Prediction of Martensite Start Temperature by Neural Network Analysis

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Abstract. Commercial steels are nowadays sophisticated alloys formed by a large number of alloying elements. The martensite start (M_s) temperature of such steels is of vital engineering importance, and its prediction through models allows us to enhance the design and development of industrial products. In the present work, M_s temperature dependence on chemical composition has been examined by neural network analysis. Neural networks represent powerful methods of non-linear regression modelling. The network is a mathematical function which is fitted to experimental data. The influence of alloying elements such as C, Mn, Si, Cr, Ni, Mo, V, Co, W, Al, Nb, Cu, B and N on M_s temperature was analysed. Finally, a new empirical equation for M_s temperature was derived based on the neural network results.

1. INTRODUCTION

The martensite start temperature, M_s , is a design parameter of vital importance for deciding on many process conditions, for example, the exact welding conditions necessary to avoid cracking. Hence great efforts have been made in predicting the M_s of steels. Obviously, chemical composition of steel is the main factor affecting its M_s , although the austenitising state, external stresses and stored deformation energy may sometimes play an important role as well. Martensite start temperatures are usually relatively easy to calculate as long as the steels have a low alloy content [1-6]. Even though empirical equations exist for high alloy steels, they are not sufficiently general and are known to provide inaccurate answers for the new steels which contain different alloying elements, or their compositional range are out of bounds of those used to formulate the equations.

It has been reported that additions of Mo, Co and W to the chemical composition increase the strength of steel with molybdenum (Mo_2C) and tungsten-cobalt (WC-Co) cemented carbides [7-9]. These new developed steels are materials that are widely used in applications where a good combination between abrasion resistance and corrosion resistance is required (tool steels) [10]. Likewise, new copper-bearing low carbon steels have been developed. Additions of copper increase the strength of steel by precipitation of fine copper precipitates during ageing instead of carbide particles, which considerably improve mechanical properties. Moreover, in the last decade the use of microalloying elements such as V and Nb has increased spectacularly.

Bearing in mind that M_s temperature is a parameter of considerable importance for engineering steels, to find out how Co, W, Cu, Mo, V or Nb can affect the M_s temperature is an important issue to be investigated. The aim of this work is to develop an artificial neural network model to predict the M_s temperature of steels and interpret the influence of the chemical composition.

2. BRIEF DESCRIPTION OF THE NEURAL NETWORKS

The network consisted of 14 input nodes (Table 1), a number of hidden nodes, and an output node representing the M_s temperature. Meanwhile in a traditional linear regression each input is multiplied by a random weight w_i and the products are summed together with a constant θ to give the output node $y = \sum_i w_i x_i + \theta$, in neural network analysis the input data x_j are also multiplied by weights ($w_j^{(1)}$), but the sum of all these products forms the argument of a hyperbolic tangent. The output is linear combinations of these hyperbolic tangent functions:

$$h = \tanh\left(\sum_j w_j^{(1)} x_j + \theta_j^{(1)}\right)$$

$$y = w^{(2)} h + \theta^{(2)}$$
(1)

where $w^{(2)}$ is a weight and $\theta^{(2)}$ another constant. The weights were determined by training the network and the details are described elsewhere [11]. The model developed in this work consists of 7 hidden nodes and it is developed under a Bayesian framework [12], which allows the calculation of error bars representing the uncertainty in the fitting parameters. The method recognises that there are many functions which can be fitted or extrapolated into uncertain regions of the input space, without unduly compromising the fit in adjacent regions which are rich in accurate data. Instead of calculating a unique set of weights, a probability distribution of sets of weights is used to define the fitting uncertainty. The error bars therefore become larger when data are spare or locally noisy.

Table 1. Variables that influence Ms temperature. The values are in wt.-%. S.D. is the standard deviation. P.T. is the number of points in the training.

	C	Mn	Si	Cr	Ni	Mo	V	Co	Al	W	Cu	Nb	B	N
Min.	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0
1														
Max.	1.62	3.76	3.40	17.90	27.20	5.10	4.55	30.00	1.10	12.90	0.98	0.23	0.01	0.06
Mean	0.36	0.889	0.343	1.182	1.379	0.298	0.073	0.474	0.012	0.111	0.050	0.002	0.001	0.002
S.D	0.20	0.53	0.41	1.44	3.81	0.57	0.25	2.78	0.08	0.87	0.10	0.01	0.001	0.001
PT	360	339	260	287	235	254	165	50	90	20	112	28	65	25

3. USE OF THE MODEL

The main advantage of the neural network model as compared with other empirical models is the ability of analysing separately the influence on Ms temperature of each one of the alloying elements. In this sense, the role of alloying elements such as Cu, W, Co, Mo, Nb and V on Ms has been analysed in this section and the results are presented in Fig. 1. Figure 1(a) shows that copper addition has not influence on Ms although the increase in error bars indicate a lack of data for high copper concentrations. On the other hand, Fig. 1(b) shows that tungsten increases the value of Ms. Likewise, Fig. 1(c) shows that cobalt concentrations lower than 3 wt.-% does not affect Ms temperature. However, the higher cobalt concentration up to 30 wt.-%, the higher Ms temperature. From Figs. 1(d), 1(e) and 1(f) it is shown the evolution of Ms as the content of strong carbide-formers such as Mo, Nb and V increases. It is clear from these figures that the strongest carbide former, the highest increases on Ms temperature. This behaviour could be attributed to the influence of alloying elements on the activity of carbon in the solid solution. Keeping this in mind, we can expect that interactions between carbon and carbide-forming elements tend to weaken the role of carbon, and give rise to an increase in Ms temperature.

Table 2. Fitting parameters estimated by non linear regression analysis to a $M_s = y_0 + ax + by$ equation type

	y_0	a	b	R
Mn	768.40	-301.49	-30.61	0.99812820
Si	769.84	-311.31	-14.46	0.99867290
Cr	759.55	-290.79	-8.99	0.99832584
Ni	759.22	-299.09	-16.63	0.99939313
Mo	769.85	-306.08	2.37	0.99821097
V	761.12	-286.77	5.35	0.99712654
Co	738.63	-281.20	8.58	0.98232872
Al	797.36	-328.45	40.40	0.99283463
W	770.85	-312.88	7.42	0.99876925
Cu	777.31	-318.52	-11.34	0.99740703

Figure 1. Effect of (a) Cu, (b) W, (c) Co, (d) Mo, (e) V, and (f) Nb on Ms temperature.

With the aim of finding an empirical equation for Ms temperature upon the steel chemistry, the neural network predictions are plotted by pairs of elements (C-Mn, C-Ni, etc). For instance, Fig. 2 shows the evolution of Ms with carbon and chromium concentrations ranging from 0.001 to 0.9 wt.%, and from 0 to 17 wt.-%, respectively. These values are fitted to a plane regression equation ($M_s = y_o + ax + by$, where x **corresponds to** carbon concentration values in wt.-%, and y **corresponds to** the alloying element) by non-linear regression analysis. The regression coefficients a and b for the different alloying elements are listed in Table 2. R in Table 2 is the correlation factor between the neural network data and the parameters of the $M_s = y_o + ax + by$ fitting equation.

According to that procedure, the relative effect of alloying elements is indicated in the following empirical relationship for predicting the Ms temperature of steels:

$$M_s (K) = 767.7 - 305.4w_C - 30.6w_{Mn} - 14.5w_{Si} - 8.9w_{Cr} - 16.6w_{Ni} + 2.4w_{Mo} + 5.3w_V + 8.58w_{Co} + 40.4w_{Al} + 7.4w_W - 11.3w_{Cu} + 510.4w_{Nb} \quad (2)$$

The effect of carbon has been considered as the mean value of the ' a ' values listed in Table 2. Likewise, it should be notice the large value corresponding to Nb, which is consistent with the stronger carbide former, highest Ms temperature.

Figure 2. Effect of binary interaction C-Cr on Ms temperature.

Figure 3. Comparison between experimental and estimated Ms values for the steels listed in Table 3.

Figure 3 shows a comparison between the results predicted by equation (2) and the experimental Ms temperature in six very different steels whose actual compositions are listed in Table 3. **The steels listed in Table 3 have not been used in the fitting procedure.** It could be concluded from this figure that the neural network model **provides** an excellent accuracy on Ms temperature predictions. All of these steels are used for commercial purposes and, therefore, the accurate determination of Ms temperature is very **important** from an industrial point of view.

Table 3. Chemical composition of the six steels analysed.

C	Mn	Si	Cr	Ni	W	Co	Mo	V	Al	Cu	Nb
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S1	0.45	0.4	0.32	13.0	0.38	0	0	0	0	0	0	0
S2	0.8	3.52	1.67	1.1	0	0.99	1.44	0.24	0	0.01	0	0
S3	0.07	1.5	0.37	0.039	0.49	0	0	0.021	0.004	0.045	0.039	0.03
S4	0.31	1.22	0.253	0.138	0.098	0	0	0.03	0.004	0	0	0
S5	0.09	1.03	0.16	9.1	0.99	0	0	0.99	0.19	0	0	0.04
S6	0.09	0.99	0.18	8.94	0	0.98	1.87	0.96	0.18	1.87	0	0.05

4. CONCLUSIONS

A neural network method based within a Bayesian framework has been used to rationalise an enormous quantity of published experimental data on Ms temperature of steels. It is now possible, therefore, to predict the Ms temperature as a function of the chemical composition. The influence of the alloying elements is considered by means of the C-X pair interactions. The results predicted by the neural network model were compared with the experimental Ms temperature of six very different commercial steels. It is concluded that an excellent agreement between experimental and predicted Ms temperature was found.

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