Journal of Achievements in Materials and Manufacturing Engineering
VOLUME 21 ISSUE 2 April 2007

Employment of rough data for modelling of materials properties

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Received 09.11.2006; accepted in revised form 15.11.2006

Analysis and modelling

ABSTRACT

Purpose: The paper presents the method of high - speed steels' secondary hardness modeling, basing on chemical composition and heat-treatment parameters.
Design/methodology/approach: The computer modeling using statistical regression method were carried out basing on results of investigations of newly developed high - speed steels and rough data included in standards containing information about these steels.
Findings: The models developed in the work was experimentally verified. The verification procedure consists of the evaluation of the conformity of the computational results with the experimental data. The obtained results indicate good conformity of calculations with experimental results since the error of calculations is c.a. 0.8 HRC.
Research limitations/implications: The results presented are valid in the ranges of mass concentrations of alloying elements occurring in analyzed steels group and presented in the paper.
Practical implications: The worked out model may be used in computer systems of steels' designing for cutting tools.
Originality/value: The use of rough data for modeling of materials properties.
Keywords: Computational material science; Modelling; Mechanical properties; Metallic alloys

1. Introduction

High-speed steels are still an important group of engineering materials. Their common industrial application justifies carrying out research on new types of steel with better functional qualities. A fast development in computer science and its widely spread modern technologies brings about the successful application of steels in research concerning the material engineering. Artificial intelligence method, including neural networks, as well as advanced computational methods make it possible to broaden the examinations over the high-speed steels in order to reduce costs of their manufacturing by replacing laborious and expensive metallurgical processes with computer analyses and simulations. Another vital factor is a significant reduction of time of analyses done, as the application of new technologies makes it possible to avoid lots of laborious empirical research and replacing it by computer simulations whose correct results are often a basic source of consecutive analyses. Modern applications of computer sciences in the material engineering including the artificial intelligence methods are more and more of the interest of the materials science environment. Years to come will definitely bring new solutions that will indicate other areas of practical use of these methods, and our own works [1-8] are an example.

In the paper there has been a mathematical model presented, made with the use of multiple regression method, helpful when calculating the secondary hardness of high-steels after the heat-treatment on the basis of the chemical composition and heat treatment parameters.

2. Material and method

The base of the mathematical model are results of investigations of expeirmental HSS steels with addition of Si as a partial substutite of W or/and Mo and addition of Ti and Nb as a substituetes of V with chemical composition presented in table 1. The steels were austenitised at temperatures of 1120°C to 1240°C varied in 30°C steps and next tempered at temperatures of 480°C to 630°C varied in 30°C steps [9-14]. As a result, hardness examinations for 5 austenitising temperature values and 6 tempering temperature values have been made, what cumulatively gave the results for 30 variants of the heat-treatment for each of the analyzed types of steel.

Table 1.
Chemical composition of the experimental high-speed steels

Steel grade	Mass concentration of the alloying element, %									
	C	Mn	Si	Cr	W	Mo	V	Ti	Nb	Co
SW9M2S	0.94	0.48	0.58	4.5	9.0	1.72	1.8	0.0	0.0	0.0
SW9M2STi	0.93	0.46	0.78	4.5	9.0	1.88	1.7	0.23	0.0	0.0
SW9M2STi1	0.93	0.52	0.63	4.7	8.9	2.0	1.5	0.6	0.0	0.0
SW9M2SNb	0.94	0.45	0.65	4.5	9.0	1.85	1.67	0.0	0.54	0.0
SW9M2SNb1	0.92	0.43	0.66	4.5	9.1	1.87	1.3	0.0	0.95	0.0
SW9M2K5S	0.94	0.63	0.71	4.4	8.8	2.4	1.6	0.0	0.0	5.2
SW11S	0.93	0.42	0.54	4.5	11.2	0.0	1.8	0.0	0.0	0.0
SW11STi	0.98	0.5	0.74	4.6	10.8	0.0	1.6	0.34	0.0	0.0
SW11STi1	0.93	0.51	0.72	4.4	10.6	0.0	1.4	0.56	0.0	0.0
SW11SNb	0.94	0.47	0.64	4.5	11.4	0.0	1.6	0.0	0.43	0.0
SW11SNb1	0.93	0.46	0.63	4.5	11.5	0.0	1.3	0.0	0.85	0.0
SW11K5S	0.91	0.51	0.63	4.5	10.9	0.0	1.8	0.0	0.0	5.2
SW11M2S	1.1	0.37	0.64	4.4	11.3	1.88	1.8	0.0	0.0	0.0
SW11M2STi	1.05	0.44	0.63	4.5	11.2	1.9	1.7	0.3	0.0	0.0
SW11M2STi1	1.04	0.44	0.69	4.2	11.1	1.8	1.5	0.56	0.0	0.0
SW11M2SNb	1.0	0.4	0.56	4.4	11.2	1.95	1.7	0.0	0.46	0.0
SW11M2SNb1	1.02	0.42	0.54	4.5	11.3	1.82	1.4	0.0	0.86	0.0
SW11M2K5S	1.03	0.42	0.65	4.5	11.3	1.94	1.8	0.0	0.0	4.9

Table 2.
Chemical composition of the high-speed steels according to PN-86/H-85022 withdrawn standard

Steel grade	Range	Mass concentration of the alloying element, %							
		C	Mn	Si	Cr	W	Mo	V	Co
SW12	Min	1.05	0.0	0.0	3.5	11.0	0.0	2.2	0
	Max	1.15	0.4	0.5	4.5	13.0	0.7	2.7	0.5
SW18	Min	0.75	0.0	0.0	3.5	17.0	0.0	1.0	0
	Max	0.85	0.4	0.5	4.5	19.0	0.7	1.4	0.5
SW2M5	Min	0.9	0.0	0.0	3.5	1.5	4.5	1.1	0
	Max	1.0	0.4	0.5	4.5	2	5.5	1.4	0.5
SK5M	Min	0.85	0.0	0.0	3.5	6.0	4.6	1.7	4.5
	Max	0.95	0.4	0.5	4.5	6.7	5.2	2.1	5.5
SW7M	Min	0.82	0.0	0.0	3.5	6.0	4.5	1.7	0
	Max	0.92	0.4	0.5	4.5	7.0	5.5	2.1	0.5
SK5MC	Min	1.05	0.0	0.0	3.5	6.4	3.5	1.7	4.5
	Max	1.2	0.4	0.5	4.5	7.4	4.5	2.1	5.5
SK5	Min	1.05	0.0	0.0	3.5	11.0	0.0	2.1	4.5
	Max	1.15	0.4	0.5	4.5	13.0	0.7	2.6	5.5
SK8M	Min	1.05	0.0	0.0	3.5	1.3	9.0	1.0	7.5
	Max	1.2	0.4	0.5	4.5	1.9	10.0	1.4	8.5
SK10V	Min	1.15	0.0	0.0	3.5	9.0	3.0	2.7	9.5
	Max	1.3	0.4	0.5	4.5	11.0	3.6	3.2	10.5
SK5V	Min	1.3	0.0	0.0	3.5	12.0	0.7	4.2	5.0
	Max	1.45	0.4	0.5	4.5	13.5	1.2	4.8	6.0

This way the appropriate set of experimental data has been obtained which describes the secondary steel hardness' values depending on the chemical composition and heat–treatment parameters containing 540 examination results. Additionally, to obtain the mathematical model adequate for a wider concentration range of alloy elements, one has used the data included in the standard specification PN-86/H-85022 "High-Speed Steels", withdrawn at present, embracing information about 10 types of the high-speed steels. This standard involves requirements concerning the chemical composition shown as allowable ranges of particular alloy elements – minimal and maximal (Table 2). Moreover, it presents approximate diagrams of tempering curves (for different values of tempering temperatures) for the optimal austenitising temperature for a given type of steel. It needs to be mentioned that with these diagrams have not been associated any specific chemical compositions, assuming that they occur in the limits suitable for any type of steel. These approximate data have been used for extending the data set by additional 171 results and this number results from the quantity of data in the above mentioned tempering diagrams and from the accepted method of formulating the approximate data, presented below in the paper.

3. Methodology of handling the approximate data

The proposed in the paper method allows for obtaining the approximate data indispensable for working out the mathematical method. There have been used the diagrams of the tempering curves of high-speed steels included in the PN-86/H-85022 standard. A sample tempering diagram obtained for SK5V steel subjected to austenitising temperature of 1240º has been presented in Figure 1.

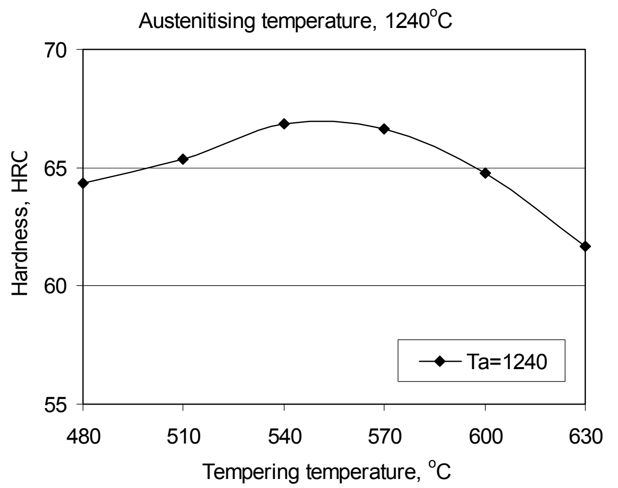

Fig. 1. Tempering curve of the SK5V steel grade austenitising temperature 1240°C (according to PN-86/H-85022 withdraw Polish Standard)

Similar diagrams for other types of steel included in the standard have been placed in the paper. They are of informational character as one does not know for which chemical composition they have been obtained. In the proposed in the paper method one has assumed that these diagrams correspond to the so-called average chemical composition what corresponds to the values from the middle of the permissible range for concentrations of particular elements. Furthermore, it has been assumed that in case when the chemical composition of steel changes in allowable limits, there are possible some hardness deviations for respective tempering temperatures by 1,25% which do not go beyond the value of 1 HRC. As a consequence of such the assumption, one gets, instead of the tempering curve, a special type of a tempering band, limited by an adequate value of "raised" or "lowered" curves (in HRC units) in relation to the basic tempering curve (Fig.2). It has additionally been accepted that the limiting tempering curves are related to the chemical compositions of steels when the concentrations of the alloy elements correspond to the bottom allowable concentration limit (the so-called "lowered" curve) or the upper limit of the concentration of the element (the so-called "raised" curve). The assumed, in this way, chemical compositions are presented in Table 3. It needs to be also mentioned that in case of the alloy elements that occur in these steels and are not treated as the basic alloy addition, manganese and silicon here, their concentrations have been accepted as equal: manganese = 0.24% and silicon= 0.3%. The proposed approach allows for obtaining data describing changes of hardness of the secondary steel depending on the changing chemical composition of steel and the heat-treatment parameters. This approach is undoubtedly a subject matter if the assumptions made are right and the described method fulfill them, as it is obvious that there are other approaches possible for handling the data included in standards, catalogues or other publications, e.g. with the application of the rough set theory[15].

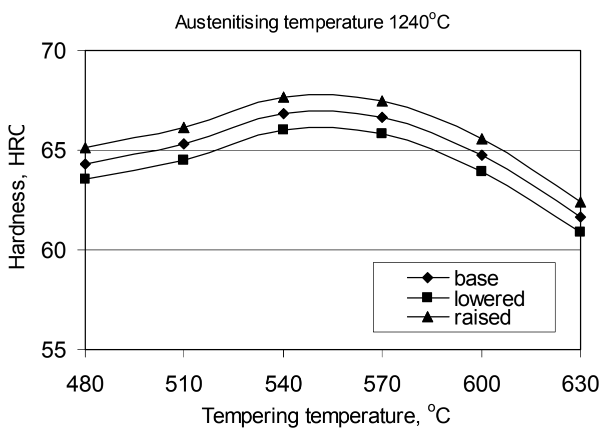

Fig. 2. Tempering band of the SK5V steel grade for chemical compositions presented in table 3

Table 3.
Assumed chemical compositions of the SK5V steel

Tempering curve	Mass concentration of the alloying element, %							
	C	Mn	Si	Cr	W	Mo	V	Co
base	1.375	0.24	0.3	4	12.75	0.95	4.5	5.5
lowered	1.3	0.24	0.3	3.5	12	0.7	4.2	5.0
raised	1.45	0.24	0.3	4.5	13.5	1.2	4.8	6.0

4. Model of the steels' hardness

For working out the mathematical model enabling the calculation of hardness of the analyzed high-speed steels only on the basis of the chemical composition and the austenitising and tempering temperatures, the statistical method of multiple regression has been used. The calculations have been made using Statistica v.5.5 program. Because the analysis of the physical interrelations connected with the secondary hardness effect does not allow for defining the appropriate physical model, many forms of phenomenological method have been considered, based solely on the knowledge, experience and intuition of the researchers. When judging the adequacy of the worked out models, one has based on the error analysis between the calculated hardness and the corresponding hardness measured empirically (or read from the standard according to the methodology described in Item 3). As a criterion, an average error for a tested data set has been accepted:

$$R=\frac{1}{N}\sum_{i=1}^{N}\left(\left|H_{ci}-H_{mi}\right|\right) \tag{1}$$

where: N – testing set size, H_{ci} – calculated hardness, H_{mi}- measured hardness.

It has been accepted that the adequate is the model which allows for obtaining the values of the average differences in hardness in the 0.6 – 0.9 HRC range, thus corresponding to the width of the tempering band (Fig,2).

As a result of verifying calculations, the following model of hardness has been accepted:

$$\begin{aligned}H=&a_0+a_1\cdot C+a_2\cdot Mn+a_3\cdot Si+a_4\cdot Cr+a_5\cdot W+a_6\cdot Mo+a_7\cdot V+a_8\cdot Ti\\&+a_9\cdot Nb+a_{10}\cdot \%Co+a_{11}\cdot Ta+a_{12}\cdot To+a_{13}\cdot Ta^2+a_{14}\cdot To^2+a_{15}\cdot Ta^3\\&+a_{16}\cdot To^3+a_{17}\cdot(To^2\cdot Ta^2)+a_{18}\cdot(Ta\cdot To)+a_{19}\cdot(W\cdot Mo)+a_{20}\cdot(C\cdot Mn)\\&+a_{21}\cdot(Mn\cdot Mo)+a_{22}\cdot(To^3\cdot Ta^3)+a_{23}\cdot(W\cdot V)+a_{24}\cdot(W\cdot Ti)\end{aligned} \tag{2}$$

The values of a_i coefficients are as follows:
a_0=2388,15; a_1=24,48; a_2=54,23; a_3=0,407; a_4=0,354; a_5=0,335; a_6=-0,191; a_7=1,0972; a_8=-8,231; a_9=-0,984; a_{10}=-0,0303; a_{11}=-1944,13; a_{12}=-11889,61; a_{13}=191,25; a_{14}=15033,36; a_{15}=51,69; a_{16}=-8208,46; a_{17}=-6765,12; a_{18}=7831,77; a_{19}=0,0018; a_{20}=-58,7; a_{21}=1,55; a_{22}=2619,82; a_{23}=-0,159; a_{24}=0,633

The verifying calculations have shown that the model (2) allows for calculating the secondary hardness of steel with accuracy up to 0.8 HRC. It is the average error of calculations and its maximal values do not exceed 2 HRC. Moreover, the error for 65% of the calculated values is smaller than the 0.8 HRC limit value. These results allow to accept that the worked out model is adequate, and the results are compatible with the experimental results. In figures 3-4 there has been presented the sample comparison of the calculated and empirical tempering curves for SK5V and SW9M2STi steels respectively.

5. Conclusions

In the paper there has been presented the worked out model with the use of the multiple regression that enables calculating the hardness of high-speed steels on the basis of the chemical composition and the heat-treatment parameters. The obtained calculation results point at the satisfactory conformity of the model with the empirical data, as the calculation error is about 0.8 HRC. While working out the mathematical model one has based on the results of the experimental examinations of the high-speed steels and the approximate data included in the standard specification concerning the high-speed steels. The obtained results of the computer simulation are consistent with the results of the empirical research done in the source-based works [9-14].

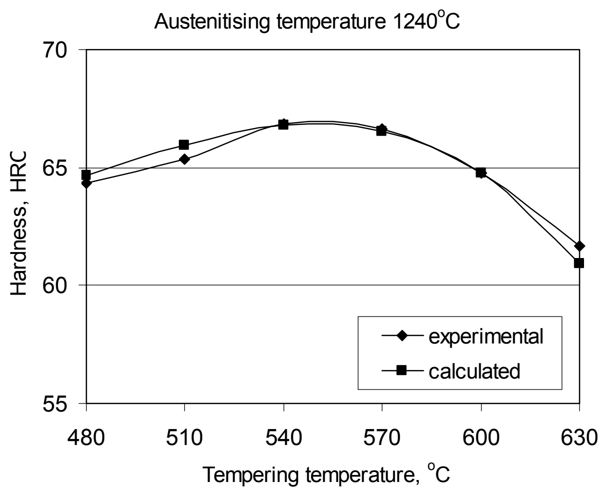

Fig. 3. Comparison of the tempering curves experimental and calculated ones of the SK5V steel grade, error of calculations 0.38 HRC

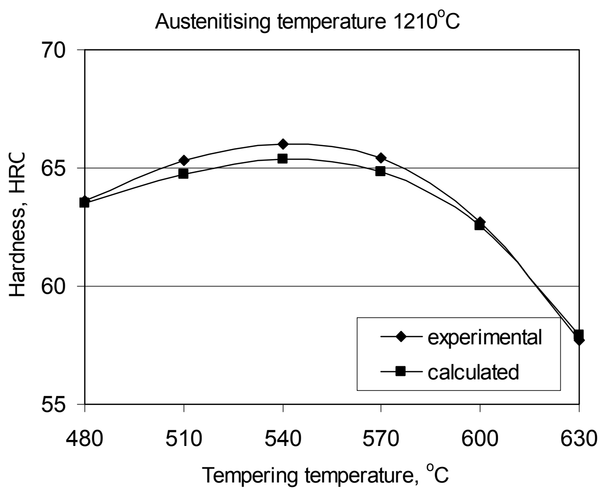

Fig. 4. Comparison of the tempering curves experimental and calculated ones of the SW9M2STi steel, error of calculations 0.57 HRC

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