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Constitutive relationship model of TC21 alloy based on artificial neural network

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Abstract: Constitutive equation is a necessary mathematical model to describe basic information of materials deformation and finite element simulation. There is a highly nonlinear relationship for flow stress as function of strain, strain rate and temperature. Based on the experimental data sets obtained from the isothermal compression tests conducted on a Gleeble−1500 thermal simulator, the flow behavior of TC21 alloy was studied systematically, and the constitutive relationship model for this alloy was developed using BP neural network. In the proposed model, the input variables are strain, strain rate and deformation temperature while the flow stress is the output variable. It was found that the established constitutive relationship model could provide a better representation of the test data and better describe the whole deforming process compared to the traditional method.

Key words: TC21 alloy; BP neural network; constitutive relationship

1 Introduction

Constitutive relationship of materials is the basic function of flow stress and hot processing parameters, such as strain (ε), strain rate ($\dot{\varepsilon}$) and deformation temperature (T). Traditionally, the constitutive equations are usually built by the multivariate non-linear regression analysis with the experimental results [1,2]. However, many factors affecting the flow stress present the highly non-linear relationship, and the response of the deformation behaviors of the materials under strain rates and temperatures has complicated interaction, which makes the accuracy of the flow stress predicted by the regression methods at the low level and the range of application limited. In addition, these constitutive equations will be established across the regions of phase transformation. Therefore, in order to represent data over large domains, different equation parameters or separate equations ought to be employed.

In recent years, artificial neural network (ANN) provides a fundamentally novel and different approaches for materials modeling and processing control from statistical or numerical methods [3]. Basically, ANN approach, which is well known as a type of evolutionary computation method, is an intelligent data information treatment system with the characterization of adaptive learning, and is especially suitable for dealing with the complex problems with highly non-linear relationship and complicated interactive correlations. Based on these advantages, it has been widely adapted in various scientific areas [4]. Moreover, ANN has been successfully developed and widely applied to investigating the hot deformation behavior of titanium alloys [5−9].

TC21 alloy, which is a recently developed alpha-beta damage tolerance titanium alloy, is characterized by high strength, high toughness and damage tolerance. In the previous reports, a number of research groups have systemically and deeply carried out some contributory work with respect to this alloy [10−12]. However, there are few reports about the application of ANN for TC21 alloy to develop the constitutive relationship model and study the hot deformation at elevated temperature. Therefore, in the present investigation, on the basis of the experimental data sets obtained by the isothermal compression tests of TC21 alloy, the constitutive relationship model was

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established using artificial neural network with back-propagation learning rule.

2 Experimental

The beta-transus temperature of the TC21 alloy, as determined by metallographic phase disappearing techniques, was approximately (950±5) °C. The raw material was rolled into a bar with diameter of 18 mm in the α+β phase region. The specimens for hot compression tests, which were obtained from the bar, were machined into cylinder with 8 mm in diameter and 12 mm in height, and the cylinder ends were grooved for retention of the glass lubricants. Isothermal compression tests were carried out on a thermo mechanical simulator Gleeble−1500. Tests were conducted at the deformation temperature ranging from 900 °C to 1000 °C and the strain rates ranging from 0.01 s^{-1} to 50 s^{-1}. The height reduction of the experimental specimens was 70%. The specimens prior to isothermal hot compression were heated and held for 10 min at the deformation temperature in order to obtain a uniform deformation temperature. The stress—strain curves were recorded automatically in the isothermal compression which are shown in Fig. 1.

3 Modeling constitutive relationship of TC21 alloy using ANN

In general, artificial neural network is an intelligent information-treatment system with the characteristics of adaptive learning and treating complex and non-linear relationships. To be specific, an artificial neural network model learns from data obtained from isothermal compressing experiments and recognizes patterns in a series of input and output data sets without any prior assumptions. Generally, each neural network consists of an input layer, an output layer and one or more hidden layers. As sigmoid functions are easily differentiable, the processing units for computational convenience are employed in the present model:

$$f(x)=\frac{1}{1+\exp(-x)} \tag{1}$$

It is quite essential to determine the learning algorithm for the artificial neural network model. Because the back-propagation (BP) algorithm is one of the most typical methods of supervised learning method, and the network weight of each layer in backward process is continuously adjusted, the output value can be

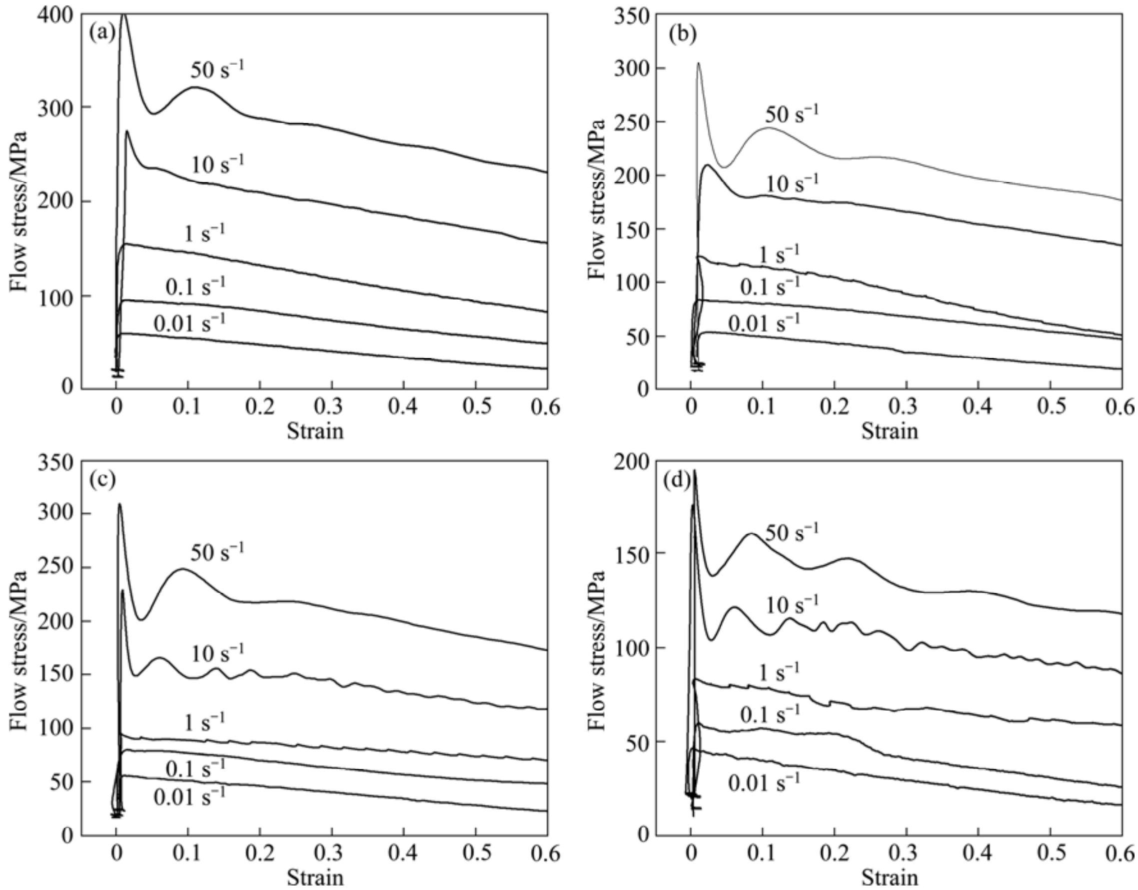

Fig. 1 Stress—strain curves of TC21 alloy obtained by isothermal compression tests at different temperatures: (a) 900 °C; (b) 930 °C; (c) 950 °C; (d) 1000 °C

desirably lost to the target value, So the back-propagation learning algorithm has become the most popular in the field of practical engineering applications. The basic principle and architecture of the BP learning algorithm were introduced in Ref. [13] in detail. In order to develop a desired constitutive relationship model using the technique of artificial neural network model, the procedures listed as follows have to be obeyed: determination of input/output parameters; data collection; analysis and pre-processing of the data; training of the neural network and using the trained network for prediction.

Before training the network, both input and output variables were normalized within the range from 0 to 1 in order to achieve a usable form for the network to read. As a result, the experimental data must be unified to make the neural network training more efficient. The widely used method of unification is presented as:

$$X' = \frac{X - 0.95X_{\min}}{1.05X_{\max} - 0.95X_{\min}} \tag{2}$$

where X is the original data; $X_{\min}$ and $X_{\max}$ are the minimum and maximum values of X, respectively; X' is the unified data of the corresponding X.

The influence of the number of neurons in the hidden layer on the performance of network is complicated. If the architecture of model is too simple, the trained network might not have sufficient ability to learn the process correctly and obtain the correlation between input and output variables. Conversely, it may not converge during training or the trained data may be over fitted. Therefore, various network structures with varying number of neurons in the hidden layer were examined. In this work, the value of mean square error (MSE) was employed to check the ability of a particular architecture, which is presented as

$$E_{\mathrm{MSE}} = \frac{1}{N}\sum_{i=1}^{N}(E_i - P_i)^2 \tag{3}$$

where E and P are the experimental and predicted values, respectively; N is the total number of training data employed in the investigation. In all the calculations involved in this model, a convergence criterion of MSE is set. Figure 2 shows the influence of the number of neurons in the hidden layer on the network performance. It is obviously observed that the MSE of network decreases to the minimum value when the number of hidden-layer neurons is 12, indicating that the network model with 12 neurons in the hidden layer can exhibit the best performance.

During developing the artificial neural network model, the available data sets at temperatures of 900, 930 and 1000 °C were used to train the network, and the data at 950 °C was used to verify the generalization capability of the network. Finally, the constitutive relationship model of TC21 alloy was developed based on artificial neural network, whose schematic diagram is shown in Fig. 3. It can be clearly seen from Fig. 3 that the optimized parameters for the proposed model are 3 input neurons, a single hidden layer with 12 neurons and 1 output neuron with tansig and purelin as transfer function and trainlm as training function.

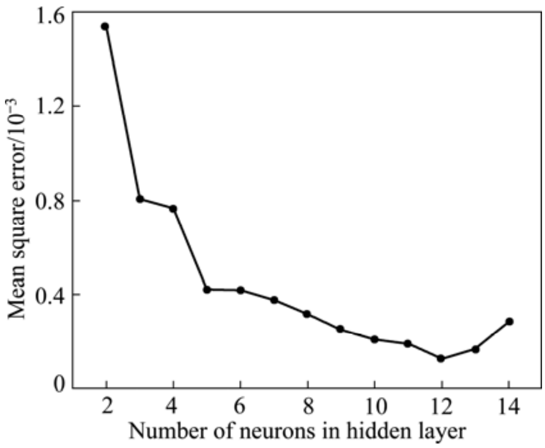

Fig. 2 Influence of number of hidden-layer neurons on network performance

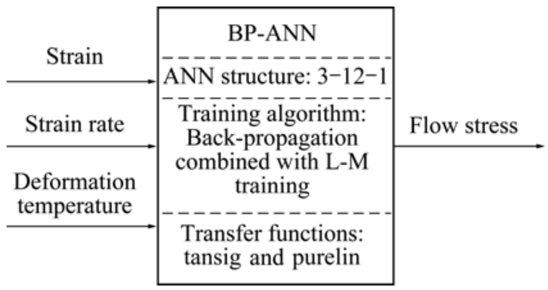

Fig. 3 Schematic diagram of constitutive relationship of TC21 alloy using artificial neural network

4 Results and discussion

The stress—strain curves of TC21 alloy during the isothermal compression deformation at various temperatures are shown in Fig. 1. It can be obviously observed that the stress—strain curves exhibit peak stress at the initial strain, then the flow stress decreases with increasing the strain. In addition, the stress level decreases with decreasing the strain rate and increasing the deformation temperature because high temperature and low strain rate provide longer time for the energy accumulation, growth of dynamically recrystallized grains and dislocation annihilation. Consequently, the effect of the deformation temperature and strain rate on the flow stress traces is significant for all the tested conditions, which can be explained in terms of dynamic recrystallization and dislocation mechanism. The constitutive relationship among flow stress, strain rate and deformation during the hot deformation at a given strain can be usually expressed with an equation known as the classical sine hyperbolic relation as follows [14]:

$$\sigma = \frac{1}{\alpha}[\sinh^{-1}(Z/A)]^{\frac{1}{n}} \tag{4}$$

$$Z = \dot{\varepsilon}\exp(\frac{Q}{RT}) \tag{5}$$

where $\dot{\varepsilon}$ is the strain rate; σ is the flow stress; A, α and n are the material constants for the particular strain; Q is the apparent activation energy for deformation; R is the gas constant; T is the thermodynamic temperature; Z is known as Zener−Hollomon parameter. It is necessary to demonstrate that although these constants in Eqs. (4) and (5) depend on the material considered differently in both phase regions, they cannot fit the whole data set to one set of equation parameters conveniently. Fortunately, the artificial neural network is available to deal with such kind of problem very well.

Training is the process in which the network predictions are refined to fit the experimental data. After the training procedure, the network is tested for the purpose to check whether the predicted results agree with the experimental results. The neural network model is tested by the unused data sets. The performance of the ANN model trained with BP algorithm is evaluated in terms of the indicator of the correlation coefficient (R) described as

$$R = \frac{\sum_{i=1}^{N}(E_i - \overline{E})(P_i - \overline{P})}{\sqrt{\sum_{i=1}^{N}(E_i - \overline{E})^2 \sum_{i=1}^{N}(P_i - \overline{P})^2}} \tag{6}$$

where N is the total number of data employed in the present investigation; E is the experimental value; P is the predicted value obtained from the network model; $\overline{E}$ and $\overline{P}$ are the mean values of E and P, respectively. Figure 4 shows the comparison of predicted flow stress by ANN model with the experimental value of flow stress. For the perfect prediction, all the data points should lie on the 45° line from horizontal. As shown in Fig. 4, most of the data points lie quite close to the line of perfect prediction and the correlation coefficient for the dataset is 0.998, which means that a good correlation between the predicted and experimental values is achieved. Accordingly, it can be suggested that the developed network, which possesses excellent performance and favorable network architecture, has the predicted ability of flow stress for the unseen data sets of TC21 alloy.

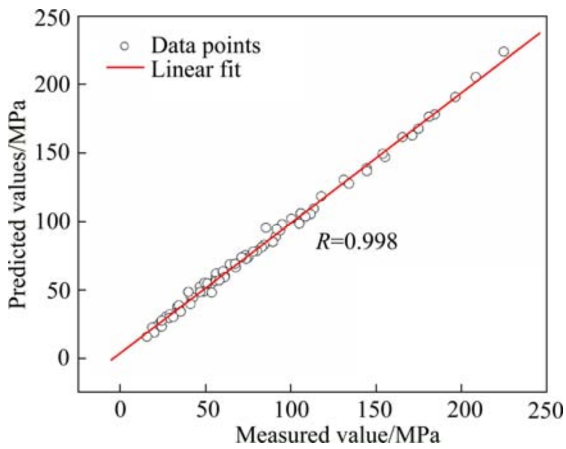

Fig. 4 Comparison of measured stress and predicted stress by BP neural network

Subsequently, the established artificial neural network model is tested by the unused data sets. The validation data sets at the deformation temperature of 950 °C are not used earlier for the training purpose. Comparison of the experimental data with the predicted data by the artificial neural network is listed in Table 1.

Table 1 Comparison of absolute errors between experimental value and predicted value by ANN at 950 °C

Strain	Strain rate/s^{-1}	Experimental stress/MPa	Predicted stress/MPa	Absolute error/MPa
0.1	0.01	50.1	49.6	−0.5
	0.1	77.0	74.3	−2.7
	1	89.6	98.4	8.8
	10	149.8	157.9	8.1
	50	248.5	240.3	−8.2
0.2	0.01	45.9	43.5	−2.4
	0.1	70.9	70.0	−0.9
	1	86.4	93.2	6.8
	10	148.9	146.6	−2.3
	50	215.6	207.1	−8.5
0.3	0.01	39.7	32.9	−6.8
	0.1	62.5	64.3	1.8
	1	82.4	88.3	5.9
	10	143.5	136.9	−6.6
	50	211.6	206.5	−5.1
0.4	0.01	33.4	25.4	−8.0
	0.1	56.4	56.0	−0.4
	1	79.1	83.6	4.5
	10	132.3	130	−2.3
	50	199.8	192.4	−7.4
0.5	0.01	28.0	24.4	−3.6
	0.1	51.2	50.4	−0.8
	1	75.1	76.7	1.6
	10	125	124.4	−0.6
	50	187.9	182.2	−5.7
0.6	0.01	23.1	25.8	2.7
	0.1	49.1	48.7	−0.4
	1	70.9	69.2	−1.7
	10	117.5	117.0	−0.5
	50	172.3	171.0	−1.3

The results remarkably show that the maximum absolute error between the experimental and the predicted flow stress is less than 10.0 MPa after 580 times of training. Therefore, it can be concluded that the proposed constitutive relationship model using BP neural network is a more effective tool to represent the deformation behavior of the TC21 alloy during high temperature deformation. Although the ANN model has the limitation that it cannot propose a mathematical equation which will be used in the future, once the computer model is at the condition of availability, the complicated constitutive relationship can be elaborated.

5 Conclusions

The application of the artificial neural network by the back-propagation learning algorithm was implemented in order to develop the constitutive relationship of TC21 alloy. In the present artificial neural network model, the input variables are strain, strain rate and deformation temperature, whereas the flow stress is determined as the output variable. After testing various neurons in the hidden layer, the optimal configuration of the ANN model with back propagation algorithm was 3−12−1. The generalization performance of the model was quantitatively evaluated using the correlation coefficient and the absolute error, respectively. It was found that the trained ANN model was available to predict the flow stress of TC21 alloy with a favorable accuracy. The good agreement of the predicted flow stress from the ANN model with the experimental results represents a solid correlation between the flow stress (σ) and hot processing parameters (ε, $\dot{\varepsilon}$ and T). It can be suggested that the method of artificial neural network can be used for the estimation and analysis of flow stress as a function of strain, strain rate and deformation temperature for titanium alloys, which can avoid the evaluation of a large number of constants associated with empirical/semi empirical constitutive models.

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基于神经网络的 TC21 合金本构关系模型

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摘　要：本构方程是描述材料变形和有限元模拟基本信息必要的数学模型，它反映流动应力与应变、应变率和温度综合作用的高度非线性关系。基于 Gleeble−1500 热模拟机上进行等温压缩试验获得的实验数据，系统研究 TC21 钛合金的流变行为，并采用 BP 人工神经网络建立该合金的本构关系模型。在该模型中，输入变量为应变、应变速率和变形温度，输出变量为流动应力。与传统方法相比，利用 BP 人工神经网络所建立的本构关系模型能够更好地表征试验数据及描述整个变形过程。

关键词：TC21 合金；BP 人工神经网络；本构关系

(Edited by Hua YANG)