Constitutive Model of TC21 Titanium Alloy Based On BPNN

Hongbo Dong*, Chengtong Sun
School of Mechanical and Vehicle Engineering, Linyi University, Linyi, China
*Corresponding author e-mail: donghbo@163.com

Abstract. TC21 alloy is a new two-phase titanium alloy with good comprehensive properties of high strength, toughness and damage tolerance. The isothermal thermal compression deformation test of TC21 titanium alloy is carried out on the Gleeble-3500 thermal simulation test machine. Based on the stress-strain data at different temperatures and strain rates, the constitutive relation model of TC21 alloy was established by using BPNN (Back Propagation Neural Network), which has high prediction and generalization ability, and the predicted flow stress value is very close to the experimental data.

1. Introduction
TC21 titanium alloy is a new α+β titanium alloy[1,2], It belongs to Ti-Al-Mo-Nb-Sn-Zr-Cr-X system with good comprehensive properties of strength, toughness and high damage tolerance. For this reason, it has the widespread application in aviation, aerospace and other fields.

In the process of metal deformation, flow stress is one of the most important factors, which is affected by strain rate, deformation temperature and deformation amount. In recent years, linear regression analysis and BP neural network are commonly used methods to establish constitutive model relations of alloys. However, the prediction accuracy of BP (back propagation) neural network is higher than that of regression model, which is a good way to solve the problem of constitutive model. Liu Xuefeng[3] et al. established high-precision artificial neural network model of aluminum lithium alloy to predict rheological stress during high temperature deformation; Zhang Xingquan[4] et al. established constitutive model of Ti-17 alloy based on artificial neural network model.

In this paper, a reasonable method is proposed to select the number of hidden layers and the number of node based on MATLAB software platform, and then to train the BP neural network by 'trainbr' algorithm [5-7].

2. Experimental
The chemical composition of TC21 alloy used in the experiment is Ti-6Al-2Sn-3Mo-1Cr-2Zr-2Nb, developed by Northwest Nonferrous Metal Academe with self-determinate intellectual asset, its phase transition point is (950±5)℃. The original microstructure of alloy is shown in Fig.1. The material is mainly composed of isometric and strip-shaped primary α and β transformation phases.
The TC21 titanium alloy samples were subjected to thermal compression test on Gleeble -3500 thermal simulation test machine. The sample size is 8×12 mm. The deformation temperature is in the range of 870-990 °C with a temperature interval of 30 °C. The strain rate is in the range of 10^{-2}-10s^{-1}, the heating velocity is 10°C/s and holding time is 3min. Then the specimens were deformed to a true strain of 0.6. In addition, during the whole testing process, the samples were protected by argon to prevent high temperature oxidation. The resistance heating method was used to control and measure the temperature of the sample by welding a platinum-platinum rhodium thermocouple in the center of the sample. Finally, the specimens were immediately water-cooled to room temperature after deformation ended.

The deformed samples were cut parallel to the compression direction, followed by mechanical grinding and polishing. The metallographic specimens were etched using Kroll reagent of HF:HNO3:H2O (1:2:5). The microstructures of the specimens were investigated by optical microscopy using an OLYMPUS/PMG3 microscope.

3. Constitutive relation of TC21 alloy based on BPNN model

3.1. Principles of BP artificial neural network model

Artificial neural network is emerging edge discipline developed in modern neuroscience research, it is also an artificial intelligence pattern recognition method established by simulating cranial nerve to learn the external environment. This method has remarkable functions such as self-learning, self-organization, self-adaptation and nonlinear dynamic processing. In addition, it has many excellent characteristics and is a new type of information processing tool. It has been successfully used in the modeling of nonlinear systems, fault diagnosis, performance prediction and other fields for research.

As seen from Fig.2, neural network based on BP algorithm is a network structure model composed of input layer, hidden layer and output layer. Each layer is closely connected with each other, and the input data information of each layer shall be propagated forward to the node of the hidden layer, and
then, after the activation function operation of each layer cell, the output data information of the hidden node shall be propagated to the output node, and finally the output result shall be given.

3.2. Constitutive model of TC21 alloy based on BPNN

The constitutive relationship of TC21 titanium alloy describes the variation of flow stress with deformation temperature, strain rate and strain variable at high temperature. The experimental data \((T, \varepsilon, \dot{\varepsilon})\) are taken as the input factors of the network structure and \(\sigma\) as the output factor of the network. Before the training, in order to make data meet input requirements, all the data need to be normalized processing to make them within the scope of \([-1,1]\). According to the traditional empirical formula to determine the number range, then repeated experiments and choose the best. For TC21 titanium alloy, the 4-layer BP network structure model of \(3 \times 10 \times 16 \times 1\) is the most appropriate choice in this paper.

In consideration of the value range of input and output vectors, the tangent function 'tansig' is adopted as the activation function of implicit layer 1 and of the input layer of the material. The activation function between the hidden layer 1 and the hidden layer 2 propagated forward also selects the tangent function, while the linear function 'purelin' is selected as the activation function between the hidden layer 2 and the output layer. Trainbr algorithm was used to improve the prediction and generalization ability of BP neural network. The network model set according to the above parameters can achieve the target accuracy of \(10^{-4}\) after the training of MATLAB software.

3.3. Generalization ability of BP neural network

When the network training error of the material has reached a very small value, a new input value will appear, making the training error of the network become much larger in an instant. This kind of network training simulation without good generalization ability is of no great significance and will directly lead to the decline of network prediction ability.

Trainbr algorithm was proposed to improve the network prediction ability of the material. Trainbr algorithm is mainly based on the theory of Bayesian regularization principle, the network structure model of the material parameters such as weights and threshold as the data of change. The normalized parameters are associated with the changed data, and the values of these parameters can be estimated by statistical methods, so that the size of performance parameters can be adjusted adaptively in the process of network training to achieve the optimal value required by materials.

4. Results and discussion

The hot compression test data were taken as the network sample data of TC21 titanium alloy. In order to verify the network generalization ability of the material, the experimental data were divided into sample data and non-sample data, and the neural network structure model of the material was trained according to the sample method set in the experiment of this topic. When the values of SSE (Sum of Squared Errors) and SSW (Sum of Squared Weights) tend to the constant value respectively after several iterations, it indicates that the result of network training is convergent. The number of parameters of the current effective network is 212.601 (as shown in Fig.3).
The comparison between the neural network predicted value and the experimental value of TC21 alloy is shown in Table 1. It can be seen from the data that the stress value predicted by the neural network is very close to the stress value obtained by the experiment, and the relative error range of the results is all within 6%, indicating that the BP neural network has a strong ability to deal with the nonlinear function of the material.

| deformation temperature T/℃ | strain rate ė/s⁻¹ | strain ε | training sample values ln(σ/MPa) | network predicted values ln(σ/MPa) | relative error % |
|-----------------------------|-------------------|----------|----------------------------------|-----------------------------------|------------------|
| 870                         | 0.001             | 0.10773  | 3.88                             | 3.89                              | -0.98            |
| 870                         | 0.001             | 0.20343  | 3.84                             | 3.86                              | -3.2             |
| 870                         | 0.001             | 0.30636  | 3.81                             | 3.79                              | 1.7              |
| 870                         | 0.001             | 0.40886  | 3.77                             | 3.78                              | -0.37            |
| 870                         | 0.001             | 0.51077  | 3.74                             | 3.75                              | -0.16            |
| 870                         | 0.001             | 0.60403  | 3.72                             | 3.75                              | -2.5             |
| 870                         | 0.001             | 0.7108   | 3.73                             | 3.72                              | 0.7              |
| 870                         | 0.001             | 0.81926  | 3.78                             | 3.75                              | 2.6              |
| 930                         | 0.001             | 0.1182   | 3.47                             | 3.45                              | 2.0              |
| 930                         | 0.001             | 0.50335  | 3.38                             | 3.36                              | 1.6              |
| 930                         | 0.1               | 0.4364   | 4.38                             | 4.39                              | -0.6             |
| 930                         | 0.1               | 0.60907  | 4.37                             | 4.36                              | 0.5              |
| 960                         | 0.01              | 0.10778  | 3.74                             | 3.75                              | -0.7             |
| 960                         | 1                 | 0.8008   | 4.75                             | 4.76                              | -0.2             |

The comparison of non-sample experimental values and network predicted values of TC21 alloy is shown in Table 2. It can be seen that the non-sample values of the alloy are basically consistent with the predicted values of the network.

The results show that the constitutive relationship of TC21 titanium alloy based on the network structure model of trainbr algorithm has quite good predictive and data promotion ability. In addition, the error analysis and calculation show that the average error between the test sample data of this model training and the flow stress value predicted by the network is 1.5%. The average error between the test sample data and the network prediction of the flow stress value reached 5.5%, which fully met the error requirements of the material during the thermal forming process.
### Table 2. Comparison of non-sample experimental values and network predicted values

| Deformation temperature T/℃ | Strain rate ε / s⁻¹ | Strain ε | Non-sample experimental values ln(σ/MPa) | Network predicted values ln(σ/MPa) | Relative error % |
|-----------------------------|---------------------|----------|------------------------------------------|-----------------------------------|------------------|
| 870                         | 0.01                | 0.10859  | 4.49                                     | 4.492                             | -0.1             |
| 870                         | 0.01                | 0.21492  | 4.4                                       | 4.45                               | -0.4             |
| 870                         | 0.01                | 0.31868  | 4.397                                    | 4.396                               | 0.07             |
| 870                         | 0.01                | 0.41341  | 4.372                                    | 4.37                               | 0.2              |
| 870                         | 0.01                | 0.52055  | 4.31                                     | 4.29                               | 1.1              |
| 870                         | 0.01                | 0.61703  | 4.28                                     | 4.27                               | 0.9              |
| 870                         | 0.01                | 0.7127   | 4.24                                     | 4.23                               | 0.3              |
| 930                         | 0.01                | 0.81536  | 4.21                                     | 4.24                               | -2.8             |
| 930                         | 0.01                | 0.35128  | 4.92                                     | 4.93                               | -0.7             |
| 930                         | 0.01                | 0.57871  | 4.9                                      | 4.93                               | -2.1             |
| 930                         | 0.01                | 0.64149  | 4.93                                     | 4.9                                | 2.1              |
| 990                         | 0.01                | 0.43409  | 3.7                                      | 3.69                               | 0.2              |
| 990                         | 0.01                | 0.72648  | 3.67                                     | 3.68                               | -0.8             |
| 990                         | 0.01                | 0.55724  | 4.746                                    | 4.747                              | -0.1             |

5. Conclusion

The constitutive relation of TC21 alloy based on BP neural network was established according to the experimental data of thermal simulation compression. By using trainbr algorithm to train BP neural network, the BP neural network model of TC21 titanium alloy has high precision and prediction and generalization ability, and can better reflect the change rule of the rheological stress in the thermal deformation process of TC21 alloy.

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