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A DESIGN OF NEW BRANDS OF MARTENZITE STEELS BY ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

The paper proposes a model-based approach for the design of martenzite structure steels with improved mechanical and plastic characteristics using proper composition and thermal treatment. For that purpose, artificial neural models approximating the dependence of steels strength characteristics on the percentage content of alloying components were trained. These non-linear models are further used within an optimization gradient procedure based on backpropagation of utility function through neural network structure. In order to optimizing the steel characteristics via its chemical composition, several steel brands with high values of tensile strenght, yield strenght and relative elongation were designed. A steel composition having economical alloying and proper for practical application was determined comparing several obtained decisions. The usage of that steel will lead to lightening of the hardware for automobile industry.

KEYWORDS: metal materials, high strength steels, composition optimization, neural networks

1. Introduction

Metallurgy and, in particular, steel production for motor industry have develop faster during the last decades. On the one hand, methods and technologies for characteristics optimization of known steel brands are looked for, on the other hand, a lot of research efforts are targeted to designing new steel brands with improved physical-chemical and mechanical characteristics.

Especially for the steels used in motor industry, the research aim is to decrease the weight of the final product applying high strength steels. The number of high strength steels application increase because they are able to meet at the same time the contradictive requirements for better deformability, weldability, resistance to stress, fatigue, and corrosion.

Since the motor vehicles are the biggest source of pollutants of the environment (producing harmful emissions of CO_2= 0,2 kg/km), nowadays a lot of efforts are targeted to their weight decreasing. This will lead to improvement of their combustible efficiency and as a result, to the decrease of harmful emissions decrease. In [1] several innovative approaches related to economy of fuel, the decrease of harmful emissions and recycling are described. It is demonstrated that the use of high strength steels allows decreasing car carriage weight with 25%, and it is expected to achieve even 35 % weight decrease using the new generation of high strength steels that are still under development.

While the strength of the most common application steels varies in the range of 440–590 MPa, a part of special components of steels have tensile strength about 980–1180 Mpa. High strength foliate steels still have restricted application because of their restricted plasticity. In Nippon Steel Corporation, three brands of high strength steels (980 MPa) are designed and introduced into vehicle production. [2].

Moreover from the functional and economic point of view the high strength steels appear to be the best material for the mentioned application. The iron based materials ensure such a structure and properties that absorb the shock energy. The quick elaboration of the steels applied for motor-car construction leads to definition of steel classes denoted by AHSS (Advanced High Strength Steels). In 2002 a project ULSAB - AVS (Ultra _ Light Steel Autobody) started. Fig. 3 shows that the average value of the tensile strength for the developed steels increases from 413 MPa to 758 MPa [3]. Together with the increasing values of the strength there is also a tendency towards improved deformability. The ULSAB - AVS project applies the high strength steels for parts of the entire car. In an investigation of the model Audi A1, one can see that the quota of the high strength steels is approximately two times greater than the conventional low carbon steels. Farahani [4] gives an investigation published by the International Council on Clean Transportation that represent different ways for development.

The short-term plan foresees that in 2014 the mild steel will be changed with the high strength steels. For the analysis a Toyota Venza (model from 2009) has been chosen. The aim is a reduction of the total mass with 20%.

This study presents a new contemporary method for design of optimized iron-based alloy composition using artificial neural networks (ANN) accounting for economic alloying at the same time.

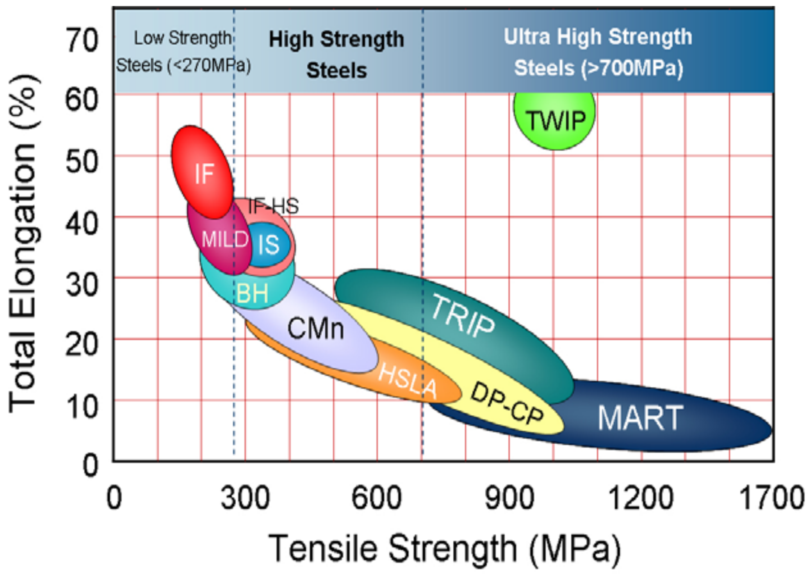

Fig. 1. *Areas of variance of steels quality characteristics according to the program ULSAB–AVC.*

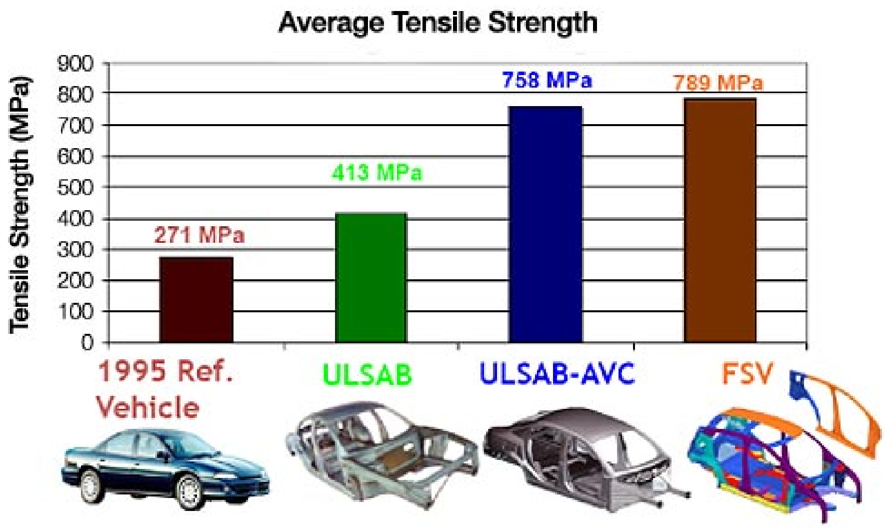

Fig. 2*. Change of the average value of the materials tensile strength at different motor-car construction projects.*

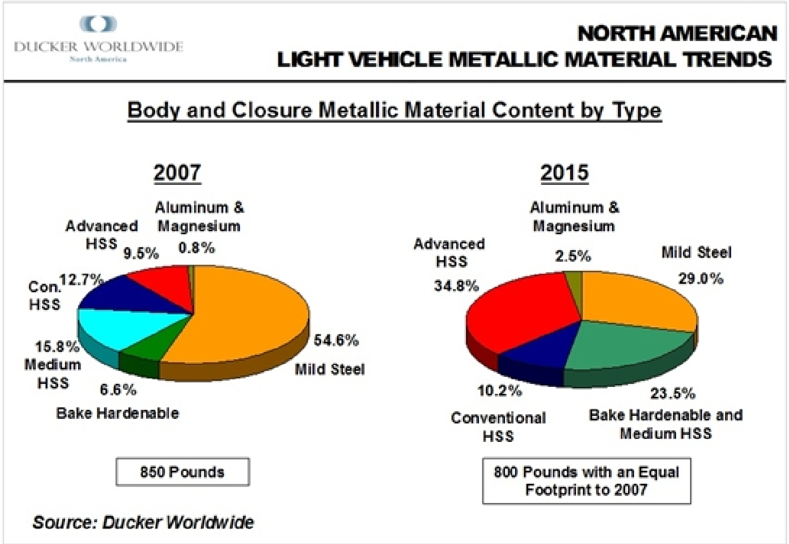

***Fig. 3**. Distribution of the steel types used by the motor-car construction.*

2. Steel types and contemporary trends

During the reduction of elements amount in the steels there is need to keep the design balance of the system "composition – treatment regime – characteristics" that will allow to improve its strength and plastic characteristics.

Steels used in vehicle production can be classified based on different indications, as it is shown on Figure 1.

Diphase (DP) steels structure consists of ferrite matrix containing hard martenzite part and of soft ferrite phase.

The lather insures good conditions for shape changing.

The increase in martenzite volume leads to the increase of steel strength.

In TRansformation Induced Plasticity (TRIP) steels residual austenite of about 5% is included into ferrite matrix together with different amounts of hard phases martenzite and bainite. During deformation, residual austenite is converted into martenzite. Complex phase (CP) steels on similar to the TRIP steels microstructure but they do not contain residual austenite.

In MART steels, the final structure is obtained from austenite that is converted entirely into martenzite matrix containing small amounts of ferrite and/or bainite during hot roll forging. Martenzite MART steels possess higher tensile strength, up to 1700 MPa, and at the same time lower ability to plastic deformation.

As can be seen in the above figure, increase in strength of different types of steel is related the decrease of its total elongation. This unfavorable feature of high strength steels leads to deterioration of their deformability but also improves their stress resistance without increasing product weight.

Steels chemical composition is of crucial importance for product quality. The quality is determined by the mechanical characteristics of steel obtained after their plastic and thermal treatment. Manganese, chrome, molybdenum, and nickel added as alloying elements in combination or separately help to increase steels strength. Increasing of carbon amount leads the increase of martenzite. Variations in carbon and other alloying elements during optimization must improve not only steels mechanical characteristics but also their technological properties such as weldability, deformability etc.

3. Design of martenzite steel with optimal characteristics

The design of steels includes determination of their chemical composition, parameters of thermal treatment regime and obtained mechanical characteristisc.

Here we propose a design procedure that relates the mechanical characteristics aimed at to chemical steels composition using multiple criteria optimization. Optimization criteria contain complex of targeted for given application steel characteristics defined as objective functions.

In the present study a data base of 92 alloys from [5] was used. It contain alloys chemical compositions and their corresponding to mechanical characteristics. The alteration intervals of the considered alloying elements are given in Table 1 and Table 2 contains the change intervals of mechanical characteristics after thermal treatment (tempering and low temperature lukewarming).

***Table 1**. Alteration intervals of investigated steels alloying elements*

Element	**C**	**Si**	**Mn**	**Ni**	**S**	**P**	**Cr**	**Mo**	**V**
min, %	0.12	0.27	0.27	0	0.025	0.025	0.15	0	0
max, %	0.5	1.4	1.6	4.22	0.035	0.35	2.5	1.5	0.15

***Table 2**. Alteration intervals of investigated steels mechanical characteristics*

Mechanical characteristic	**Rm**, MPa	**Re**, MPa	**A**, %	**Z**, %	**KCU**, KJ/m^2	**HB*10^{-1}**, MPa
min	500	300	7	30	290	179
max	1670	1375	26	70	1830	541

For steel composition optimization purposes, developed in [6] a methodology based on ANN was applied.

The first step is to train neural network model approximating non-linear dependence between alloying elements amounts and obtained after thermal treatment of the mechanical characteristics of the given steel. Our former investigations [6] showed that due to insufficient data it is impossible to train a single accurate NN model for predicting all investigated mechanical characteristics. Here we trained separate NN models for each of the mechanical characteristics from Table 2. Since the amounts of sulfur and phosphorus in all investigated steels are equal, they are considered as one variable. The NN structure as in [4] is 8:40:1. The number of inputs is defined by the number of alloying elements, i.e. eight. All NN models have single output neuron for the modeled one of the mechanical characteristics. The number of hidden units was determined by trail and error as in [6].

We also had to account that the database we have is relatively small and it do not contain all the possible combinations between alloying elements. Because of that we divide the available data into 18 smaller data sets used for training of 18 NN models excluding each time one of the data sets for testing. Then the best model for each of the mechanical characteristics was chosen based on smaller testing error.

Because the investigated input/output space is multidimensional and the modeling dependencies are non-linear, in order to find global optima during optimization we need to explore the entire input space. However, due to huge number of possible combinations, this is a time and resource demanding task. That is why here we apply gradient the procedure proposed in [6]starting from numerous different initial points. Finally, the obtained optimal compositions are compared and the best ones were chosen.

Figure 4 presents the main optimization procedure known as "backpropagation of objective function" [7]. The optimization task is the following: find values of input vector X that maximize (minimize) the objective function:

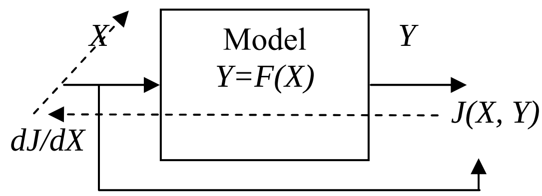

***Fig. 4**. Optimization procedure. Dashed lines represent gradient calculation direction.*

$$J = J(X, Y) \quad (1)$$

Here Y is output variables vector that is related to the input one via a given function (here NN model) F as follows:

$$Y = F(X, p) \quad (2)$$

and p is model parameters vector.

The gradient procedure needs calculation of objective function derivatives with respect to optimized variables as follows:

$$dX = \frac{dJ}{dX} = \frac{\partial J}{\partial X} + \frac{\partial J}{\partial Y}\frac{\partial F}{\partial X} \quad (3)$$

In the cases when J do not depend explicitly on X, the first term in equation (3) is zero, i.e. the derivative depends only on function F.

The layered structure of neural network models offer a convenient way for calculation of derivatives from (3) using backpropagation procedure.

The next step is the iterative determination of the optimal values of X as follows:

$$X_i = X_{i-1} \pm \alpha \Delta X_i \quad (4)$$

Here α is a parameter called learning rate and ΔX_i is a step change of *X* at i-th iteration calculated as follows:

$$\Delta X_i = g(dX_i) \tag{5}$$

Here g is a function defining the gradient. Usually it is proportional to dX_i but in some cases it could depend also on previous values of ΔX_i. Here we used simple gradient procedure with $\Delta X_i = dX_i$. The learning rate α is chosen relatively small and stopping criteria were very small change in objective function.

In our case the input vector X consists of concentrations of 8 alloying elements and the output vector – of corresponding steel mechanical characteristics.

The following optimization tasks were solved:

A.Single criteria optimization- maximization of ***Re***:

$$J_1 = \mathrm{Re} \to \max \tag{6}$$

Table 3*. Chosen optimal compositions,%*

Decision Compounds/ characteristics	№1	№2	№3
C	0.27	0.3	0.26
Si	1.10	1.02	1.24
Mn	1.06	1.2	1.18
Ni	2.36	2.35	2.78
S	0.02	0.02	0.02
P	0.02	0.02	0.02
Cr	1.04	0.96	1.26
Mo	0.15	0.18	0.23
V	0.0087	0.0087	0..022
Rm, MPa	1666.9	1678.	1647.5
Re, MPa	1370.3	1355	1370.9
A, %	11.4	12.8	12.2
Z, %	51.1	52.3	54.1
HB	281.6	284.3	287.4

B.Two-criteria optimization: simul-taneous maximization of ***Re*** and of the ratio ***Rm/Re***:

$$J_1 = \mathrm{Re} \to \max,$$

$$J_2 = \frac{Rm}{\mathrm{Re}} \to \max \tag{7}$$

In both cases, the restriction C≤0.3 was imposed aimed at obtaining low carbon steels.

After applying the above optimization procedure, three optimal decisions were chosen. They are shown in Table 3 below. The first two of them maximize ***Re*** while the third one maximizes the ration ***Rm/Re***.

Finally, composition № 2 is chosen because it is the most economical one.

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Conclusion

Here we presented an approach to design optimal steel compositions for transport vehicles industry. The applied methodology on bases in artificial neural networks. Via optimization of mechanical characteristics on base of the chemical composition of the steel, the values of tensile strength and yield strength are kept high at total elongation of about 12%.

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