UDK 620.172.2:621.3.015:519.7
Original scientific article/Izvirni znanstveni članek

ISSN 1580-2949
MTAEC9, 51(6)883(2017)

INCREASING THE TENSILE STRENGTH AND ELONGATION OF 16MnCrS5 STEEL USING GENETIC PROGRAMMING

POVEČEVANJE NAPETOSTNE TRDNOSTI IN RAZTEZKA 16MnCrS5 JEKLA Z UPORABO GENETSKEGA PROGRAMIRANJA

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Prejem rokopisa – received: 2016-09-29; sprejem za objavo – accepted for publication: 2017-05-05

doi:10.17222/mit.2016.293

Štore Steel Ltd. is one of the largest spring-steel producers in Europe. Štore Steel makes more than 1400 steel grades of different chemical composition. Among them is 16MnCrS5 steel. It is generally used for the fabrication of case-hardened machine parts for various applications (e.g., bars, rods, plates, strips, forgings), where a combination of wear resistance, toughness and dynamic strength is essential. These properties can be easily correlated with tensile strength, which depends on the chemical composition and heat treatment after rolling. In addition, the elongation should be taken into account. In the paper, modeling of tensile strength and elongation with genetic programming is presented and compared with linear regression modeling. The chemical composition data (content of C, Mn, S and Cr) and the heat-treatment regime data (GKZ or BG annealing) were used for modeling. The modeling results show that a higher tensile strength with improved elongation were achieved.

Keywords: 16MnCrS5, tensile strength, elongation, modeling, genetic programming, linear regression

Štore Steel je največji proizvajalec vzmetnega jekla v Evropi. Štore Steel izdeluje več kot 1400 različnih kvalitet jekla z različnimi kemijskimi sestavami. Med njmi tudi 16MnCrS5, ki spada v skupino jekel za cementacijo, ki so namenjena za strojno obdelavo različnih delov (npr. palic, plošč, trakov, odkovkov), kjer se zahteva kombinacija obrabne odpornosti, žilavosti ter trajnonihajne trdnosti. Le-te lastnosti lahko povezujemo z natezno trdnostjo, ki je odvisna predvsem od kemične sestave in toplotne obdelave po valjanju. Prav tako je pomemben raztezek. V članku je predstavljeno modeliranje natezne trdnosti in raztezka s pomočjo genetskega modeliranja in linearne regresije. Za modeliranje smo uporabili vsebnosti kemijskih elementov (C, Mn, S in Cr) ter način toplotne obdelave (GKZ ali BG). Glede na rezultate smo povečali natezno trdnost pri izboljšanem raztezku.

Ključne besede: 16MnCrS5, natezna trdnost, raztezek, modeliranje, genetsko programiranje, linearna regresija

1 INTRODUCTION

In the modern steel-production and steel-consumption industry, it is essential to know the material properties and behavior. There are several well-known commercial types of software available for modeling material properties but steel producers are often forced on using inventive experiments, methods and approaches due to their unique production, equipment, time constraints and niche applications.[1–6]

The literature review reveals that tensile strength and elongation optimization of steel products in general incorporates multi-criteria optimization approaches,[1,2,7–9] based also on artificial intelligence methods.[10–14]This is the case for rated material properties in both quantitative and qualitative terms.[1,10]

The required tensile strength and elongation are obtained by changing:

- chemical composition,[2,12,14]
- plastic deformation parameters (i.e., influencing microstructure, grain size),[8,15–17]
- heat-treatment parameters after plastic deformation.[2,7,14]

The article presents the practical implementation of tensile strength and elongation optimization for long-rolled products made of 16MnCrS5 steel, which is generally used for the fabrication of case-hardened machine parts for several applications (e.g., bars, rods, plates, strips, forgings).

First, we provide the experimental background, then the methods used, and, lastly, we present the practical implementation and draw conclusions.

2 EXPERIMENTAL BACKGROUND

In general, production starts with scrap melting in an electro arc furnace (EAF).[18] After the scrap and carburizing agents have been melted, dephosphorization is conducted. The melting bath is heated up to the tapping temperature and, after secondary steel treatment, is discharged into the casting ladle.

After discharging from EAF, the melting bath is deoxidated, desulphurized, the nonmetallic inclusions are filtered out, the slag metallic oxides are reduced, the hydrogen and nitrogen are partly degassed, the melting bath and temperature field are homogenized, and then the formed slag exchange and the major alloying are carried out. The melt is poured from the casting ladle into the tundish on the continuous casting device, where 180 mm square billets from 2 m to 4 m in length are cast. All billets are cooled before the rolling operation.

The billets are heated, in accordance with the prescribed temperatures, in the continuous heating furnace. After heating, the billets are hot rolled on the rolling stands. Depending on the various shapes and dimensions of the grooves, cylindrical, square or flat steel bars can be produced. Steel bars are cooled on the cooling bed. After cooling they are cut into different lengths using hot shears. During cutting, the samples for examination of the material are taken (e.g., tensile strength, hardenability, micro-cleanliness).

After cooling, the bars can be additionally heat treated in accordance with the customers' orders.

In Štore Steel there are 7 different quality prescriptions (chemical compositions) for 16MnCrS5.[19] Only the most representative one (**Table 1**) was used in the research. From October 2008 to February 2016, 70 consecutively cast batches (orders) with diameters from 20 mm to 55 mm were produced. In all cases the data on tensile strength and elongation is available. For some orders the bars were also heat treated:

- GKZ (Glühen auf kugeligen Zementit) – spheroidization annealing or
- BG annealing – isothermal annealing (for excellent machinability properties and a better micro-structure homogenizing).
- The heat treatment is conducted using the tunnel heat-treatment furnace.[3]

Table 1: Chemical composition in mass fractions (*w*/%) of the most representative quality prescription (17) for 16MnCrS5

	C	Mn	Cr	S	Mo	Ni
Minimum	0.14	1.00	0.8	0.020		
Maximum	0.19	1.30	1.1	0.040	0.08	0.30

During the microstructure examination, also the pearlite content and percentage of spheroidization (after GKZ annealing) were assessed. The micro-cleanliness (*K*3) was determined according to DIN 50602, method K. All the metallurgical examinations and tensile testing were conducted by the head of the metallurgical laboratory and by the person responsible for mechanical testing. The collected data is presented in **Table 2**. In the same table, besides quantitative (i.e., chemical composition, content of pearlite, percentage of spheroidization and micro-cleanliness), also the qualitative parameter is included (heat treatment), where the prediction of material properties is often aggravated.[1,10]

Table 2: The collected data on 16MnCrS5 (quality prescription 17)

Batch #	C (%)	Mn (%)	S (%)	Cr (%)	*K*3	Pearlite (%)	Spherodization (%)	Heat treatment	Rm (N/mm^2)	A (%)
1	0.17	1.26	0.03	1	7	40	0	/	669	24.5
2	0.17	1.22	0.027	0.99	5	40	0	/	604	17.2
3	0.17	1.22	0.027	0.99	6	45	0	/	658	16.1
4	0.18	1.2	0.025	0.97	6	40	0	/	654	16.2
5	0.17	1.19	0.023	0.99	7	45	0	/	666	16.8
6	0.19	1.29	0.023	1.09	9	40	90	GKZ	437	29.5
7	0.15	1.05	0.033	0.82	3	45	80	GKZ	454	30.4
8	0.15	1.02	0.028	0.82	11	40	90	GKZ	440	28.9
9	0.19	1.3	0.019	1.06	9	40	95	GKZ	446	30.5
10	0.19	1.27	0.021	1.07	15	40	0	BG	570	22.2
11	0.15	1.02	0.03	0.85	7	40	0	BG	593	22.3
…	…	…	…	…	…	…	…	…	…	…
70	0.16	1.09	0.029	0.92	5	40	0	/	644	15.2

3 MODELING OF TENSILE STRENGTH AND ELONGATION

In **Table 2** the percentage of spheroidization depends on GKZ (Glühen auf kugeligen Zementit) – spheroidization annealing. Accordingly, both "qualitative" parameters of GKZ and BG annealing can be replaced, respectively, by the quantitative values 0 and 1 (0 for when no heat treatment is used; 1 for when the heat treatment is used).

For the model fitness the average relative deviation between the predicted and the experimental data was selected. It is defined as Equation (1):

$$\Delta = \frac{\sum_{i=1}^{n} \left| E_i - P_i \right|}{n} \qquad (1)$$

where n is the size of the collected data, and E_i and P_i are the actual and the predicted total tensile strength or elongation, respectively.

The tensile strength and elongation were modeled using linear regression and genetic programming. The results of the modeling are presented hereafter.

3.1 Linear regression

Based on the linear regression results regarding tensile strength only the percent of spheroidization and heat treatment are statistically significant influential parameters ($p < 0.05$). The average relative deviation between the predicted and the experimental data is 3.06 %. The linear-regression model for the tensile-strength prediction is in Equation (2):

$$Rm = 500.0126 \cdot \mathrm{C} - 198.777 \cdot \mathrm{Mn} + 119.686 \cdot \mathrm{S} + 128.071 \cdot \mathrm{Cr} - 0.0738 \cdot K3 + 1.815 \cdot \mathrm{Pearlite} - 1.66 \cdot \mathrm{Spherodization} + 587.2196 \qquad (2)$$

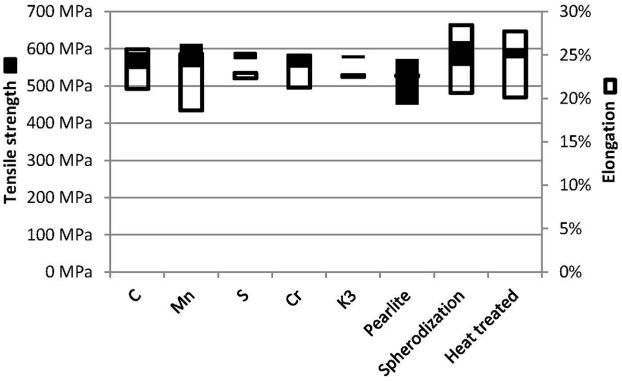

Figure 1: Calculated influences of individual parameters on the tensile strength and elongation, while separately changing them within the range from **Table 2**

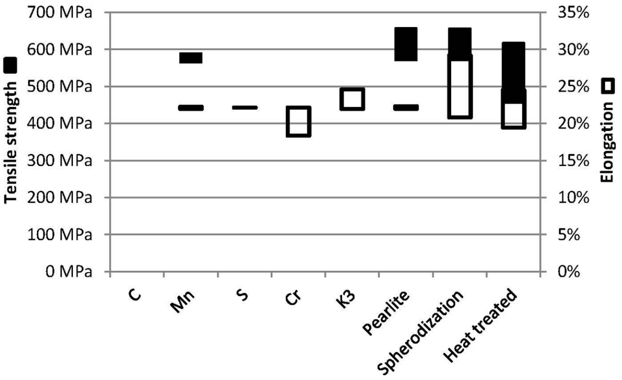

Figure 2: Calculated influences of individual parameters on the tensile strength and elongation, while separately changing them within the range from **Table 2**

During the elongation modeling only the percentage of spheroidization and heat treatment are statistically significant influential parameters ($p < 0.05$). The average relative deviation between the predicted and the experimental data is 7.56 %. The linear regression model for the tensile-strength prediction is:

$$A = -57.295 \cdot C + 21.749 \cdot Mn \pm 44.973 \cdot S - 12.498 \cdot Cr - 0.0093 \cdot K3 - 0.0247 \cdot Pearliten + 0.07823 \cdot Spherodization + 16.718 \tag{3}$$

It must be emphasized that the percentage of spheroidization and heat treatment statistically significantly influences both the tensile strength and the elongation. However, it does so conversely (i.e., if tensile strength is increased by the influence of both parameters, the elongation is decreased and vice versa).

Figure 1 shows the calculated influences of individual parameters on the tensile strength and elongation using the developed models, while separately changing the individual parameter within the range from **Table 1**. It can be concluded that the C, Mn, S and Cr content, the percentage of spheroidization and the heat treatment are the most influential factors.

3.2 Genetic programming

Genetic programming has already been found useful for several different applications in Štore Steel Ltd.[3,6,18,19] Genetic programming is a population-based algorithm that is similar to a genetic algorithm and many other heuristic optimization techniques.[20–23] In the present paper 100 models for tensile strength and also for elongation were obtained through a genetic programming method. During the simulated evolution the organisms (with basic ingredients – function and terminal genes) are generated and afterwards changed through different changing algorithms. The following function genes were selected: addition (+), subtraction (-), multiplication (*) and division (/). The selected terminal genes were: weight percentage of C (*C*), Mn (*MN*), S (*S*), Cr (*CR*), the micro-cleanliness K3 (*K*3) determined according to DIN 50602, method K, content of pearlite in % (*PEARLITE*), percentage of spheroidization (*SPHER*) and heat treatment (*HT*).

The AutoLISP-based in-house genetic programming system was run 100 times in order to develop 100 independent civilizations. Each run lasted approximately 4 h and 40 min on a 3.0-GHz processor with 4 GB of RAM.

$$\begin{aligned}
&\frac{5.65484 + \mathrm{C} + 5.21897\,\mathrm{PEARLITE} + 5.21897\,(\mathrm{Mn} + \mathrm{PEARLITE}) + 1 - \left(-5.21897 + \frac{27.2376\mathrm{HT\,Mn}}{\mathrm{HT\,Mn+PEARLITE}}\right)\left(\mathrm{Mn} - \frac{27.23764(16.1979+2\,\mathrm{Mn})}{-42.2681770815+\mathrm{PEARLITE}} - \frac{0.1916\mathrm{Mn}}{\mathrm{SPHER}}\right) - 5.21897\,(\mathrm{Mn} + \mathrm{SPHER})}{\mathrm{PEARLITE}} + \\
&\frac{-\mathrm{Mn}\left(-5.21897 + \frac{741.8894\,\mathrm{HT\,Mn}}{(\mathrm{Mn+PEARLITE})(\mathrm{HT\,Mn+PEARLITE})}\right) + \frac{27.2376(8.09895+2\,\mathrm{Mn})}{\mathrm{PEARLITE}-5.21897\mathrm{SPHER}} - \frac{16.1979+2\,\mathrm{Mn}}{\mathrm{PEARLITE}-5.21897\mathrm{SPHER}} + \frac{\mathrm{Mn}}{\mathrm{SPHER}+\frac{8.09895+\mathrm{HT\,Mn+SPHER}}{\mathrm{PEARLITE}}}}{\mathrm{SPHER} + \frac{8.09895+\mathrm{HT\,Mn+SPHER}}{\mathrm{PEARLITE}}} + \\
&\frac{-\mathrm{Mn}\,(-5.21897 + 2\,\mathrm{Mn}\,(\mathrm{HT} + \mathrm{HT\,Mn})) + \frac{5.21897(\mathrm{PEARLITE}-5.21897\mathrm{SPHER})}{\mathrm{SPHER}} + \frac{\mathrm{Mn}}{5.21897\mathrm{SPHER} - \frac{27.2376\,\mathrm{Mn}}{\mathrm{PEARLITE}+\mathrm{SPHER}} + \frac{\mathrm{Mn+HT\,Mn}+\frac{\mathrm{HT\,SPHER}}{\mathrm{PEARLITE}}}{(-5.21897+\mathrm{HT\,Mn})\,\mathrm{SPHER}}}}{\mathrm{SPHER} + \frac{8.09895+(-5.21897+2\,\mathrm{Mn}\,(\mathrm{HT+HT\,Mn}))\,(2\,\mathrm{HT\,Mn+SPHER})}{\mathrm{PEARLITE}}}
\end{aligned} \tag{4}$$

$$
\begin{aligned}
&15.70195+\mathrm{Mn}+4.96016\left(\mathrm{HT}+\frac{\mathrm{HT}+\mathrm{SPHER}+\frac{\mathrm{Cr}+\mathrm{HT}+\mathrm{SPHER}}{0.3709+2\,\mathrm{HT}+\mathrm{K3}+0.10849\mathrm{SPHER}}}{9.21726+\frac{\mathrm{SPHER}}{\mathrm{S}}+\frac{\mathrm{Cr}+\mathrm{SPHER}}{\mathrm{PEARLITE\ SPHER}}}\right)+\\
&\frac{\mathrm{SPHER}+\frac{\mathrm{SPHER}}{\mathrm{K3}}-\frac{-3.41876+\mathrm{Cr}+\mathrm{HT}}{-\mathrm{Cr}+\frac{3.41876}{\mathrm{HT}}+\mathrm{HT}+2\,\mathrm{K3}-\mathrm{PEARLITE}+\frac{\mathrm{SPHER}}{\mathrm{K3}}}+\frac{3.41876}{-\frac{3.41876}{\mathrm{HT}}+\mathrm{K3}-\frac{\mathrm{SPHER}+\frac{\mathrm{SPHER}}{\mathrm{K3}}+\frac{3.41876\ \mathrm{PEARLITE}}{\mathrm{Cr}+\mathrm{SPHER}}}{9.21726+\mathrm{Cr}+\frac{\mathrm{SPHER}}{\mathrm{PEARLITE}}}}}{9.21726+\mathrm{HT}+\frac{\mathrm{SPHER}+\frac{\left(9.21726+\mathrm{Cr}+\frac{1-\frac{3.41876}{\mathrm{HT}}}{9.21726+\mathrm{Cr}+\mathrm{HT}+\mathrm{PEARLITE}}+\frac{3.41876\ \mathrm{HT}}{\mathrm{SPHER}}-\frac{3.41876}{\mathrm{K3\ SPHER}}\right)\left(0.3709+\mathrm{HT}+\mathrm{K3}+\mathrm{SPHER}+\frac{\mathrm{HT}+\mathrm{SPHER}}{9.21726'+\mathrm{HT}+0.10849\ \mathrm{SPHER}}\right)}{-9.21726-\mathrm{HT}+\mathrm{K3}+\mathrm{SPHER}-\frac{\mathrm{SPHER}}{\mathrm{PEARLITE}}}}{\mathrm{PEARLITE}}}
\end{aligned}
\tag{5}
$$

The selected maximum number of generations was 100. The selected size of the population of organisms 100, the reproduction probability 0.4, the crossover probability 0.6, the maximum permissible depth in the creation of the population 6, the maximum permissible depth after the operation of crossover 10, and the smallest permissible depth of the organisms in generating new organisms 2. For the selection of organisms the tournament method with tournament size 7 was used.

For the tensile-strength modeling, the most succesful organism from all of the civilizations is presented in Equation (4).

The average relative deviation between the predicted and the experimental data is 2.89 %. The model consists of 235 genes. Its depth is 14. It must also be emphasized that the parameters (genes) *CR*, *S*, *K*3 are not included in the model.

For elongation modeling, the most succesful organism from all of the civilizations is presented in Equation (5).

The average relative deviation between the predicted and the experimental data is 5.18 %. The model consists of 189 genes. Its depth is 14. It must also be emphasized that parameters (genes) *CR*, *S*, *K*3 are not included in the model.

Figure 2 shows the calculated influences of the individual parameters on the tensile strength and elongation using the genetically developed model (Equations (4) and (5)), while separately changing the individual parameter within the range from **Table 2**. It can be concluded that Cr and pearlite content, the percentage of spheroidization and the heat treatment are the most influential factors.

4 IMPLEMENTATION OF MODELING RESULTS

Up until February 2016, six consecutively cast batches (16MnCrS5, quality prescription 17) were used for the implementation of the modeling results. The collected data are presented in **Table 3**. Depending on the chemical composition and the pearlite content, the plan for the heat treatment is determined in order to achieve the optimal tensile strength at moderate elongation.

Table 3: The collected data on 6 16MnCrS5 (quality prescription 17) consecutively cast batches

Batch #	C (%)	Mn (%)	S (%)	Cr (%)	*K*3	Pearlite (%)
1	0.17	1.09	0.035	0.87	4	40
2	0.17	1.13	0.025	0.86	8	45
3	0.16	1.08	0.026	0.85	6	40
4	0.18	1.09	0.022	0.85	7	40
5	0.15	1.07	0.023	0.87	6	40
6	0.17	1.13	0.025	0.99	7	40

Figure 3 presents the prediction of tensile strength using linear regression and genetic programming for the 6 batches (from **Table 3**). There are statistically significant differences (one-way ANOVA, $p < 0.05$) between the predicted tensile strength when the heat treatment is used and when it is not used – for both methods: linear regression and genetic programming. GKZ annealed material has the statistically significantly lowest tensile strength (one-way ANOVA, $p < 0.05$).

Figure 4 presents the prediction of elongation using linear regression and genetic programming for 6 batches (from **Table 3**). There are statistically significant differences (one-way ANOVA, $p < 0.05$) between the predicted elongation when the heat treatment is used and when the heat treatment is not used – for both methods: linear regression and genetic programming. GKZ annealed ma-

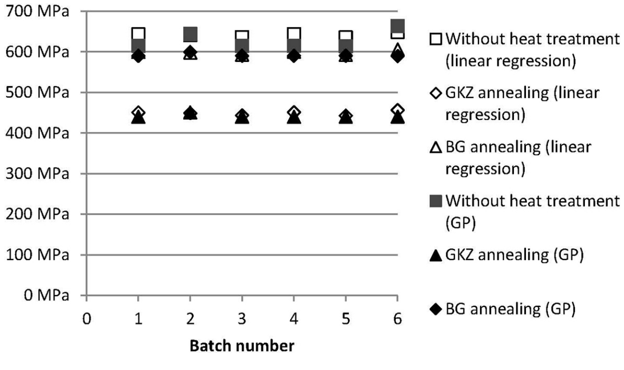

Figure 3: Calculated influences of the individual parameters on the elongation, while separately changing them within the range from **Table 2**

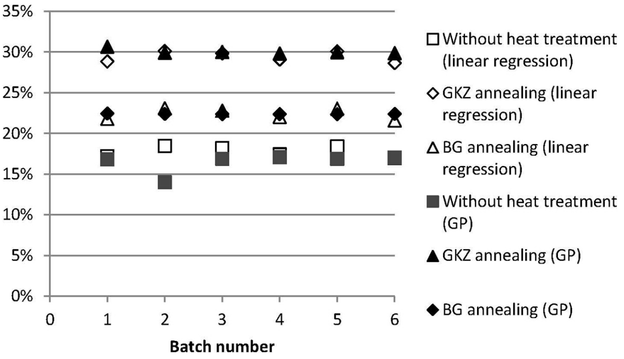

Figure 4: Calculated influences of the individual parameters on the elongation, while separately changing them within the range from **Table 2**

terial has the statistically significantly highest elongation (one-way ANOVA, $p < 0.05$).

In accordance with the predictions presented in **Figures 3** and **4** the BG annealing was selected in order to achieve a higher tensile strength at moderate elongation.

The tensile-test results (tensile strength and elongation) and linear-regression results are presented in **Table 4**.

The average relative deviation between the predicted and the experimental data for the tensile strength for linear regression and genetic programming is 3.55 % and 3.08 %, respectively. The average relative deviation between the predicted and the experimental data for elongation for linear regression and genetic programming is 3.56 % and 2.65 %, respectively.

5 CONCLUSIONS

The 16MnCrS5 steel grade is generally used for the fabrication of case-hardened machine parts for several applications (e.g., bars, rods, plates, strips, forgings), where having a combination of wear resistance, toughness and dynamic strength is essential. These qualities can be easily correlated with tensile test results (e.g., tensile strength, elongation), which depends on the chemical composition and the heat treatment after rolling.

Accordingly, from October 2008 to February 2016, 70 consecutively cast batches with diameters from 20 mm to 55 mm were produced. In all cases the data on the tensile strength and elongation is available. For some orders the bars were also heat treated:

- GKZ (Glühen auf kugeligen Zementit) – spheroidization annealing or
- BG annealing – isothermal annealing (for excellent machinability properties and a better microstructure homogenizing).

The chemical composition (content of C, Mn, S and Cr) and heat-treatment regime (GKZ or BG annealing) data were collected. During the microstructure examination also the pearlite content and the percentage of spheroidization (after GKZ annealing) were assessed. The micro-cleanliness (*K*3) was determined according to DIN 50602, method K.

The tensile strength and elongation were modeled using linear regression and genetic programming.

The ANOVA results obtained using linear regression show that only the percentage of spheroidization and heat treatment are statistically significant influential parameters ($p < 0.05$) for tensile strength. The average relative deviation between the predicted and the experimental data is 3.06 %. At elongation only the percentage of spheroidization and heat treatment are statistically significant influential parameters ($p < 0.05$). The average relative deviation between the predicted and the experimental data is 7.56 %.

The average relative deviation between the predicted and the experimental data for the best genetically developed mathematical model for predicting tensile strength is 2.89 %. The model consists of 235 genes. Its depth is 14.

The average relative deviation between the predicted and the experimental data for the best genetically developed mathematical model for predicting elongation is 5.18 %. The model consists of 189 genes. Its depth is 14.

Up until February 2016, six consecutively cast batches (16MnCrS5, quality prescription 17) were used for the implementation of the modeling results. To achieve the optimal tensile strength at moderate elongation, the plan for the heat treatment has to be determined on the basis of the chemical composition and the pearlite content. The tensile strength and the elongation were predicted using linear regression and genetic programm-

Table 4: The collected data on 6 16MnCrS5 (quality prescription 17) consecutively cast batches

Batch #	C (%)	Mn (%)	S (%)	Cr (%)	*K*3	Pearlite (%)	R_m (MPa)	R_m – linear regression (MPa)	R_m – GP (MPa)	*A* (%)	*A* – linear regression (%)	A – GP (%)
1	0.17	1.09	0.035	0.87	4	40	622.0	600.28	590.53	22.60	21.82	16.85
2	0.17	1.13	0.025	0.86	8	45	641.0	598.63	599.92	22.00	23.10	14.02
3	0.16	1.08	0.026	0.85	6	40	578.0	593.48	590.74	21.90	22.81	16.91
4	0.18	1.09	0.022	0.85	7	40	613.0	600.94	590.54	23.00	22.05	17.10
5	0.15	1.07	0.023	0.87	6	40	607.0	592.67	590.98	22.70	23.05	16.89
6	0.17	1.13	0.025	0.99	7	40	598.0	606.28	589.95	22.30	21.61	17.05

ing. Based on the obtained results the BG annealing was selected in order to achieve a higher tensile strength at moderate elongation.

The average relative deviation between the predicted and the experimental data for the tensile strength for linear regression and genetic programming is 3.55 % and 3.08 %, respectively. The average relative deviation between the predicted and the experimental data for elongation for linear regression and genetic programming is 3.56 % and 2.65 %, respectively.

In the future the proposed concept will be used for analyzing the properties of selected steel grades.

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