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Prediction of Transition Temperature of Alloy steel Austenite Based on Self-Organizing Neural Network

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Abstract. In order to determine the key chemical elements of the austenite transformation temperature (Ac1/Ac3) of alloy steel, this paper uses stepwise regression so that the number of neurons in the input layer of Kohonen self-organizing neural network is also determined and the network structure will be optimized. The learning algorithm is improved by combining non-tutor learning and supervised learning. Based on the optimized Kohonen neural network, an Ac1/Ac3 transition temperature predictive model was established. The prediction accuracy of this model which is based on Kohonen self-organizing neural network is higher in tests. The relative error of Ac1 is less than 3.01%, and the relative error of Ac3 is also below 3.02%, which is significantly better than the prediction accuracy of stepwise regression. With predicting the critical temperature of Ac1/Ac3 based on Kohonen Network, the actual heating temperature can be determined, which has important practical application value in both steel heat treatment to guarantee quality and shortening the physical experiment period.

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1. Introduction

In the course of heat treatment of the metal material, the steel is heated to a certain temperature so that its tissue partially or completely transform into austenite, or the austenite composition is homogenized. The actual heating temperature is calculated based on the critical temperature, which directly affects the performance of the heat treatment. In the supercooled austenite transformation curve of steel, Ac1 represents the critical temperature at which pearlite transforms to austenite during heating; Ac3 represents the final critical temperature at which free ferrite is completely transformed into austenite during heating. In the above chart, Ac1 and Ac3 provide a reliable basis for the actual heating temperature. Generally, when quenching, the quenching heating temperature of the hypoeutectoid steel is above Ac3 temperature (20-40) °C, and the quenching temperature of the hypereutectoid steel is above Ac1 temperature (30~50) °C. For newly developed steels, knowing the temperature of Ac1 and Ac3 before heat treatment provides an extremely valuable reference for the actual heating temperature.

The thermodynamic software and empirical formula were used to calculate the Ac1 and Ac3 critical temperature lines of CL50D steel and Fe-C binary system by Yaquin N, and he carried out comparative analysis [1]. Zhongqi S adopted the transmission electron microscopy technique to determine the critical temperature AC1 of A508-3 steel. The measurement result is about 25 °C lower than the result of the dilatometer method. The reason is that the electron microscopy technique can find the phase transition occurring in a very small area and it is closer to equilibrium state [2]. The expansion method was employed by Xiaoning Z[3]. The effect of the austenite transformation



temperature Ac1 of nuclear power SA738Gr.B Steel on different heating speeds was studied by Gleeble-3500 thermal simulator[3]. Baoqun N systematically studied the austenitizing temperature of 20MnSi rebar at different heating speeds on DIL805A/D dilatometer. The results show that the heating rate significantly affects the austenite formation starting temperature Ac1 and the ending temperature Ac3 of 20MnSi steel[4]. In recent years, many scholars have used artificial neural networks to predict various parameters and properties of alloy steel, which include mechanical properties [5], heat treatment process [6], martensite transformation temperature [7], The supercooled austenite continuous cooling phase transition curve [8], achieving higher prediction accuracy.

The aim of this essay is to combine stepwise regression to optimize the structure of Kohonen self-organizing neural network, improve the network learning algorithm, establish the prediction model of Ac1 and Ac3 austenite transformation temperature, and analyze its prediction performance so that a new method for predicting the single point critical temperature of Ac1 and Ac3 in the actual production of alloy steel is explored.

2. Construction of austenite transformation temperature prediction model

2.1 Network structure and optimization

The Kohonen neural network structure consists of an input layer and an output layer, as shown in Figure 1 [6]. The Kohonen network structure includes an input layer and an output layer, and a weight vector between the input layer and the output layer, and the determination of the neighborhood structure is also involved in the output layer. There are two ways to determine the neighborhood structure of the Kohonen output layer generally. One way is to define a neighborhood centered on the competitive winning neurons. The neighborhood is represented by a square or a circle. Another way is to directly determine the neighborhood changes by using the neighborhood function.

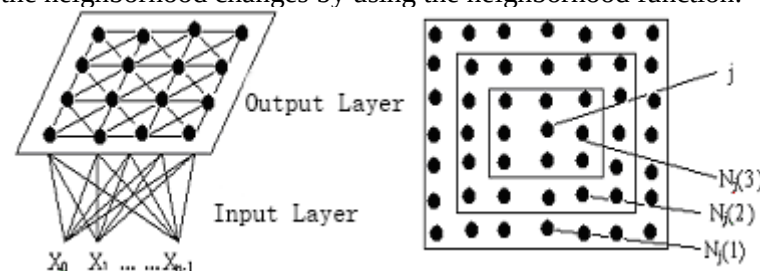


Figure 1. Kohonen network structure and neighborhood structure.

The key to establishing the Ac1/Ac3 temperature prediction model based on Kohonen neural network is how to determine the number of neurons in the input layer and the structure of the competition layer neurons. In order to find the main elements affecting the temperature of Ac1/Ac3, this paper combines stepwise regression analysis to determine the input parameters of Kohonen neural network.

According to the stepwise regression analysis, among the listed chemical components, the contents of P, S, Mo and C have no significant effect on Ac1 temperature, while the contents of P, S, Mo and Cr have no significant effect on Ac3 temperature. Since the temperature of the alloy steel Ac1/Ac3 is predicted at the same time by the Ac1/Ac3 temperature prediction model based on the Kohonen neural network, the percentages of the chemical components C, Si, Mn, Cr, Ni, and V which have a great influence on the temperature of the alloy steel Ac1/Ac3 are selected as the input parameters of the Ac1/Ac3 temperature prediction model, that is, the number of input layer neurons in the Kohonen prediction model is 6. For the competitive layer structure, due to the limited number of training samples, the output layer is set to a 7x7 two-dimensional planar structure based on experience and multiple experiments.

2.2 Improved network learning algorithm

Kohonen learning is a self-organizing process without tutor learning, which cannot be used directly for applications such as forecasting. Reference [7], combined with the non-tutor learning and supervised learning process, improved Kohonen learning algorithm for the prediction of Ac1/Ac3 critical temperature.

The random samples are used in the first phase to conduct initial training on the network. The basic ideas are as follows:

1) Let the initial learning rate be η_0 . Set the initial neighborhood to be N_{c0} . The maximum number of iterations to be T . The random initialization weight w_j ;

2) Input all random samples X , calculate the distance d_j from the sample X to the output layer neuron node j , select the minimum distance node j^* as the output layer winning neuron according to the distance, and the node j^* and its neighbors, the output layer, and the input layer weight vector w_j are updated:

$$\begin{cases} w_{ij}(t+1) = w_{ij}(t) + \eta(t) * h(j, j^*) * (x_i(t) - w_{ij}(t)), & j \in N_c(t) \\ w_{ij}(t+1) = w_{ij}(t), & j \notin N_c(t) \end{cases} \quad (1)$$

In the above formula, $\eta(t)$ is the learning rate at time t , $N_c(t)$ is the feedback neighborhood of the winning neurons at time t , and $h(j, j^*)$ is the neighborhood function.

3) Order $t = t + 1$, and the learning rate $\eta(t)$ and the neighbor $N_c(t)$ are updated according to the following formula:

$$\eta(t) = \eta_0 * (1 - \frac{t}{T}), \quad N_c(t) = N_{c0} * (1 - \frac{t}{T}) \quad (2)$$

4) If the sum of the squared weights of the two iterations is less than the set minimum threshold, or $t > T$, the loop ends; otherwise, turn 2).

The supervised training samples were used to further train the neural network in the second phase. Learn from the literature based on Kohonen's supervised classification. In this essay, the improved reward and punishment supervised learning algorithm is used to predict the critical temperature of Ac1/Ac3. The specific algorithm is as follows:

Enter the supervised training sample x , find the smallest output neuron c of $\|x - w_c\|$, set the expected value of x to s , and the actual output of neuron c is o , then use the reward and punishment formula to complete the supervised learning process:

$$\begin{cases} w_c(t+1) = w_c(t) + \eta(t) * (x_i(t) - w_c(t)), & fabs(s - o) < e \\ w_c(t+1) = w_c(t) - \eta(t) * (x_i(t) - w_c(t)), & fabs(s - o) \geq e \\ w_i(t+1) = w_i(t), & i \neq c \end{cases} \quad (3)$$

Where e is the minimum threshold for controlling the actual output and the expected output, the learning rate $\eta(t)$ is decremented with the number of iterations t , and its initial value and calculation method are the same as the unsupervised training phase. The basic idea of equation (3) is: input supervised samples, and the output layers compete with each other to produce winning neurons. If the output of the winning neurons is consistent with the expected value of the supervised sample, the weight vector of the neuron is brought closer to the supervised sample; Otherwise, away from the supervision sample.

3. Experiment and analysis

3.1 Training sample preprocessing and network training

In actual production, the critical point of steel is affected by many factors, but under basically similar process conditions, the chemical composition of steel has the most significant effect [11]. A total of 136 samples of low- and medium-carbon alloy steels were selected from references [12-14], and the

chemical composition ranges are shown in Table 1. One hundred of the samples were taken as training samples and the other 36 samples were used as test samples.

Table 1. Range of values of the sample(% , °C).

	C	Si	Mn	Cr	Ni	Mo	P	S	V	Ac3	Ac1
min	0.09	0.22	0.22	0	0	0	0	0	0	770	700
max	0.55	1.63	2	5.43	3.6	1.29	0.03	0.05	0.37	980	840
mean	0.24	0.51	1.01	0.90	0.71	0.41	0.014	0.011	0.074	844	743

It can be seen from Table 1 that the sample data differ greatly, and the training samples need to be preprocessed. The specific method is to normalize the chemical composition (% by mass) and the measured temperature (°, °C) of Ac1/Ac3 to 0~1, which is convenient for network training [7, 9].

In the first stage of clustering in network training, the maximum number of iterations is 10000, the mean square error is $1e-3$, and the learning rate is 0.01 when the weight is adjusted. The second stage is the supervised fine adjustment stage, the maximum number of iterations is 15000, and the mean square error is $1e-5$. While the weight is adjusted, the learning rate is 0.01. 48 samples are taken as training samples, and after training by inputting the training sample set, a network model with predictive ability is obtained.

3.2 Experimental results and analysis

(1) Analysis of Ac1/Ac3 temperature prediction results based on Kohonen network

In order to test the prediction accuracy of the network model, 36 test samples were input into the network to obtain the predicted Ac1/Ac3 temperature, and the results are shown in Fig. 2.

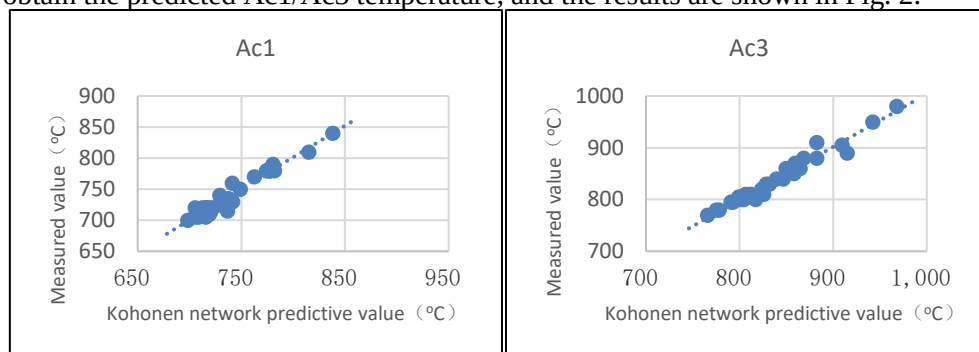


Figure 2. Ac1/Ac3 temperature prediction based on Kohonen network.

Figure 2 shows that the Ac1/Ac3 temperature prediction accuracy based on Kohonen network is ideal, and the predicted value is very close to the measured value. Looking at the predicted temperature value, the prediction error value of most steel grades is in the range of 50°C, and some of the values are close to the original value. Only the predicted temperature of a few steel grades differs from the actual temperature by 10~20 (°C) .

(2) Comparison with stepwise regression prediction results

Based on stepwise regression analysis, a multivariate regression model of chemical composition and Ac1/Ac3 was established, which is compared with Kohonen neural network results. In the course of using stepwise regression to establish the optimal multiple regression, the chemical composition of Ac1 and Ac3 is not significantly affected. Only the elements with significant influences on the temperature of Ac1 and Ac3 are used to establish the multiple regression models of Ac1 and Ac3. The specific equations are as follows:

$$Ac1 = 755.68 + 14.39 \cdot Si - 26.86 \cdot Mn + 16.32 \cdot Cr - 18.5 \cdot Ni + 88.91 \cdot V \quad (R^2 = 0.866) \quad (4)$$

$$Ac3 = 928.66 - 236.37 \cdot C + 30.44 \cdot Si - 32.68 \cdot Mn - 27.51 \cdot Ni + 141.65 \cdot V \quad (R^2 = 0.869) \quad (5)$$

From the stepwise regression equations (4) and (5), the influence of chemical composition on the critical temperatures Ac1 and Ac3 can be found: the temperature of Ac1 increases with the increase of Si, Cr and V content, decreases with the increase of Mn and Ni content, and V has the greatest influence on Ac1 temperature. The temperature of Ac3 increases with the increase of Si and V content, and decreases with the increase of C, Mn and Ni content. C has the greatest influence on the temperature of Ac3 relative to other elements. This conclusion is consistent with the law of the influence of alloying elements of steel on the critical temperature in [15].

The 36 test samples used in the Kohonen neural network model were input into the AC1 and AC3 regression models, and the prediction results were obtained and compared with the prediction results of the Kohonen neural network, as shown in Fig. 3.

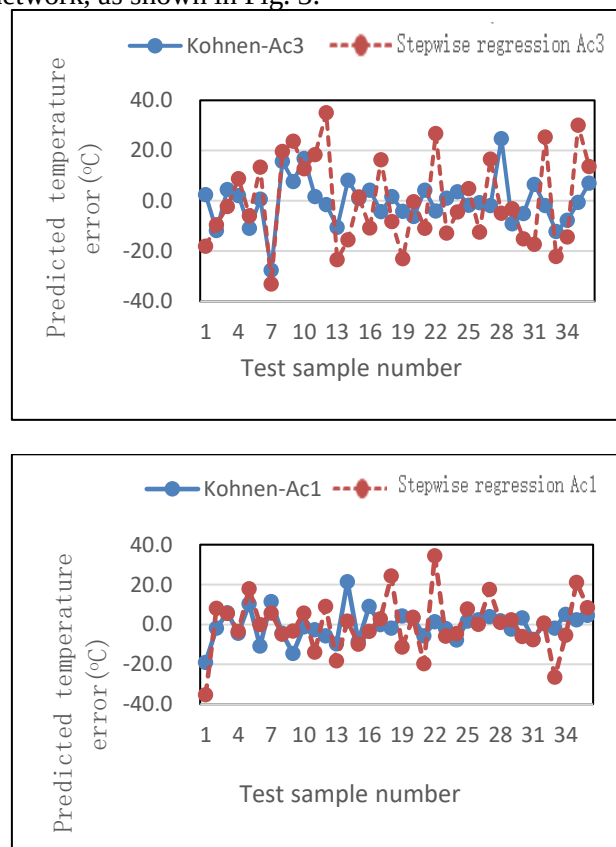


Figure 3. Kohonen network prediction and stepwise regression prediction error comparison.

It can be clearly seen from Fig. 3 that the Kohonen neural network prediction error is generally smaller than the temperature error value predicted by the stepwise regression equation. Further statistics on the prediction error of Kohonen neural network and stepwise regression are shown in Table 2.

Table 2 Comparison of Kohonen network prediction and stepwise regression prediction error value. (°C)

	Kohonen Prediction error		Stepwise regression prediction error	
	Ac3	Ac1	Ac3	Ac1
Minimum value	-27.53	-18.91	-33.07	-35.26
Maximum	24.76	21.54	35.03	34.46
Absolute value mean	7.44	6.32	15.50	11.02
Standard deviation	9.25	7.62	17.50	13.70

The Ac1 error range predicted by Kohonen network is -18.91~21.540C, Ac3 error range is -27.53~24.760C; the absolute value of Ac1 error does not exceed 22°C, the relative error is less than 3.01%; the absolute value of Ac3 error does not exceed 28°C, and the relative error is less than 3.02%. The Ac1 error range of the stepwise regression prediction is -35.26~34.460C; and the Ac3 error is -33.07~35.030C. At the same time, the absolute value and standard deviation of the Kohonen network prediction error are significantly smaller than the stepwise regression prediction error, further indicating that the Kohonen neural network predicts the accuracy of Ac1/Ac3 temperature is relatively high.

4. Conclusion

In this paper, stepwise regression is used to determine the key chemical elements affecting the transition temperature of Ac1 and Ac3, and then the number of neurons in the input layer of Kohonen neural network is also determined. The output layer is set to a 7x7 two-dimensional planar structure to establish the Kohonen neural network structure. And combined with the non-tutor to learn and supervise the learning process, improve the Kohonen learning algorithm. The Ac1/Ac3 transition temperature prediction model is established, which is based on the optimized Kohonen neural network structure and improved learning algorithm. Experiments show that the accuracy of the Ac1/Ac3 prediction model based on Kohonen neural network is higher. The absolute value of Ac1 does not exceed 22°C, and the relative error is less than 3.01%. The absolute value of Ac3 error does not exceed 28°C, and the relative error is less than 3.02%. At the same time, the prediction accuracy of the Kohonen network is significantly better than that of the stepwise regression.

In the supercooled austenite transformation curve of steel, the critical temperatures of Ac1 and Ac3 mainly depend on the chemical composition of steel, but it is difficult to determine the relationship with chemical composition. In actual production, according to the chemical composition of steel, based on Kohonen network to predict its critical temperature, and then determine the actual heating temperature, which is of practical guiding significance to guarantee the quality of steel heat treatment and shorten the physical experiment cycle.

References

- [1] Nie, Y.Q., Han, L.Z., Gu, J.F. (2015) Calculation of critical temperature and maximum ferrite transformation of low alloy hypoeutectoid steel[J]. Heat Treatment of Metals, 02: 8-12.
- [2] Sheng, Z.Q., Xiao, H. (1996) Electron microscopic determination of critical temperature AC1 of A508-3 steel[J]. Large Castings, 2 :26-28.
- [3] Zhang, X.N., Jing, Y., Yu, Y. (2013) Effect of heating rate on austenite transformation temperature of SA738Gr.B steel[J]. thermal processing technology, 42 (6): 38-41.
- [4] Ning, B.Q., Zhao, J., Liu, Y.C. (2011) Effect of Heating Rate on Austenite Transformation Temperature of 20MnSi Steel[J]. Thermal Engineering Technology, 40 (4): 149-150.
- [5] Liu H., Zou D.N., Yan D.N., et al. (2011) Prediction of quenching mechanical properties of super martensitic stainless steel based on artificial neural network[J]. Hot Working Technology, 40(20):150-153.
- [6] Zuo X.R., Chen Y.B., Wang Y.H., etc. (2010) Heat treatment process of P20 steel based on artificial neural network[J]. Journal of Materials Heat Treatment, 31(4): 62-66.
- [7] Zhao W.Y. (2014) Prediction of Martensite Start Transition Temperature Based on RBF Neural Network[J]. Thermal Engineering, 43(6): 47-49.
- [8] Long S.P., Zhou X.D. (2012) Continuous Cooling Phase Transition Curve of Undercooled Austenite in 42CrMoA Steel[J]. Thermal Engineering, 41(22): 83-85.
- [9] Zhao W.Y.(2014) Research on Prediction of CCT Curve Based on BP Neural Network Based on Optimization[J]. Hot Working Technology, 43(4):95-102.
- [10] Luo X.B., Chen D., Deng L. et al. (2011) Remote sensing image classification based on Kohonen neural network [J]. Journal of Chongqing University of Posts and Telecommunications (Natural Science Edition), 23(5): 616-620.

- [11] Zhao Z.D. (1999) Effect of chemical composition of steel on critical temperature [J]. Mechanical engineering materials. 23(1): 39-40
- [12] Zhang S.Z. (1993) Atlas of supercooled austenite transformation curve of steel[M]. Metallurgical Industry Press, Beijing.
- [13] Lin H.G., Fu D.Z. (1988) Austenite transformation curve of steel - principle, test and application [M]. Mechanical Industry Press, Beijing.
- [14] Xu G. (2009) Determination and drawing of CCT curves of metallic materials[M]. Chemical Industry Press, Beijing.
- [15] Dahe J.Z.(1986) Heat treatment 150 questions [M]. Science and Technology Press, Beijing.