A R C H I V E S O F M E T A L L U R G Y A N D M A T E R I A L S
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THE PREDICTION OF HARDENABILITY USING NEURONAL NETWORKS

SYMULACJA HARTOWNOŚCI OPARTA O ZASTOSOWANIE SZTUCZNYCH SIECI NEURONOWYCH

The data base which was used for development of the model consists from measurements of hardness profile from jominy test samples. It contains almost twenty thousand data vectors with extensive range of chemical composition.

The model was developed on the basis of neuronal networks and its successfulness was verified.

For each of four most influential chemical elements (carbon, nickel, chromium and molybdenum) two different diagrams are presented in this work. One gives the information how the change of alloying element influences the hardness close to surface. Other shows the change of hardenability with respect to change in chemical composition.

In the article it was publicized that, in spite of great variations in chemical compositions of each steel grade and data base it self, very accurate predictions of hardenability can be maid.

Keywords: neuronal networks, hardenability, chemical composition, jominy test

Baza danych zastosowana do stworzenia modelu hartowności składała się z pomiarów uzyskanych metodą Jominy'ego. Baza zawierała prawie dwadzieścia tys. rekordów z dużym zakresem zmienności składów chemicznych. Stworzony model został oparty o sztuczne sieci neuronowe i został pozytywnie zweryfikowany.

Dla każdego z czterech najsilniej oddziałujących pierwiastków (węgiel, nikiel, chrom i molibden) przedstawiono dwie zależności w postaci wykresów. Pierwsza podaje wpływ zawartości pierwiastka na twardość na powierzchni próbki. Drugi wpływ odległości od czoła próbki i zawartości pierwiastka na hartowność.

W pracy wykazano, że pomimo dużego zróżnicowania składów chemicznych różnych grup stali otrzymano zadowalającą dokładność obliczeń modelu.

1. Introduction

The simple analysis of the jominy test results could not give the exact answer about the influence of the chemical composition on the material hardness or hardenability. The reason is in the chemical composition variances within the particular steel grade prescribed tolerances. We have to deal with great number of data points which can be mutual dependence, commonly also with unlinear dependence.

Common methods for the representation of the link between influential parameters are linear and unlinear regression methods [1]. Nowadays the artificial intelligence methods are frequently used, i.e. neuronal networks [2-5].

In the presented work the use of the neuronal networks for the prediction of the hardenability of the constructional steel will be discussed.

2. Determination of the chemical composition on the hardenability

The data base for the determination and further predictions of the hardenability depend from the chemical composition are the results of hardness measurements of jominy tests which were made in Metal Ravne. The measurements were made on the distances from 1,5 mm to 70,0 mm starting from the quenched surface.

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2.1. The neuronal network selection and data base configuration

The program *STATISTICA Neuronal Networks* was used. The main advantage of this program is that it contains various types of the neuronal networks and that make it suitable for solving problems from different areas, for regression as well as classification cases.

The problem which was studied is typical regression problem thus MLP (multilayer perceptrons) type neuronal network was used. It contains three layers, ten input parameters in first layer, five neurons in hidden layer and one output parameter – hardness (figure 1). Ten input parameters corresponds nine chemical elements which were considered in the analysis, and tenth input parameter was distance between quenched surface and measuring point.

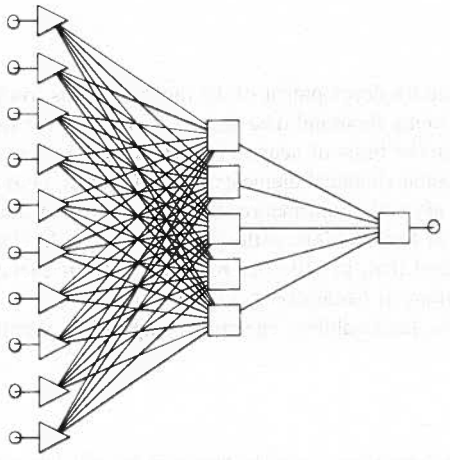


Fig. 1. The schematic presentation of neuronal network with 3 layers; 10 input parameters, 5 neurons in hidden layer and one output parameter

For the MLP training the Levenberg-Marquardtov algorithm was used because it gives the best results for the smaller neuronal networks (up to about hundred neurons) with only one output parameter. It is generally known as one of the best unlinear optimization algorithms and one of the quickest algorithms for neuronal networks training [6].

In the data base the results of the hardness measurements on predetermined distance from quench surface and the chemical composition of the corresponding constructional steel sample were collected. The average, minimum and maximum content of particular element is presented in table 1 as illustration of chemical composition variations. Average content of particular chemical element is here meant the average content in whole data base. It was calculated from equation $w = \frac{\sum_{j=1}^{n} w_j^i}{n}$;

i: i^{th} element and

n: number of data points.

TABLE 1

Chemical composition of all constructional steel samples

	C	Si	Mn	P	Cr	Mo	Ni	Al	Cu
W	0,341	0,261	0,627	0,014	1,213	0,244	1,090	0,020	0,164
$w_{min.}$	0,120	0,105	0,165	0,003	0,004	0,010	0,030	0,000	0,000
$w_{max.}$	1,550	1,520	1,650	0,370	15,620	1,910	4,110	0,920	0,420

TABLE 2a

Statistical evaluation of predictions for the whole data base (n_{rmT} = 17326)

	training
data mean	46,43
data S.D.	10,51
error mean	-0,46
error S.D.	4,02
absolute error mean	2,60
S.D. ratio	0,38
correlation R	0,92

TABLE 2b

Statistical evaluation of predictions and representativeness for devided data base (n_T = 11609; n_T = 5717)

	training	verification
data mean	46,43	46,43
data S.D.	10,55	10,43
error mean	-0,06	-0,14
error S.D.	3,97	3,97
absolute error mean	2,50	2,51
S.D. ratio	0,38	0,38
correlation R	0,93	0,92

The data base was constructed as matrix with 17.326 model vectors. In the model vector all for analysis necessary data were collected, i.e. in our case one output parameter – hardness and ten input parameters – 9 chemical compositions and distance from quench surface.

The quality of the predictions was verified with statistical evaluation of results and the representativeness with the comparison from different distributions between training and verification data bases. In first case the whole data base was used for training (Table 2a) and in the second case the data base was divided into training and verification data base in the ordinary 2:1 ratio (11609 + 5717 model vectors) – Table 2b.

From the comparisons of Tables 2a and 2b it can be seen that the results are almost identical regardless if one or two data bases were used. Also no significant difference between prediction results for training and verification data bases can be observed. This convinced us that the chosen data base is representative and also that over learning of the neuronal network did not occurred.

2.2. Results and discussion

The influence of particular prediction parameter, i.e. chemical element or distance to the quenched surface, on the hardness is presented in Table 3. Factor $N_{inf.}$ is the order of parameter importance or its influence on the predictions, with E is presented the mean absolute error in case of no consideration of particular parameter and F is relative weight of parameter influence, i.e. the value 2,0 for F means that the error of the prediction without particular parameter is twice as big as in the case of whole data base. From the Table 3 it can be clearly seen that the order of parameter importance is the same for the predictions in training and verification data base.

TABLE 3

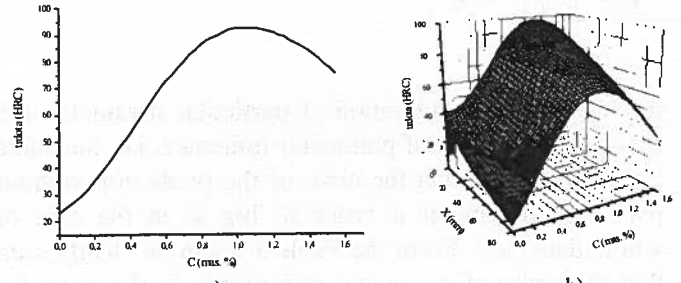
The results of the sensitivity analysis. In *upper section* there are calculations for the *training data base* and in the lower part for the verification data base

	dist.	C	Si	Mn	P	Cr	Mo	Ni	Al	Cu
$N_{inf.}$	3	1	7	6	9	4	5	2	10	8
E	7,11	9,04	4,12	4,60	4,00	6,01	5,09	7,61	3,97	4,00
F	1,80	2,28	1,04	1,16	1,01	1,51	1,28	1,92	1,00	1,01
$N_{inf.}$	3	1	7	6	9	4	5	2	10	8
E	7,06	9,10	4,09	4,65	4,00	5,91	4,96	7,67	3,97	4,00
F	1,78	2,30	1,03	1,17	1,00	1,49	1,25	1,93	1,00	1,01

The aim of our work was prediction chemical composition influence on the hardness profile after quenching, i.e. jominy test.

Carbon influence

The biggest influence on the accuracy of the hardness prediction has carbon (Table 3). The carbon content for constructional steels which were in our data base has varied between 0,12 mass. % and 1,55 mass. %. On the Fig. 2a is diagram hardness vs. carbon content at the distance 1,5 mm from surface. Almost linear dependence up to 0,6 mass. % C can be seen, between 0,7 and 1,0 mass. % C the gradient of increase is smaller and further carbon increase can even decrease hardness. With distance from the sample surface the hardness decrease but the tendency of carbon influence stays the same (figure 2b).

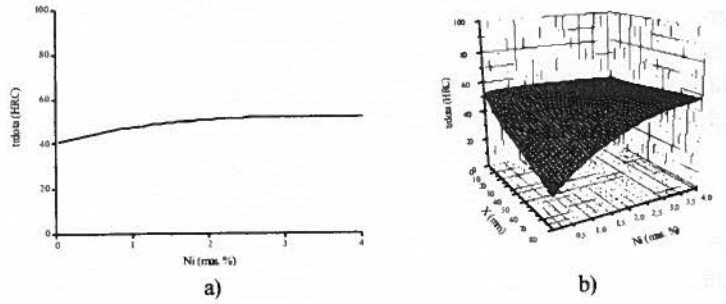


a) b)

Fig. 2. Carbon influence at the distance 1,5 mm (a) and on the whole area of the hardness measurements (b)

Nickel influence

Second on the influence factor scale is nickel (Table 3) which content is within the limits between 0,03 mass. % in 4,11 mass. %. From the graph on Fig 4a it can be seen that its influence at 1,5 mm distance is much smaller. On next Fig. 4b, the nickel content influence is presented with surface in the 3D graph. It can be seen that for lower nickel contents the influence of distance from quench surface is noticeable, but at higher nickel values stays almost the same.



a) b)

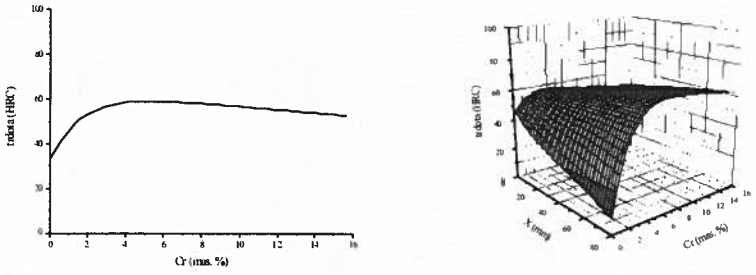
Fig. 3. Nickel influence at the distance 1,5 mm (a) and on the whole area of the hardness measurements (b)

Chromium influence

In the analyzed data base the chromium content varies from almost 0,0 up to almost 16,00 mass. % (0,004 – 15,62 mass. %). The variations have visible influence up to 4,0 mass. %, the hardness has increased from 30 up to 55 HRC. Further chromium content has even opposite influence; it decreased for 5 – 10 HRC (Fig. 4a).

Figure 4b presents the whole area of analysis. It can be seen that the hardness at lower chromium contents drastically decrease with the distance, and even slight increase for the chromium content over 3,0 mass. %.

It has to be stressed that in the data base only 0,7 % model vectors have chromium content over 4,5 mass. % and only 5,8 % model vectors over 2,0 mass. %.

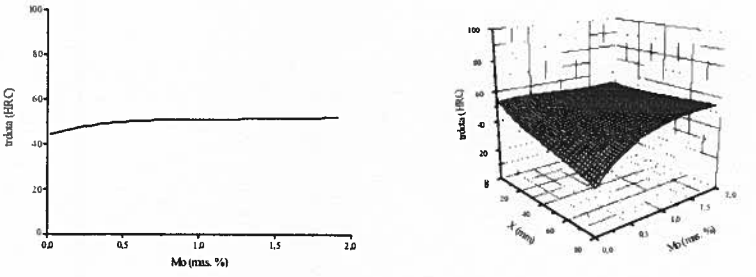


a) b)

Fig. 4. Chromium influence at the distance 1,5 mm (a) and on the whole area of the hardness measurements (b)

Molybdenum influence

Molybdenum has on the whole section of chemical composition and distance changes small influence, similar to nickel (figure 5a and 5b). Some influence can be seen at 1,5 mm for lower molybdenum contents (0,0 – 0,5 mass. %), additional increase of molybdenum has no noticeable influence. Also the increase in distance from sample surface has no noticeable effect on hardness (figure 5b).



a) b)

Fig. 5. Molybdenum influence at the distance 1,5 mm (a) and on the whole area of the hardness measurements (b)

3. Conclusions

In the article the capability of the neuronal networks is presented. Even for large data base and big variations in alloying elements, i.e. chemical composition the predictions were good.

The main aim of this study was to establish possibility to predict hardness profile – hardenability on the basis of constructional steel chemical composition. It was confirmed that not only for minor changes in chosen alloying element amount, but also for wide variety in chemical composition the hardenability can be determined. The calculations can be made for one or more chemical elements and also mutual influence of alloying elements can be studied.

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