Prediction of Austenite Formation Temperatures Using Artificial Neural Networks

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Abstract. For the modeling and design of heat treatments, in consideration of the development/ transformation of the microstructure, different material data depending on the chemical composition, the respective microstructure/phases and the temperature are necessary. Material data are, e.g. the thermal conductivity, heat capacity, thermal expansion and transformation data etc. The quality of thermal simulations strongly depends on the accuracy of the material data. For many materials, the required data - in particular for different microstructures and temperatures - are rare in the literature. In addition, a different chemical composition within the permitted limits of the considered steel alloy cannot be predicted. A solution for this problem is provided by the calculation of material data using Artificial Neural Networks (ANN). In the present study, the start and finish temperatures of the transformation from the bcc lattice to the fcc lattice structure of hypoeutectoid steels are calculated using an Artificial Neural Network. An appropriate database containing different transformation temperatures (austenite formation temperatures) to train the ANN is selected from the literature. In order to find a suitable feedforward network, the network topologies as well as the activation functions of the hidden layers are varied and subsequently evaluated in terms of the prediction accuracy. The transformation temperatures calculated by the ANN exhibit a very good compliance compared to the experimental data. The results show that the prediction performance is even higher compared to classical empirical equations such as Andrews or Brandis. Therefore, it can be assumed that the presented ANN is a convenient tool to distinguish between bcc and fcc phases in hypoeutectoid steels.

1. Introduction

For the modeling and design of heat treatment processes of steels, a large number of different material data is required. Such data comprises, e.g. thermal conductivity, heat capacity, thermal expansion and transformation data (TTT/CCT). For the transformation behavior, start- and finish-temperatures of the austenite formation are of major significance. These temperatures are relevant for the determination of the temperature required in different heat treatment processes and to distinguish between bcc and fcc lattice structure.

In figure 1, the different phases of a three-component steel (system of iron, carbon and metallic alloying element, with low content of the alloying metal M in accordance with [1]) are illustrated. The different phase areas and limits as well as the associated temperatures are distinctly marked. The start and finish temperatures of the austenite transformation during heating are described e.g. in time-tem-
perature-austenitization diagrams (TTA), time-temperature-transformation diagrams (TTT) or continuous-cooling-transformation diagrams (CCT), which, for example, can be found in [2–8]. According to [4], the start and finish temperatures can be classified by dilatation curves as shown in figure 2.

Figure 1. Section through a 3-component system iron-carbon-alloying element M at low and constant concentrations of M in accordance with [1].

The start of the austenite formation is usually denoted as $A_c^1$ or $A_{cm}$. A deviation from a linear dependency between temperature and dilatation occurs, when at least 1% of the volume has transformed from ferrite to austenite [4]. The temperature $A_c^3$ denotes the end of the ferrite/austenite transformation. If hypoeutectoid steels have a volume fraction of pearlite less than 60% the finish of the perlite transformation $A_c^{1e}$ is visible in the dilatation curve [4], figure 2. However, the transformation temperatures $A_c^{1e}$ and for high-alloyed and hypereutectoid steels $A_{cm}$ or $A_c^c$ are not considered in this paper due to the very limited accessible data situation.

As already mentioned above, material data for a large number of different steels are available in the literature. It is, however often not possible to find data for a very specific chemical composition or the found data show an insufficient quality. To calculate the temperatures $A_c^1$ and $A_c^3$ according to a given chemical composition, several empirical equations exist [9, 10]. In particular, the formulas of Andrews [9]

\[
A_c^1 = 723 - 10.7 Mn - 16.9 Ni + 29.1 Si + 16.9 Cr + 290 As + 6.38 W \\
A_c^3 = 910 - 203 \sqrt{C} - 15.2 Ni + 44.7 Si + 104 V + 31.5 Mo + 13.1 W
\]

and Brandis [10]

\[
A_c^1 = 739 - 22 C + 2 Si - 7 Mn + 14 Cr + 13 Mo - 13 Ni + 20 V \\
A_c^3 = 902 - 255 C + 19 Si - 11 Mn - 5 Cr + 13 Mo - 20 Ni + 55 V
\]

are often used to identify the start and finish temperatures of the ferrite/austenite transformation in steels. The symbols of the chemical elements represent the percentage by mass of these elements in the alloys. In [9] and [10], the limitations of the range of the chemical composition of these equations are described. According to [11], it is not certain whether the intrinsic relations between the chemical composition and $A_c^1$ or $A_c^3$ are considered by the empirical equations, which is why inaccuracies of the prediction can occur.

As it is shown in several publications [11–15], another more convenient mathematical approach to predict the material data is given by Artificial Neural Networks (ANN). ANN are advantageous in many cases, especially if the intricacy of the problem is immense and simplifications are not possible. Thus, ANN are used in materials science to predict effects and properties of welding processes, superalloys,
fatigue properties, transformations, steel processing, machining and processing and many more [12]. The successful prediction of the austenite formation temperatures $A_c_1$ and $A_c_3$ using ANNs is already described in [11–15]. In the literature, two ANNs - each calculating one transformation temperature and one hidden layer with logistic activation function [13] or hyperbolic tangent transfer function [15] - were used. The prediction of both temperatures using a single ANN (but again only one hidden layer) is described in [11, 14]. The literature indicates that the architecture of the ANN and the activation functions influence the prediction accuracy of the neural network.

In this study a systematic procedure to train an ANN on the prediction of the austenite formation temperatures for a steel with given chemical composition is shown. The focus is on the prediction for hypoeutectoid steels using available literature data. The number of hidden layers as well as of different activation functions is varied, and the network with the highest prediction accuracy is compared to the accuracy of the classical empirical equations of Andrews and Brandis.

2. Modeling of Artificial Neural Network (ANN)

To model an ANN predicting the austenite formation temperatures of a given steel with high accuracy, data from a large number of steels with different chemical compositions were collected from the literature [2–8]. Often, elements such as N, Co, B, As, Sn, Zr, O, W, Ti were not measured but may influence the transformation temperatures. An element is used as input if it is considered in at least half of the surveyed data and if it is set to zero in the case of steels with no information about the element content. If the experimental alloys have varying contents of alloying elements, which are not considered as input parameter, the alloying effects cannot be considered by the model either, and significant errors can occur [16]. Therefore, if a surveyed steel type had measured elements, e.g. boron, which were not considered as input data this steel would not be used for the ANN presented in this work. Because of the low variety of chemical compositions and due to the consideration of only unalloyed and low alloyed hypoeutectoid steels, the input data are reduced from 406 to 206 steel types with different chemical compositions. The elements considered, the content range, the mean content as well as the standard deviation (of the percentage of mass) of the 206 steels, which were used to model the neural network, are shown in Table 1.

| Variable | Minimum | Maximum | Mean | Standard deviation |
|----------|---------|---------|------|--------------------|
| C        | 0.043   | 0.76    | 0.297| ± 0.160            |
| Si       | 0.010   | 1.80    | 0.340| ± 0.272            |
| Mn       | 0.040   | 2.11    | 0.744| ± 0.420            |
| P        | 0.003   | 0.071   | 0.019| ± 0.009            |
| S        | 0.004   | 0.090   | 0.018| ± 0.009            |
| Cr       | 0.000   | 3.52    | 0.709| ± 0.675            |
| Cu       | 0.000   | 0.98    | 0.112| ± 0.123            |
| Mo       | 0.000   | 1.10    | 0.166| ± 0.244            |
| Ni       | 0.000   | 4.28    | 0.432| ± 0.887            |
| V        | 0.000   | 0.87    | 0.039| ± 0.090            |
| Al       | 0.000   | 0.14    | 0.010| ± 0.018            |
| Output in °C | |         |       |                    |
| $A_c_1$  | 657     | 800     | 733.3| ± 23.07            |
| $A_c_3$  | 740     | 954     | 823.1| ± 39.60            |

To train the net the selected data from the literature were randomly divided ten times and arranged in groups of three: a training set (60% of the data), a validation set (20%) and a test/unseen set (20%). The test set was used to identify an over-trained network at the beginning as well as to compare the prediction
accuracy between the ANN and the classical empirical equations of Andrews and Brandis afterwards (cf. section 3).

To find the best ANN with a minimum error between the experimental and ANN calculated temperatures, the hidden layer size and the number of neurons within one layer were systematically varied for each randomly grouped dataset (figure 3). Also the activation functions (logsig and tansig) of the hidden layer neurons were changed. The activation function of the output layer was always set to be the identity function. The input and output data were normalized between zero and one.

A total of 8400 different ANNs were trained using the Levenberg-Marquardt algorithm which is implemented in the used MATLAB software. In so doing, the algorithm minimized the mean square error (MSE) between the predicted and experimentally measured temperatures adjusting the biases $b$ and the weights $w$ of all neurons. It was stopped, in the moment when the MSE of the training set was less than a predefined threshold value. At the end, the biases, weights and activation functions of the ANN with the lowest MSE, according to the validation set, were selected.

Figure 3. Schematic illustration of the trained feedforward network with the variation of the number of neurons and the activation functions in the hidden layers.

3. Results and Discussion

The mean square errors are illustrated in figure 4. They are represented as the radius of a sphere of all trained neural network configurations. A sphere with a small radius implies a low MSE. In figure 4 it can be seen that the MSE varies on a low level over the whole range of the number of neurons in the two hidden layers, except for an ANN with one neuron in the first hidden layer. As it is also shown in the literature [11–15], an ANN with only one hidden layer has an MSE which is in an acceptable magnitude. The ANN with the lowest MSE (further denoted as “best ANN”) of all trained configurations has seven neurons in the first and sixteen neurons in the second hidden layer. The activation function of the hidden layers is the logsig function (see also black filled sphere in figure 4).

Figure 4. Mean square errors represented as the radii of a sphere of all trained ANN configurations. Black filled sphere: Configuration with the minimum MSE. Note: For reasons of clarity only the half of the configurations of the randomly selected dataset with the minimum MSE are illustrated.
To quantitatively estimate the prediction accuracy of the best ANN the mean relative estimation errors (MREs)

\[ MRE_{1,2} = \frac{100}{n} \sum_{i=0}^{n} \left| \frac{A_{c_{x}}^{ex} - A_{c_{x}}^{ANN}}{A_{c_{x}}^{ex}} \right|, x \in \{1,3\} \]  

(5)

(in which \(n\) denotes the number of different steel compositions and \(A_{c_{x}}\) the \(A_{c_{1}}\) or \(A_{c_{3}}\) temperature) are compared to the corresponding values of the Andrews equations (1–2) and Brandis equations (3–4).

The predicted temperatures of the steel compositions used to train and validate the ANN show a higher accuracy than the values of the equations, figure 5. The average MRE of 1.24% of the best ANN (compared to 1.76% of the Andrews and 1.80% of the Brandis equations) confirms this statement, table 2. However, it is not unusual that an ANN has a very high prediction accuracy for trained data.

**Table 2.** Summary of the mean relative estimation errors of the best ANN and the empirical equations.

| Model     | ANN | Andrews | Brandis |
|-----------|-----|---------|---------|
| MRE       | \(A_{c_{1}}\) | \(A_{c_{3}}\) | \(\bar{O}\) | \(A_{c_{1}}\) | \(A_{c_{3}}\) | \(\bar{O}\) | \(A_{c_{1}}\) | \(A_{c_{3}}\) | \(\bar{O}\) |
| Train/Val | 1.24 | 1.57    | 1.56    | 1.76    | 1.55    | 2.05    | 1.80    |
| Unseen    | 1.54 | 1.88    | 1.68    | 1.96    | 1.68    | 1.89    | 1.79    |

Therefore, the MRE of the test data, which were totally unknown during the training, is calculated. A qualitative comparison is illustrated in figure 6. Again, the ANN shows a higher prediction accuracy (average MRE of 1.55%) of the austenite formation temperatures compared to the equations of Andrews (1.96%) and Brandis (1.78%). In contrast to the equation models in which the prediction accuracy of the \(A_{c_{3}}\) temperature is always noticeably lower than the accuracy of the \(A_{c_{1}}\) temperature, the difference of the ANN is close to zero, table 2. Additionally, the difference between the MRE of the trained/validated and the unseen data of the best ANN is very low (about 0.3%). Hence, the modeled ANN should predict the temperatures of other composited steels with an equally high accuracy.

**Figure 5.** Comparison between the predicted and experimentally measured temperatures of the a) best ANN for the training and validation data and b) classical equations of Andrews (1–2) as well as Brandis (3–4) for the training and validation data.
4. Summary and Conclusions

An artificial neural network predicting the austenite formation temperatures $A_c^1$ and $A_c^3$ in dependence of the steel composition was systematically trained to achieve a minimum MSE. The ANN with the minimum MSE of all trained configurations has seven neurons in the first and sixteen neurons in the second hidden layer. The activation function of the hidden layers is the logsig function. The following conclusions can be drawn:

1. The MSE varies on a low level over the whole range of the number of neurons in the two hidden layers, except for an ANN with one neuron in the first hidden layer.
2. The prediction accuracy of the identified best ANN is very high.
3. Compared to commonly used equations of already high prediction accuracy, this best ANN shows even better results.

The developed best ANN can be used to calculate the temperatures of heat treatments (e.g. hardening) or to distinguish material data concerning fcc and bcc. In further investigations, the effect of the heating rate and of the initial microstructure will be taken into account. The ANN will also be extended to high-alloy and hypereutectoid steels, so that e.g. $A_{cm}$ or $A_c$ can be calculated.

References

[1] 1984 Werkstoffkunde Stahl (Berlin: Springer) p 200
[2] Wever F and Rose A 1961 *Atlas zur Wärmebehandlung der Stähle* (berichtigter Nachdr.) (Düsseldorf: Verl. Stahleisen)
[3] Rose A and Hougardy H 1972 *Atlas zur Wärmebehandlung der Stähle* 2 (Düsseldorf: Verl. Stahleisen)
[4] Orlich J, Rose A and Wiest P 1973 *Atlas zur Wärmebehandlung der Stähle* 3 (Düsseldorf: Verl. Stahleisen)
[5] Orlich J and Pietrzeniuk H J 1976 *Atlas zur Wärmebehandlung der Stähle* 4 (Düsseldorf: Verl. Stahleisen)
[6] 1987 *Zeit-Temperatur-Umwandlungsdiagramme* (Freital: Edelstahlwerk Freital)
[7] Seyffarth P 1982 *Schweiß-ZTU-Schaubilder* (Berlin: Verl. Technik)
[8] Seyffarth P, Meyer B and Scharff A 1992 *Großer Atlas Schweiß-ZTU-Schaubilder* (Düsseldorf: Dt. Verl. für Schweisstechnik, DVS-Verl.)
[9] Andrews K W 1965 *J. Iron and Steel Inst.* 203 721–7
[10] Brandis H 1975 *TEW-Techn. Ber.* 1 8–10
[11] You W, Xu W, Bai B and Fang H 2006 *Mater. Sci. Eng. A* 419 276–82

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**Figure 6.** Comparison between the predicted and experimentally measured temperatures of the a) best ANN and b) classical equations of Andrews (1–2) as well as Brandis (3–4) for the test/unseen data
[12] Bhadeshia H K D H 1999 *ISIJ Int.* **39** 966–79.
[13] Dobrzański L A and Trzaska J 2004 *J. Mater. Process. Technol.* **155–156** 1950–55.
[14] Rakhshkhorshid M and Teimouri Sendesi S A 2014 *J. Iron. Steel Res. Int.* **21** 246–51.
[15] Gavard L, Bhadeshia H K D H, MacKay D J C and Suzuki S 1996 *Mater. Sci. Technol.* **12** 453–63.
[16] Sha W 2011 *Mater. Sci. Eng. A* **528** 3275–76.