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 NEURAL NETWORKS

MODELOWANIE HARTOWNOŚCI STALI Z WYKORZYSTANIEM SZTUCZNYCH SIECI NEURONOWYCH

The objective of the research that has been presented was to model the effect of differences in chemical composition within one steel grade on hardenability, with a very broad and heterogeneous database used for studying hardness predictions. This article presents the second part of research conducted with neural networks.

In the previous article [1] the most influential parameters were defined along with their weights and on the basis of these results, an improved model for predicting hardenability was developed.

These developed neural networks were applied to model predictions of hardenability for three steel grades VCNMO150, CT270 and 42CrMoS4.

The results proved that the correlation between the chemical composition differences within a chosen steel grade and the hardness changes can be modeled. If the database is big enough, predictions would be accurate and of high quality. But for a less comprehensive database, the differences in hardness predictions for various chemical compositions of the steel grade concernedwere observable.

Keywords: neural networks, hardenability, Jominy test

Celem zaprezentowanych poprzednio badań było modelowanie wpływu składu chemicznego wybranego gatunku stali na hartowność. Modelowanie przeprowadzono z wykorzystaniem rozbudowanej bazy danych zawierającej informacje o składzie chemicznym próbek stali oraz wynikach prób hartowności. W artykule przedstawiono drugą część badań przeprowadzonych z wykorzystaniem sieci neuronowych.

W poprzedniej pracy [1] określono parametry modelu oraz ich współczynniki wagowe. Na podstawie uzyskanych wyników opracowano ulepszony model do predykcji hartowności stali.

Utworzone sieci neuronowe wykorzystano do predykcji hartowności trzech wybranych gatunków stali: VCNMO150, CT270 oraz 42CrMoS4.

Otrzymane wyniki wskazują na możliwość modelowania zależności pomiędzy składem chemicznym, a hartownością w ramach danego gatunku stali. Wykorzystanie do uczenia sieci neuronowej wystarczająco dużej liczby rekordów dotyczących wybranego gatunku stali powoduje, że otrzymywane wyniki charakteryzują się dobrą dokładnością. W przypadku mniej wyczerpującego zbioru danych wykorzystywanego do nauki sieci, otrzymywane wyniki charakteryzuje większy błąd prognozy.

1. Introduction

As was discussed in the previous article [1] and also in the works of several other authors [2-8], neural networks are a very useful and successful numerical tool for making predictions on the basis of a large experimental database. The capability of the applied neural network to predict the hardenability – even with a very heterogeneous database – was confirmed.

The aim of the work presented was to develop a model which can correlate the variations in the chemical composition within the prescribed tolerances of a chosen steel grade, along with the changes in its hardenability. This study was performed based on the example of several steel grades which are in Metal Ravne's regular product range.

2. Database and neural network selection and configuration

2.1. The database

The hardness profile measurements of Jominy test samples (from 1.5 mm to 50,0 mm, and in some cases up to 70.0 mm from the quenched surface) were made at Metal Ravne.

Aside from the results of the hardness measurements, the chemical composition of the corresponding steel sample was also incorporated into the database.

Various steel groups (special steel, alloyed steel and carbon steel) were included in the database, which itself contained

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about 50 different steel grades. Fewer than 10 of these contained more than 10 elements, with around half having fewer than five. The total number of distinct chemical compositions in the database was 1508.

The data was recorded as 19,469 model vectors (about 2000 more than in the previous article [1]) and was divided into training, verification and test databases at a ratio 2:1:1 (9735 + 4867 + 4867 model vectors).

Each model vector consisted of ten input parameters (nine chemical elements and the distance between the quenched surface and the measuring point) and one output parameter – hardness.

The variations in chemical composition of all the steel grades examined were condiderable, presented here in Table 1, but not as substantial as in mentioned previously (for example: $C_{max.old} = 1.55 \rightarrow C_{max.new} = 0.79$ or $Cr_{max.old} = 15.62 \rightarrow Cr_{max.new} = 4{,}75$). This has practically no influence on the average chemical composition ($C_{avg.}$: 0.341 → 0.348 or $Cr_{avg.}$: 1.213 → 1.218) but it has influenced predictions near the database margin.

TABLE 1
Chemical composition of steel samples included in the database

	C	Si	Mn	P	Cr	Mo	Ni	Al	Cu
$\overline{w}$	**0.348**	**0.258**	**0.638**	**0.013**	**1.218**	**0.237**	**1.146**	**0.016**	**0.166**
$w_{min.}$	0.100	0.105	0.165	0.003	0.080	0.010	0.030	0.000	0.000
$w_{max.}$	0.790	1.520	1.650	0.041	4.750	1.010	4.110	0.039	0.420

$$\bar{w}^i = \frac{\sum_{j=1}^{n} w_j^i}{n} (\, i: \ i^{th} \text{ element and } n: \ \text{number of data points})$$

2.2. The neural network

Figure 1 shows that hardness variations for the selected combinations of carbon content – which is the most influential parameter, along with distance (the hardness profile) – are still large despite narrowing the database.

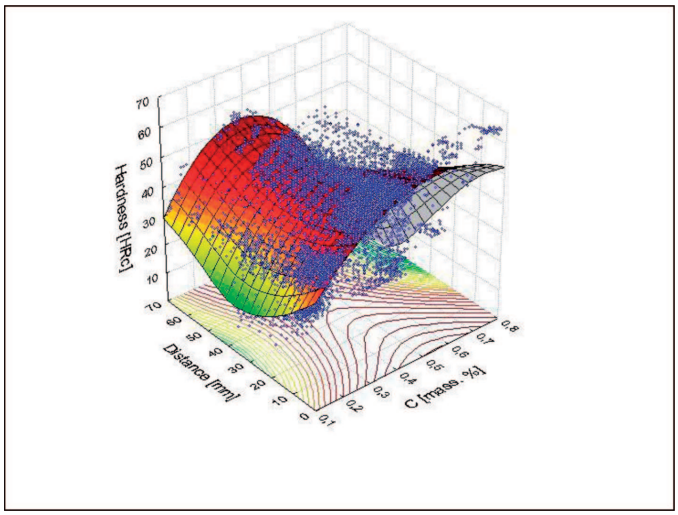

Fig. 1. Hardness versus carbon content and distance. The markers indicate the measured values, and the surface is calculated as distance weighted least squares

These findings and an analysis of similar data (graphic presentations) indicate that more than just a few influential parameters – with their interdependence as yet unknown – have to be taken into consideration if accurate predictions are required. On the basis of this consideration, along with the authors' experience from the past, neural networks were used.

As in the previous article [1] a multilayer perceptron type neural network (MLP NN) was used to solve problems with regression. To obtain a better quality of predictability, the network configuration was changed. In the new neural network, fifteen (an increase of ten from previously) neurons in the hidden layer were used (**Figure 2**). The Levenberg-Marquardtov algorithm was used for MLP NN training.

As a result of MLP NN training, a model was developed, which later was applied for the calculation of hardness profile.

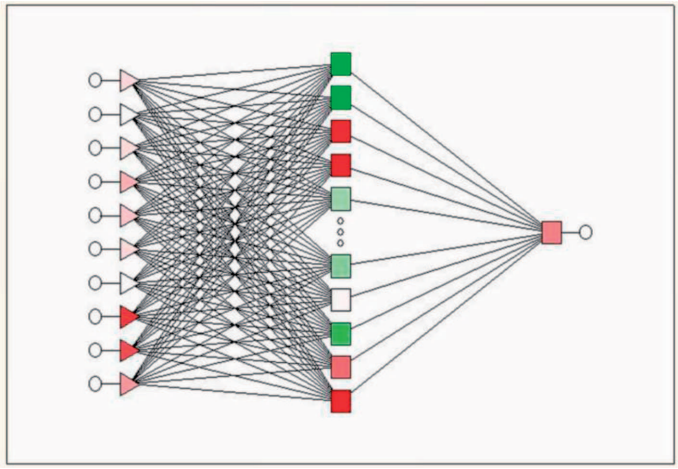

Fig. 2. A schematic presentation of a neural network with 3 layers; 10 input parameters, 15 neurons in the hidden layer and one output parameter

3. Findings and discussion

The quality and representativeness of the predictions can be seen by the comparisons of the columns in **Table 2.** Prediction quality has been improved when compared to the previous work (S.D. ratio 0.38 → 0.36) and excellent representativeness can be clearly seen from the comparison of statistical data for each database (training, verification and test database).

TABLE 2
Statistical evaluation of predictions and representativeness for 10 input variables (n_{tr} = 9735; n_{ve} = 4867; n_{te} = 4867)

	training	verification	test
data mean	47.30	47.19	46.89
data S.D.	10.29	10.37	10.54
error mean	-0.027	-0.020	-0.080
error S.D.	3.59	3.73	3.94
absolute error mean	2.15	2.19	2.25
S.D. ratio	**0.35**	**0.36**	**0.37**
correlation R	0.94	0.93	0.93

The rank and weight of a particular influential parameter on the predicted hardness is presented in **Table 3**. The ranks of the majority of influential parameters are obviously the same as in the previous work; only the last three least significant paramters have changed their positions.

TABLE 3
Results of the sensitivity analysis

	dist.	C	Si	Mn	P	Cr	Mo	Ni	Al	Cu
Rank N_{inf}	**3**	**1**	**7**	**6**	**8**	**4**	**5**	**2**	**9**	**10**
Ratio (error/ baseline) *F*	2,02	2,37	1,03	1,16	1,01	1,53	1,24	2,06	1,01	1,01

3.1. Low alloy steel VCNMO150

VCNMO150 is a heat treatable, low alloy steel containing nickel, chromium and molybdenum [9].

For this steel grade, 323 out of 1508 different chemical compositions were used for the calculation, which is more than one fifth. For each chemical composition, data from about 15 hardness measurements – which were carried out at different distances from the surface – were included in the database.

Two of the chemical compositions that were used in the process of the hardenability prediction are shown in **Table 4**.

TABLE 4
Chemical compositions of two VCNMO150 steel samples

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

Figure 3 shows variations in the hardness profile. Both marked lines present hardness predictions, one for the sample with a high carbon content (full line, white circles), and the other for the low carbon sample (dashed line, black circles).

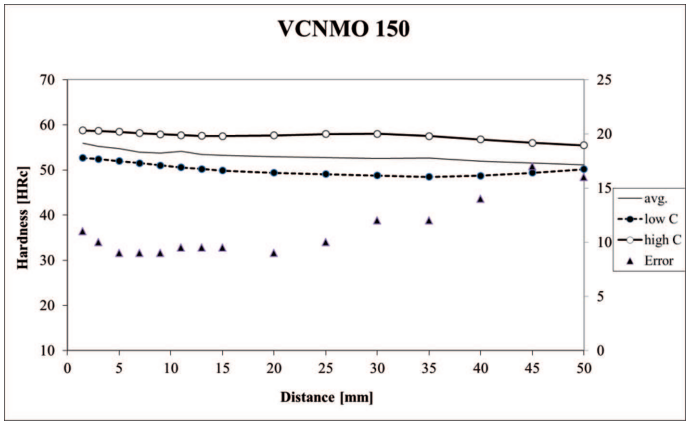

Fig. 3. Measured and predicted hardness profile for steel grade VCNMO150

The points showing dispersion of the measured data are a good indicator of the variations in the measured hardness. In this study they are considered errors with regard to the average value of all measurements at a particular distance (thin line). The variations of the measured hardness at a chosen distance were more or less constant in the whole area measured.

It is obvious from **Figure 3** that the effect of chemical composition differences on the hardenability of steel grade VCNMO150 can be predicted. The predicted hardness and the hardenability trend are in a good correlation with the results from the Jominy test measurements.

The differentiation in the prediction between the samples with a low and a high carbon contents is in this case possible due to an extensive and accurate database.

3.2. Special structural steel CT207

Steel CT207 is used for highly stressed, hardened dies for artificial resin [9].

The database for CT207 was not comprehensive, as it contained only 61 different chemical compositions out of 1508.

For steel grade CT207 two chemical compositions with the highest and lowest acceptable carbon contents were used for the prediction (**Table 5**).

TABLE 5
Chemical composition of two CT207 steel samples

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

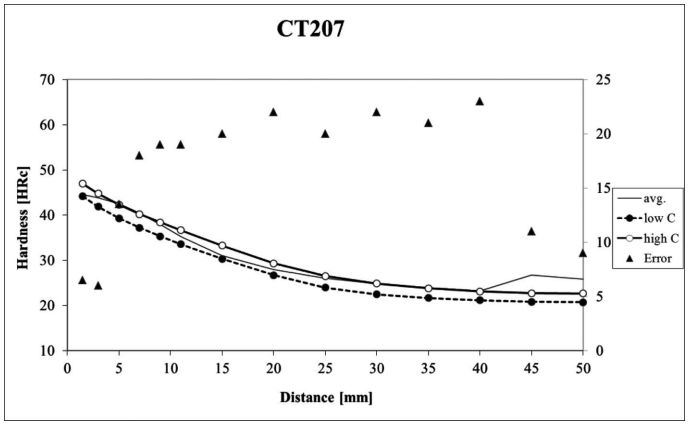

Fig. 4. The measured and predicted hardness profiles for steel grade CT207

It is clear from the error markers in **Figure 4** that there are large discrepancies amongst the measured data. However, the measured data shows that an increase in hardness at distances over 40 mm can be observed – the line represents the average value of all measurements.

The differences in the measured hardness are too wide to allow precise predictions with the use of neural networks, and consequently generalization of the hardenability profile occurs. But on the other hand it is obvious from **Figure 4** that the common effect of chemical composition differences on hardenability for steel grade CT207 can be predicted despite the huge variations in the measured data.

From what is understood, the hardenability trend correlates well up to 40 mm from the quenched end but the increase in hardness (if any) cannot be predicted.

3.3. Special structural steel 42CrMoS4

Steel 42CrMoS4 is used for highly and moderately stressed components for the automobile industry and mechanical engineering [9].

The database for 42CrMoS4 was also small, containing only 66 different chemical compositions. This representes about 4% of the total number of chemical compositions in the database.

The hardness profile predictions after the Jominy test were made for two test samples with different chemical compositions; one with a low and the other with a high (**Table 6**).

TABLE 6
Chemical composition of two 42CrMoS4 steel samples

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

Figure 5 presents variations in the predicted and measured hardness profiles – points which display errors. Within the area of the sample surface, these differences can be practically neglected (< 5 HRc), but when the distance is 20 mm or higher the variations can reach almost 20 HRc.

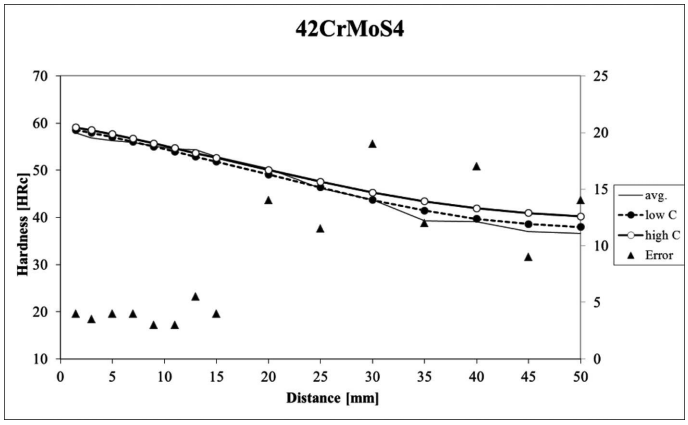

Fig. 5. The measured and predicted hardness profile for steel grade 42CrMoS4

The variations in the measured hardness near the surface are small, so it is clear that the prediction cannot effectively describe the influence of chemical composition within this particular steel grade. Also there are more substantial differences in the hardness measurements –those measured closer to the specimen center have a little effect on the differences in predictions. It is clear from the graph on **Figure 5** that in this case the predictions are highly generalized. But it has to be noted that the trend in the predicted hardenability is the same as for the measured hardenability, and the predicted values are also within in the range, or are very similar to those that have been measured.

4. Conclusions

It was successfully proven that, when focused on a narrow region, neural networks are capable of making first class and accurate predictions – in our case on a particular steel grade – even when a large and heterogeneous database was implemented.

The chemical variations within one steel grade as regards its hardness and hardenability can be described very accurately as long as the prerequisites for such description have been met. This means that the database must have sufficient and representative data for the steel grade concerned. This condition was satisfied for VCNMO150 and the influence of the carbon content on hardenability was successfully demonstrated.

In addition, for steel grades that do not have a collection of comprehensive data, it is possible to model the influence of the chemical composition on hardness. The results may not be as accurate, as in the case of a more representative database, but the basic principles can be deduced.

For both steel grades which have a less representative database the carbon content influence on their hardness was also successfully predicted in terms of quality, but quantitative predictions were less accurate.

The basic hardness profile, or the average value were successfully modelled for all the predictions which were made during this study.

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