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Application of genetic methods in materials' design

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Abstract: In the paper an optimisation method for the designing of chemical composition of high-speed steels (HSS) based on genetic algorithms (GA) is presented. The complex optimisation criterion was assumed comprising maximising secondary steel hardness with simultaneously minimising cost of material. Results of numerical simulation show that genetic algorithm-based optimisation of steel chemical composition is effective and very useful in designing of the new metallic materials.

Keywords: Genetic algorithm; High-speed steel; Chemical composition; Optimisation; Secondary hardness; Designing

1. INTRODUCTION

Since many years the investigations in the area of materials science have been carrying out to develop new materials, among them tool ones with higher working properties and fulfilling economical and ecological requirements. The main aim of this activity is the development of materials for suitable application having a few of the following required features: hardness, heat resistance, high-temperature creep resistance, wear resistance, corrosion resistance, impact strength, elasticity, strength, life, ecological manufacturing technology, recycling, low cost and other.

Fulfilling this demand is extorted by the changes still speeded up in global free-market economy where the role of inexpensive series/mass production grows up significantly.

The evolution of science at the end of the 20th century take effect in the development of new research, manufacturing and forming method of engineering materials. One can observe gradual leaving the empirical way of mastering/learning of the reality for the advantage of new, mainly computerised, methods using mathematical model of the object of investigations.

High-speed steels, which are the object of interest, are still one of the main group of steels because of their working properties and susceptibility to series production. So it justifies carrying on the research on its improvement.

Designing the chemical composition of the steel having the demanded properties, e.g. the secondary hardness, is the crucial task from the manufacturing point of view. Rapid development of computer science and technology as well as of modern computer tools among them artificial intelligence prompts their increasingly common use in different fields of science and technology.

There is a great interest in these methods, which seems to be justified, since they can be applied both to solve novel problems and to deal with the ones considered classical. For a couple of years, such trends have been presented also in the field of materials engineering.

Contemporary software tools, especially methods of artificial intelligence, make it possible to develop the method, presented in the paper, of designing of the chemical composition of high-speed steels, which still are one of the basic groups of metallic engineering materials. The methodology proposed in the work makes it possible to define precisely the chemical composition of the steel, from which the given set of mechanical properties is required as a function of the technological or other parameters (Fig. 1).

2. ASSUMPTION OF THE OPTIMISATION PROCEDURE

The problem of the optimisation of chemical composition can be formulated as the following optimisation problem:

$$Max \rightarrow Z = f(HRC(x), k(x)) = HRC(x) \cdot \frac{1}{k(x)} \tag{1}$$

where:

- Z – objective function
- Secondary hardness function:

$$HRC(x) = a_{HRC} \sum_{i=1}^{12} hrc_i(x_i) \tag{2}$$

- Cost function:

$$k(x) = a_c + \sum_{i=1}^{10} c_i x_i \tag{3}$$

Table 1.
The ranges of the optimised parameters of high-speed steels

	Mass concentration of the alloying element, %										Temperature, °C	
	C	Mn	Si	Cr	W	Mo	V	Ti	Nb	Co	Austenitising	Tempering
Min	0.75	0	0	2	1.3	0	0	0	0	0.1	1120	510
Max	1.45	0.4	0.5	4.5	19	10	4.8	1	1	10.5	1270	570

- $hrc_i(x_i)$ – partial hardness function describing an effect of a particular alloying element and temperatures of heat treatment on steel hardness
- x_i – mass concentration of the alloying elements, values of heat-treatment temperatures
- c_i – approximate cost of particular alloying elements (per 1kg of steel)
- a_{HRC}, a_c – scale parameters

Constraints for the optimisation procedure concerning limiting concentrations of the alloying elements and ranges of heat-treatment temperatures are presented in Table 1.

The hardness model model contains a summary effect of the particular alloying element, mutual effect of combination of alloying elements and effect of heat-treatment temperature on the steel secondary hardness:

$$hrcC = a_C \cdot \%C^2 + b_C \cdot \%C + c_C \tag{4}$$

$$hrcMn = a_{Mn} \cdot \%Mn - b_{MnC} \cdot \%C \cdot \%Mn \tag{5}$$

$$hrcSi = a_{Si} \cdot \%Si \tag{6}$$

$$hrcCr = a_{Cr} \cdot \%Cr - b_{CrV} \cdot \%V \cdot \%Cr \tag{7}$$

$$hrcW = a_W \cdot \%W + b_{WC} \cdot \%C \cdot \%W \tag{8}$$

$$hrcMo = a_{Mo} \cdot \%Mn - b_{MoW} \cdot \%W \cdot \%Mo \tag{9}$$

$$hrcV = a_V \cdot \%V - b_{CrV} \cdot (\%Cr + \%V) \tag{10}$$

$$hrcCo = a_{Co} \cdot \%Co - (b_{MoCo} - \%Mo)^2 \cdot \%Co \tag{11}$$

$$hTi = a_{Ti} \cdot \%Ti \tag{12}$$

$$hNb = a_{Nb} \cdot \%Nb \tag{13}$$

$$hrcT_a = a_{T_a} \cdot T_a^{\,2} + b_{Ta} \cdot T_a + c_{T_a} \tag{14}$$

$$hrcT_t = a_{Tt} \cdot T_t^{\,2} + b_{Tt} \cdot T_t + c_{Tt} \tag{15}$$

where:

- T_a – austenitising temperature
- T_t – tempering temperature
- $\%X$ – mass concentration of the alloying element X
- a_x, b_x – constant determined experimentally obtained by the use of neural network [1]

The hardness model (2) was experimentally verified. The verification procedure consists of the evaluation of the conformity of the computational results with the experimental data. The investigations were carried out on newly developed HSS steels which chemical composition is shown in table 2. 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.

Table 2
Chemical composition range of high-speed steels used in the optimisation procedure

Average mass concentration of the alloying element, %									
C	Mn	Si	Cr	W	Mo	V	Ti	Nb	Co
0,94-1,05	0,42-0,63	0,54-0,78	4,2-4,7	8,8-11,4	0-2,4	1,3-1,8	0-056	0-0,95	0-5,2

Table 3.
Approximated cost of 1-kg- addition of an alloying element in steel

Alloying element	Mn	Si	Cr	W	Mo	V	Ti	Nb	Co
Price [€*)/10kg]	0,12	0,025	0,43	1,2	38,06	83,8	215,5	71,86	35,93
*) March 2004									

The cost model is an approximated one and worked out on the basis of information published in [2] and market price of the high-speed steels.

It has been assumed that the price of an alloying element comes from the proportion of their price to the price of high speed steel in which they appear (Table 3).
The result of the mentioned assumption is the following cost model:

$$\begin{aligned} price = CC \cdot (&\%PS + p\_Mn \cdot \%Mn + p\_Si \cdot \%Si + \\ &p\_Cr \cdot \%Cr + p\_W \cdot \%W + p\_Mo \cdot \%Mo + \\ &p\_V \cdot \%V + p\_Co \cdot \%Co + p\_Ti \cdot \%Ti + p\_Nb \cdot \%Nb) \end{aligned} \tag{16}$$

where:

- CC – constant cost of manufacturing 1 kg of "pure steel", independent on steel chemical composition
- $\%PS$ – amount of "pure steel" given by the equation:

$$\begin{aligned} p\_st = 1 &- \%Mn - \%Si - \%Cr - \%W - \%Mo - \\ &- \%V - \%Co - \%Ti - \%Nb \end{aligned} \tag{17}$$

- *%X* – mass concentration of the alloying element *X*
- *p_X* – cost of the particular alloying element according to Table 3

It is necessary to emphasise that the presented model estimates only the price of the steel and the coefficients *p_X* should be treated as exemplary one for further researches.

3. OPTIMISATION PROCEDURE

As a tool the evolutionary algorithm was employed [3]. Evolutionary algorithms are stochastic search methods that mimic the metaphor of natural biological evolution. Evolutionary algorithms operate on a population of potential solutions applying the principle of survival of the fittest to produce better and better approximations to a solution. At each generation, a new set of approximations is created by the process of selecting individuals according to their level of fitness in the problem domain and breeding them together using operators borrowed from natural genetics. This process leads to the evolution of populations of individuals that are better suited to their environment than the individuals that they were created from, just as in natural adaptation. Evolutionary algorithms model natural processes, such as selection, recombination, mutation, migration, locality and neighbourhood. Evolutionary algorithms work on populations of individuals instead of single solutions. In this way the search is performed in a parallel manner.

After the preliminary one, the main calculations were made for the following genetic algorithm parameters: size of population – 300 individuals, crossover probability – 0,4, mutation probability – 0,3, umber of epochs – 150. Selected results of the optimisation of the chemical composition are presented in the full paper [4].

4. FINAL REMARKS

The paper presents a genetic algorithm optimisation approach for designing chemical composition of high-speed steels and optimal heat-treatment parameters ensuring maximal secondary hardness with the minimal costs of steel. The results of the proposed approach are the preliminary ones.

One can observe that steels being results of optimisation are tungsten-vanadium high-speed steels with increasing concentration of silicon, titanium and niobium. Obtained results of hardness cost of steel are determined by the objective function, and mainly by the hardness model. So it is advisable to continue the optimisation research by using the better hardness model i.e. based on neural network.

The work is limited to the presentation of the possibilities of the evolutionary optimisation that is why the achieved results should be treated as estimations. This research definitely indicates some directions for future work.

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