Hardenability prediction based on chemical composition of steel

Napovedovanje prekaljivosti na osnovi kemične sestave jekla

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Abstract: With use of neural networks the influence of chemical composition of steel on the hardness i.e. hardenability was determined. The chemical composition has varied within for the specified steel prescribed tolerances.
The modeling of influence of chemical composition on Jominy curve was made for three steel grades or steel groups respectively.

Izvleček: Z nevronskimi mrežami smo modelirali vpliv spreminjanja kemične sestave jekla na njegovo trdoto oz. prekaljivost. Kemična sestava se giblje v za določeno jeklo predpisanih tolerancah.
Vpliv spreminjanja kemične sestave na prekaljivost smo modelirali za tri vrste oz. skupine jekel.

Keywords: modeling, neural networks, hardenability, Jominy test
Ključne besede: modeliranje, nevronske mreže, prekaljivost, preizkus Jominy

Introduction

Steel is by production among metals by far in the first place in the world. This is due to its mechanical, physical, chemical and other properties that meet the user's demands in a wide area. One of the parameters affecting the properties of steel is also its chemical composition. For chosen steel grade it is deter-

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mined with tolerance limits.

Idea to use neural networks for modeling the influence of chemical composition on Jominy curves (hardenability) is not new. VERMEULEN et al.[1] demonstrated that Jominy curve can be modeled if chemical composition of steel is known. They also presented how the neural network parameters influenced the quality of predictions. DOBRZANSKY et al. have published their results from neural network modeling of hardenability[2, 3]. They investigations were focused on constructional steels. Results of their work gave eloquent proof that modeling of Jominy curves on the basis of chemical composition give good results. For mentioned models, i.e. data base, typically relatively small variances in chemical composition occur.

Our department has rich experiences with applying neural networks[4, 5] also with various predictions on basis of chemical composition[6–8].

First results of our Jominy curves modeling on the basis of chemical composition of steel were good[9].

In this study we focused on modeling of hardenability of various steels. Variances in chemical composition within data base were bigger then we found in literature[10].

MATERIALS AND METHODS

Three steel grades were used in the process of hardenability modeling: VCNMO 150, CT207 and 42CrMoS4.

VCNMO150 is a heat treatable, low alloy steel containing nickel, chromium and molybdenum[10]. Steel CT207 is used for highly stressed hardened dies for artificial resin[10]. Steel 42CrMoS4 is used for high and moderately stressed components for automobile industry and mechanical engineering[10]. Typical chemical compositions are presented in Table 1.

Table 1. Typical chemical composition of VCNMO 150, CT207 and 42CrMoS4 in mass fractions, *w*/% [10]

	C	Si	Mn	Cr	Mo	Ni	V	W	others
VCNMO150	0.34	max. 0.40	0.65	1.50	0.23	1.50	-	-	-
CT207	0.21	0.28	0.75	0.85	0.20	1.35	-	-	Cu < 0.25 Al < 0.035
42CrMoS4	0.41	max. 0.40	0.75	1.05	0.28	-	-	-	-

Experimental part

The Jominy test samples have length of 102 mm and a diameter of 25.4 mm. To exclude differences in microstructures due to the preliminary forging, before testing samples were normalized and later austenitised. Austenitising temperature is usually between 800 ºC and 900 ºC. The samples were quickly transferred to the device Jominy where frontend was cooled with controlled jets of water. Cooling the sample from one end simulates the effect of forging of bigger components in the water. After forging and cooling the samples were cleaned. The hardness measurements were made at prescribed intervals along the test samples from the quenched end. The Jominy curves were presented as a function of measured hardness (*HRc*) vs. distance from the quenched end.

Collecting of data base

A database was constructed from measurements of hardness at different distances from cooled surface. The database has contained nearly 20,000 measurements (exactly 19469), but they were not evenly distributed regard to the distance from the surface, as is shown in Figure 1. It can be seen that the maximum number of measurements were carried out up to a distance of 20 mm (about 60 %), as well as can be seen that the number of measurements at a distance greater than 50 mm is negligible (less than 2 %).

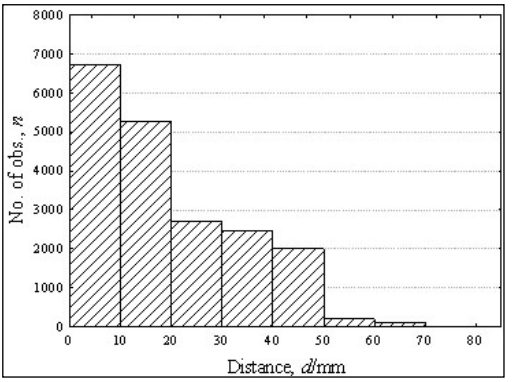

Figure 1. Distribution of measurements regard to the distance from cooled surface

Various steel groups (special steel, alloyed carbon steel and unalloyed carbon steel) were included in data base. It consists of about 50 different steel grades. Less than 10 of them contain more than 10 charges (chemical compositions), about half of them have fewer than 5 entries.

For each of the hardness measurements the chemical composition (25 elements) and distance from the forged surface was attached. These 27 figures formed the so called data vector. The whole database was presented in a matrix consisting of 19,469 lines and 27 columns. From complete data base 11 elements were used for modeling. The selection procedure is presented later. The variations in amount of elements are shown in Figure 2.

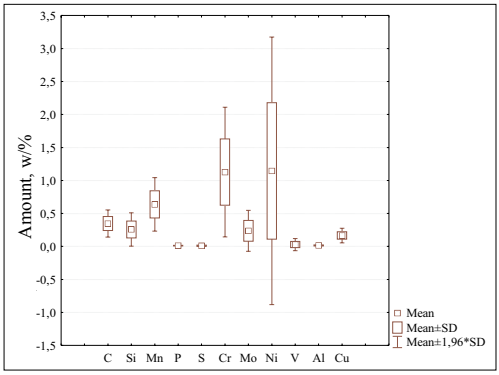

Figure 2. The amount of variation of particular element

Data was randomly divided into training, verification and test data base in the ordinary 2 : 1 : 1 proportion (9735 + 4867 + 4867 model vectors). The distribution in the three groups was automatic and random. The authenticity of the databases is guaranteed, what can be seen from a comparison of correlation coefficients (Table 2).

Table 2. Correlation coefficients for developed neural network model

	training	test	verification
Correlation coefficient	0.9526	0.9424	0.9421

Applied type of neural network

Program Statistica was used for modeling. On the base of our good experiences from previous work[9] multilayer perceptrons type neural network (MLP NN) was used. To obtain good quality of predictions 12 input and 12 neurons in hidden layer were used. Because only one output parameter was calculated also the neural network with one output neuron was applied.

The correlation coefficients for training, test and validation data base are presented in Table **2**. From comparison of those results it can be deducted that applied model is capable to accurate predict the output values and also that overtraining did not occur.

In the process of model development the sensitivity analysis was performed with special module within the program. Based on this analysis we decided that, in addition to distance, only 11 chemical elements will be used. These elements have been found as parameters with maximum correlation with the hardness. Correlation factors of the input parameters are given in Table **3**. The *p* factor indicates the amount of influence and *rang* is classification according to the importance of influence parameters.

Table 3. Factors of influence of the input parameters

	dis.	C	Si	Mn	P	S	Cr	Mo	Ni	V	Al	Cu
p	5.19	6.55	0.08	1.94	1.01	1.05	2.84	1.96	4.60	1.28	1.11	1.06
rang	2	1	9	6	12	11	4	5	3	7	8	10

Results and discussion

Before modeling of the hardness profile basic statistic evaluations of predictions for whole data base were made and results are collected in Table 4 and Table 5.

In those two tables it can be seen that we can expect hardness prediction error smaller than $HRc = 2$. It is also clear that a tiny part of data base cannot fit into developed model.

Table 4. Basic statistic parameters for the absolute error of predictions

No. of predictions	19469
Mean	1.867
Median	1.169
Min.	0.00004
Max.	38.990
25^{th} %	0.529
75^{th} %	2.207

Table 5. Frequency table of absolute error distribution

Range	Cumulative %
0–1	43.96
0–2	71.23
0–5	94.33
0–10	98.20

The results for hardness predictions for three most important chemical elements (Table **3**) – carbon, nickel and chromium are presented on Figure 3, Figure 4 and Figure 5. From higher and lower density of markers on these diagrams is evident that input data was not homogeneously distributed. Also less accurate predictions in boundary areas with no or little records in data base can be observed on these pictures.

Data base contains steel grades with the same amount of carbon but different amount of alloying elements and thus big variances in hardness value. This confirms our hypothesis that more than two input parameters must be taking into consideration if good enough predictions want to be achieved.

Nevertheless, from the pictures it can be seen the general law: carbon increase the hardness of steel and with growing distance from the quenched surface the hardness decreases. This is in agreement with results from literature[2, 3]. On Figure 4 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.

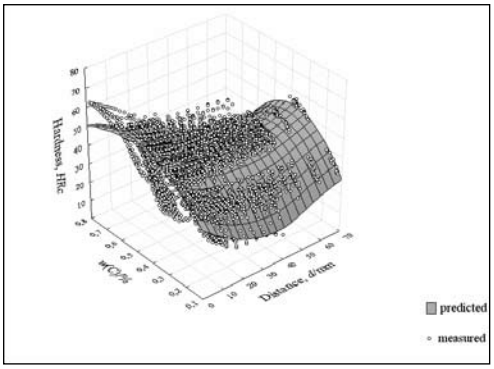

Figure 3. Dependence of hardness (measured – markers and predicted – area) upon amount of carbon and distance

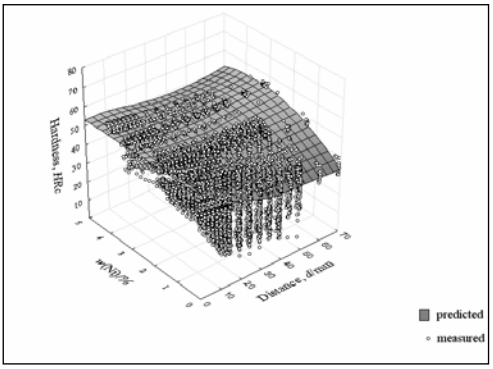

Figure 4. Dependence of hardness (measured – markers and predicted – area) upon amount of nickel and distance

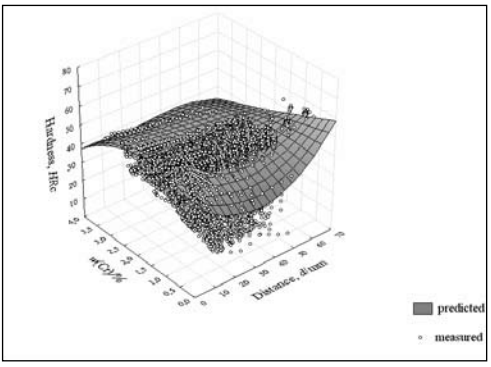

Figure 5. Dependence of hardness (measured – markers and predicted – area) upon amount of chromium and distance

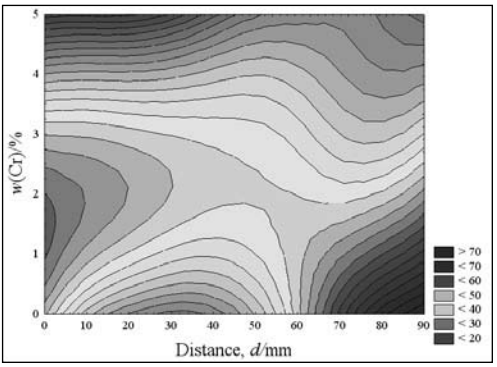

Figure 6. Results from hardness measurements dependent on amount of chromium and distance

On Figure 5 the influence of chromium is presented. It can be seen that the hardness at lower chromium contents near the quenched end decrease with the distance. But at bigger distances from cooled surface even slight increase in hardness can be observed. These unexpected results are due to lack of data but in the agreement with measurements Figure 6. At higher chromium contents the expected drop in hardness at larger distances can be observed.

Effects of charge in chemical composition – variances within one steel grade were studied on case of most influential parameter – carbon.

Table 6. Chemical composition of two VCNMO150 steel samples in mass fractions, *w*/%

	C	Si	Mn	P	Cr	Al	Ni	Mo	Cu
C_{low}	0.320	0.235	0.595	0.013	0.960	0.012	1.485	0.165	0.110
C_{high}	0.430	0.290	0.690	0.021	1.530	0.015	1.720	0.230	0.210

Low alloy steel VCNMO150

For these steel grade 323 different chemical compositions (charges) out of 1508 were used for calculation, what is more than of 1/5 of whole data base. Note; for each chemical composition data up to 15 hardness measurements on different distances from surface is included in data base.

Two chemical compositions used in the process of hardenability prediction are shown in Table 6.

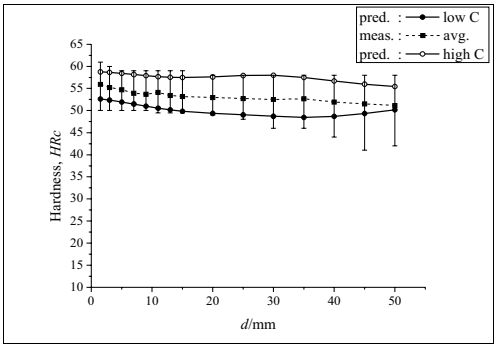

Figure 7. Measured and predicted hardness profile for steel grade VCNMO150

On Figure 7 variations in hardness profile are shown. Both full lines present hardness predictions, one for the sample with high carbon content (white circles) and other predictions for the sample with low carbon (black circles).

Good criteria for variations in measured hardness are points with error bars placed along thin dashed line. They present average value of all measurements at particular distance. The variations of measured hardness at chosen distance were more or less constant on the whole measured area.

From Figure 7 is obvious that effect of chemical composition variations on hardenability for this steel grade can be predicted. Evidently the predicted hardness and trend of hardenability are in good correlation with the results from Jominy test measurements. Differentiation between sample with low and high carbon content and accurate prediction is in this case possible due to broad and accurate data base.

Special structural steel CT207

Data base for CT207 is not comprehensive – it contains only 61 different chemical compositions (charges) out of 1508.

Two chemical compositions for steel grade CT207 with carbon content on upper and bottom border were used for prediction (Table 7). From error bars presented on Figure 8 big differences in measured data can be noticed. On the other hand increase in hardness at distances over 30 mm can be noticed – the line which represents average value of all measurements.

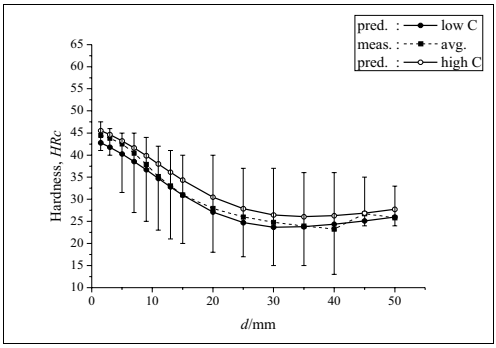

Figure 8. Measured and predicted hardness profile for steel grade CT207

From Figure 8 it is obvious that effect of chemical composition differences on hardenability for steel grade CT207 can be only roughly predicted. Differences in measured hardness are too big and thus generalization occurs. In spite of all that trend of hardenability is in good correlation; also increase in hardness can be predicted.

Special structural steel 42CrMoS4

Data base for 42CrMoS4 is also small – it contains only 66 different charges, what is a little more than 4 % of whole data base. Predictions of hardness profile after Jominy test were made for two test samples with different chemical compositions; one with low and other with high carbon content (Table 8).

Table 7. Chemical composition of two CT207 steel samples in mass fractions, *w*/%

	C	Si	Mn	P	Cr	Al	Ni	Mo	Cu
C_{low}	0.160	0.240	0.580	0.011	0.570	0.017	1.650	0.210	0.150
C_{high}	0.210	0.260	0.610	0.015	0.660	0.027	1.680	0.220	0.220

Table 8. Chemical composition of two 42CrMoS4 steel samples in mass fractions, *w*/%

	C	Si	Mn	P	Cr	Al	Ni	Mo	Cu
C_{low}	0.390	0.230	0.670	0.018	1.080	0.015	0.090	0.180	0.200
C_{high}	0.440	0.280	0.720	0.029	1.140	0.030	0.130	0.230	0.230

Variations in measured hardness near surface are small compared with those measured farther toward specimen center (Figure 9). Near sample surface the measured differences can be practically neglect (*HRc* < 5). At distances 20 mm or more those variations can be almost *HRc* = 20.

It is obvious that such big change in variations cannot be modeled very accurate with the model which was developed for whole data base. In our opinion the predictions which were made for steel grade 42CrMoS_4 can be described as successful. The differences in hardness profile for different steel chemical composition can be observed.

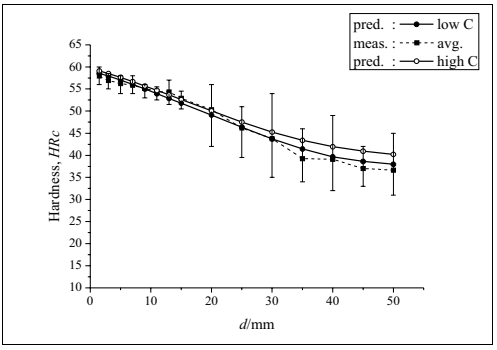

Figure 9. Measured and predicted hardness profile for steel grade 42CrMoS4

Conclusions

It was successfully proved that neural networks are capable to make good and on narrow region focused predictions. In our case even if large and heterogeneous data base was implemented.

If "necessary conditions" are fulfilled very accurate modeling of influences in chemical composition within one steel grade on hardness and hardenability can be made. The "necessary conditions" are: data base must have sufficient data vectors and they have to be representative data for treated steel grade. In the case of VCNMO150 this conditions were completely fulfilled and influence of carbon content on hardenability was successfully demonstrated.

Also for steel grades which have a lesser amount of data modeling of chemical composition influence on hardness can be made. The results are not as accurate but basic law can be deduced. For those steel grades the carbon content influence on the hardness was qualitative successfully predicted; quantitative predictions were less accurate. Basic hardness profile or average value was of course successfully modeled for all the predictions which were made during this research.

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