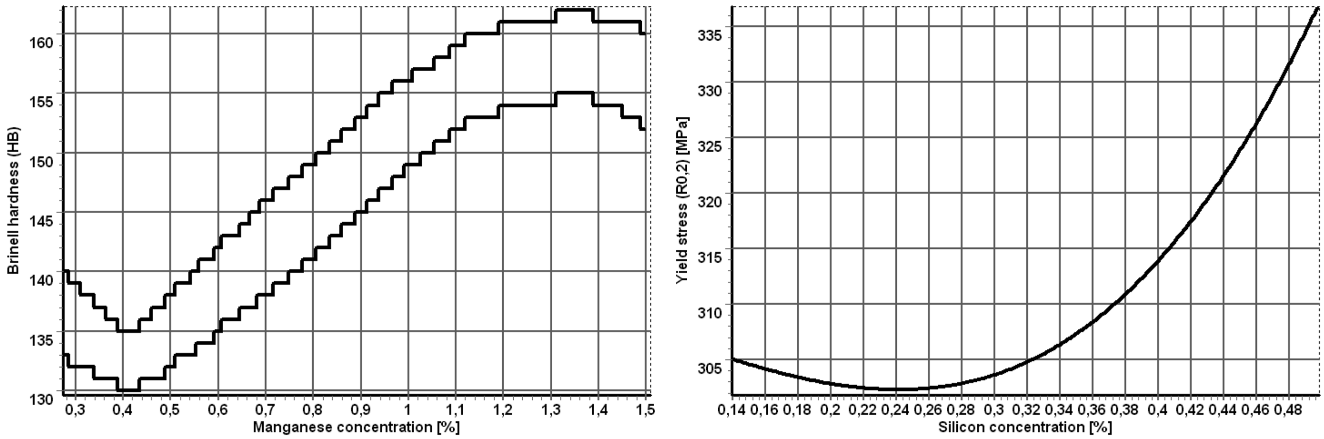

Fig. 5. Influence of manganese concentration on Brinell hardness and silicon concentration on yield stress of S275JR steel

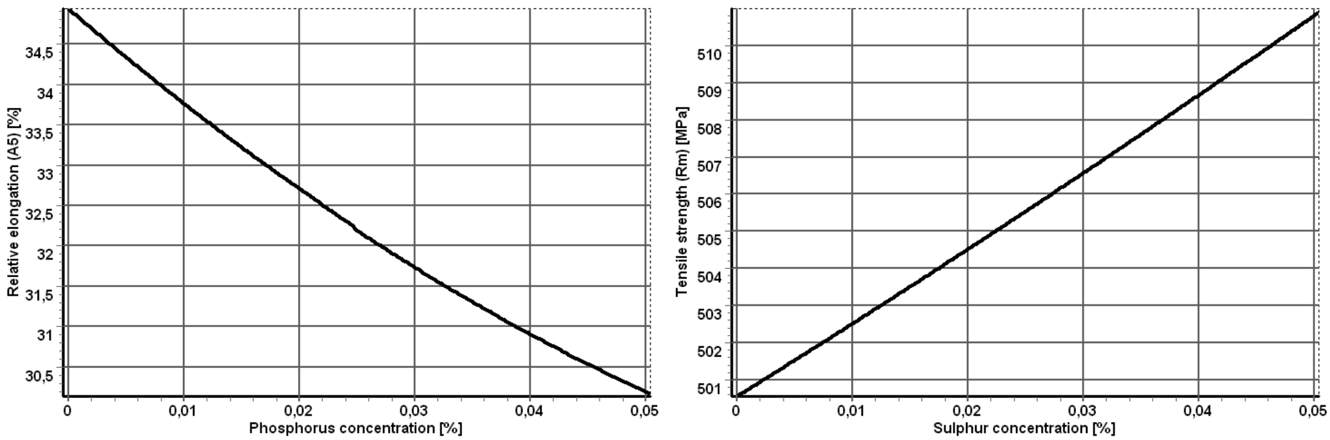

Fig. 6. Influence of phosphorus concentration on relative elongation and sulphur concentration on tensile strength of S275JR steel

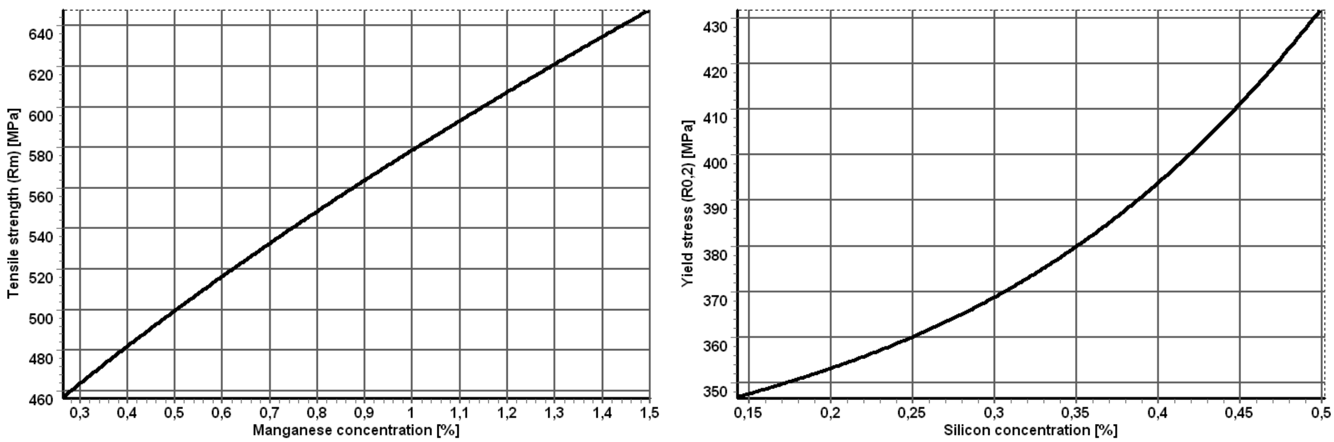

Fig. 7. Influence of manganese concentration on tensile strength and silicon concentration on yield stress of S355K2G3 steel

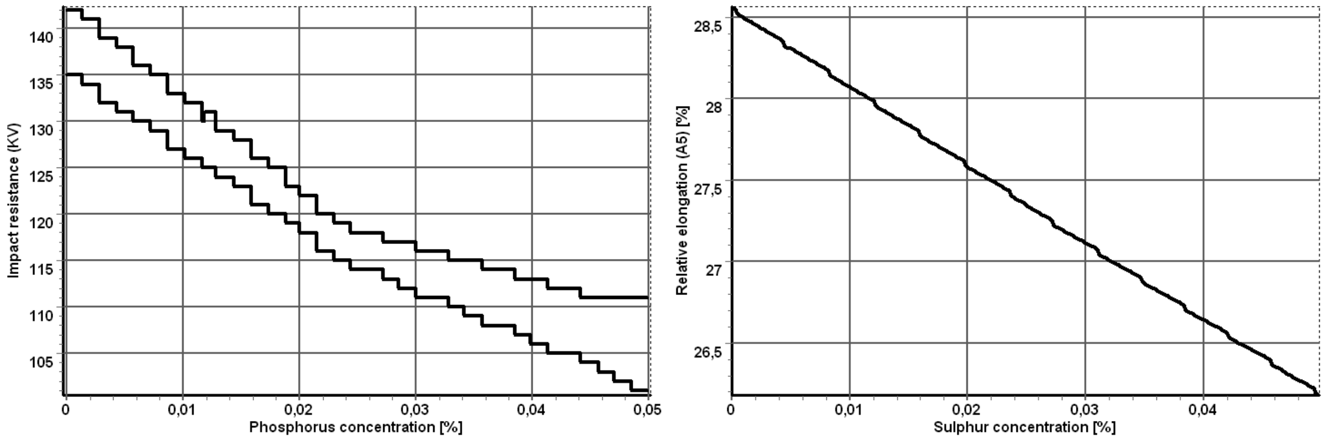

Fig. 8. Influence of phosphorus concentration on impact resistance and sulphur concentration on relative elongation of S355K2G3 steel

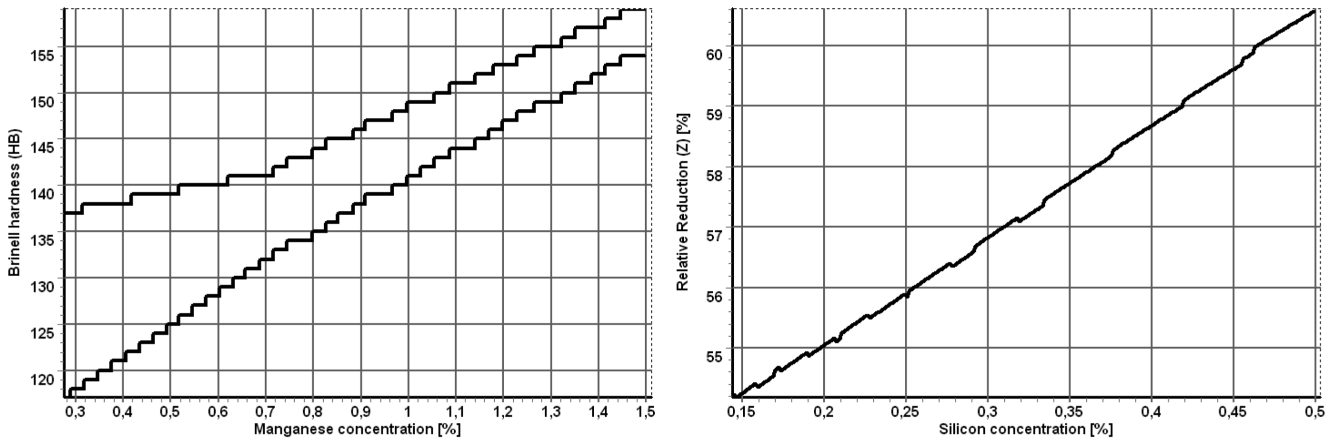

Fig. 9. Influence of manganese concentration on tensile strength and silicon concentration on yield stress of S355J2G3C steel

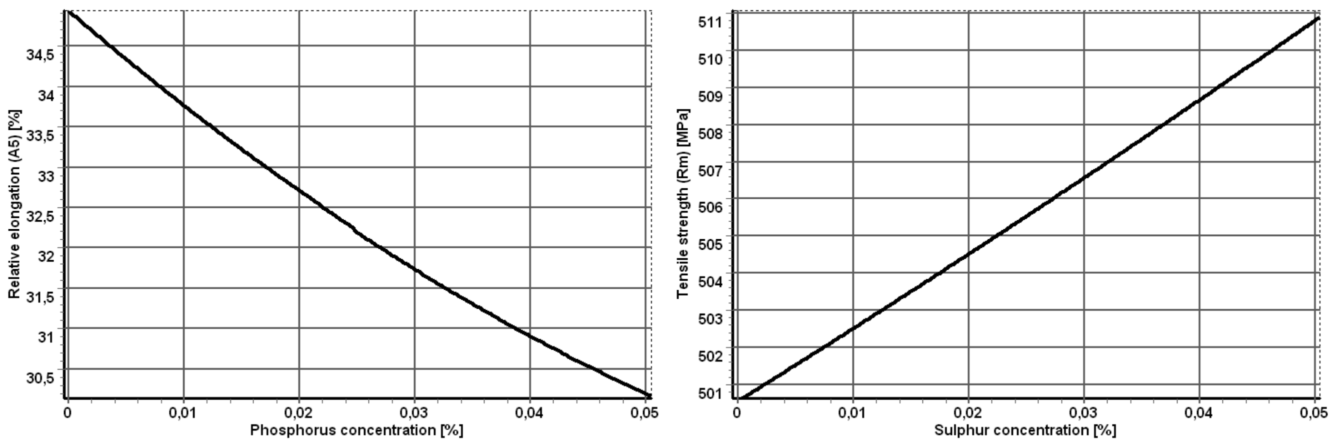

Fig. 10. Influence of phosphorus concentration on relative elongation and sulphur concentration on tensile strength of S355J2G3C steel

4. Conclusions

All estimated results are correct for all examined steel samples, because all 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.

Through the designation of relationships between the selected mechanical properties and the chemical concentration and treatment at selected ranges, it is possible to obtain data on the hypothetical and newly designed materials, which exist only in the virtual space. Ability to design new materials with unique properties strictly adjusted to client's current needs is the key in achieving market success.

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