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In the present paper, artificial neural networks (ANNs) have been applied to acquire the constitutive relationships of a Ti–5Al–2Sn–2Zr–4Cr–4Mo (wt-%) alloy at elevated temperature, using the data obtained from experiments carried out on a Thermechmastor–Z hot simulator. In establishing the neural network model for the constitutive relationship of the present alloy, deformation temperature, equivalent strain rate, and equivalent strain, were taken as the inputs, flow stress was taken as the output, and three neurons were used in the hidden layer. The activation function in the output layer of the model obeyed a linear function, while the activation function in the hidden layer was a sigmoid function. The neural network became stable after 32 500 repetitions in training. Comparison of the predicted and experimental results shows that the ANN model used to predict the constitutive relationship of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy has good learning precision and good generalisation. The neural network methods are found to show much better agreement than existing methods with the experimental data, and have the advantage of being able to treat noisy data or data with strong non-linear relationships. MST/3705

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Introduction

The constitutive relationships describing the deformation of metals are usually non-linear and complex, owing to a variation in structure during plastic deformation, particularly occurring in superalloys. For many years researchers have used statistical regression methods to conduct such studies. However, those methods are costly and time consuming and the results are not always satisfactory, because:

(i) the experimental data on flow stress generally contains random unavoidable noise

(ii) some unknown, non-linear relationships may exist between the flow stress, the microstructures, and thermomechanical parameters, which are difficult to fit into any simple pattern.

Artificial neural networks (ANNs)[1] were developed on the basis of the 'synapse hypothesis', i.e. the procedures of biological neural networks in learning information from the outside environment. The ANN is an information treatment system with the characteristics of adaptive learning. This method is especially suitable for treating non-linear phenomena and complex relationships and has been applied successfully to the prediction and control of non-linear systems and systems with unknown models.[2]

In the present paper, ANNs have been applied to acquire the constitutive relationships of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy (unless stated otherwise all compositions quoted in this paper are in wt-%) at an elevated temperature, using data obtained from experiments.

Experimental process and results

The chemical composition of the experimental Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy is given in Table 1. Homogeneous compression experiments were carried out on the Thermechmastor–Z hot simulator. The dimensions of the specimens were 8 mm dia. by 12 mm height. Lubricant notches were machined on two ends. The deformation temperature T (K) and strain rates $\dot{\varepsilon}$ (s^{-1}) were kept constant during the compression tests. The ranges of deformation temperature and strain rate were 1078–1218 K and $1{\cdot}0 \times 10^{-3}$–$8{\cdot}0 \times 10^{1}$ s^{-1} respectively.

The stress–strain curves are shown in Fig. 1, from which it can be seen that the properties of the present titanium alloy are sensitive to strain rate and deformation temperature and that there is some dynamic softening. The strain distribution becomes non-uniform during hot forming of Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy owing to the sensitivity to deformation temperature and strain rate. This might result in local overheating during hot forming and worsening of properties after hot forming. Thus, it is important that the constitutive relationships of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy are described accurately.

NEURAL NETWORK MODEL

The fundamental elements of the ANN method consists of:

(i) the characteristics of the input–output neurons

(ii) the topological structure of the network

(iii) the values of the connected weights and thresholds of neurons.

In the present work, the basic neuron model developed by Ronsenblat[3] was used, the network having a three layer forward feed structure. Figure 2(*a*) and (*b*) presents schematic drawings of the neuron model and the neural network structure. The back propagation (BP) network is especially suitable for treating non-linear systems.

The activation function in the output layer of the model obeys a linear function, while the activation function in the hidden layer was selected to be a sigmoid function

$$f(x) = 1/[1 + \exp(-x)] \qquad (1)$$

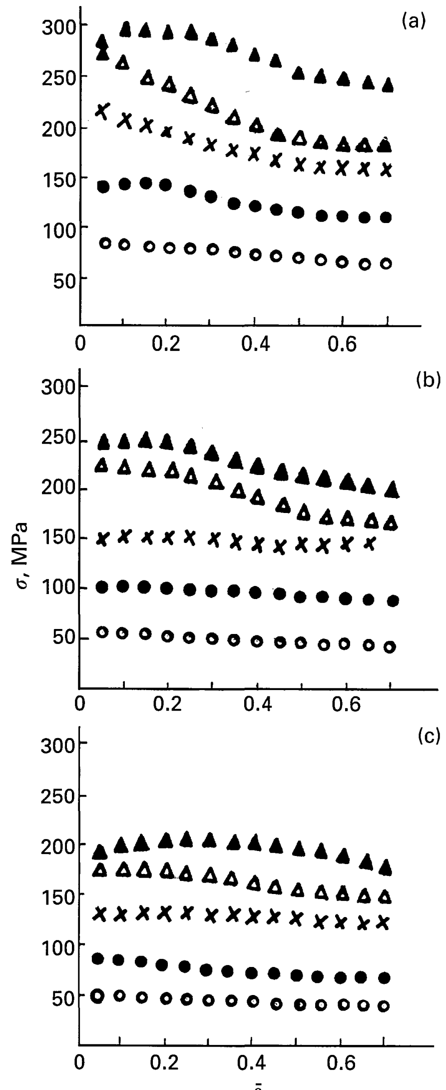
The neural networks need to be trained in a learning process before application and the BP learning algorithm applied in the present work had to follow the tasks described below.

Task 1

This determined the architecture of the neural networks used to acquire the constitutive relationships of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy (see Fig. 2*b*).

Task 2

To initialise, well distributed, random numbers between -1 and $+1$ were given to all the weights and thresholds.



▲ 0·01 s^{-1}; △ 0·1 s^{-1}; × 1·0 s^{-1}; ● 10 s^{-1}; ○ 80 s^{-1}
a 1098 K; *b* 1138 K; *c* 1178 K

1 Stress–strain curves of Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy at given deformation temperatures

Task 3

The neural network was provided with output and input vectors.

Task 4

A group of variables ($S_1^0, S_2^0, \ldots, S_{n_0}^0$) was input.

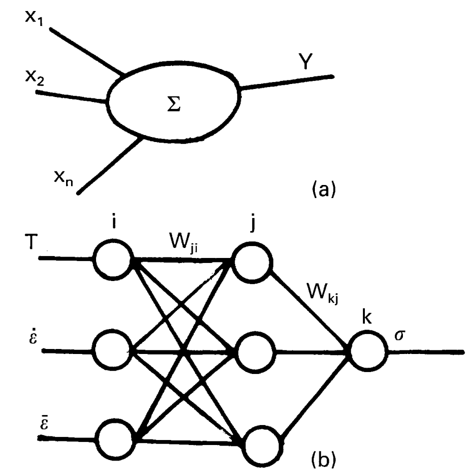
Task 5

The output of the network ($S_1^N, S_2^N \ldots S_{n_N}^N$) where N is output layer and n number of points was computed for a given input. All units on successive layers were updated by

$$S_i^n = 1/[1+\exp(-E_i^n)] \qquad (2)$$

$$E_i^n = \sum_{j=1}^{n_N-1} [W_{ij}S_j^{n-1} - Q_i^n] \qquad (3)$$

where Q_i^n is the threshold of the ith unit on the nth layer, E_i^n is total of inputs of ith point on nth layer, j is a point on the hidden layer, and W_{ij} are the weights between the



a neuron showing inside training data; *b* neural network structure showing outside training data

2 Schematic diagrams of a neuron and of neural network

ith point on the nth layer and the jth point on the $(n-1)$th layer.

Task 6

The average squared error between the measured values and these estimates was computed by

$$\text{Error} = \sum_{i=1}^{n_N-1} [S_i^* - S_i^N]^2 \qquad (4)$$

Task 7

The weights and thresholds were updated. This was accomplished by computing the weights and thresholds on the output layer first, and then propagating it backwards through the network, layer by layer, using

$$W_{ij}^{t+1} = W_{ij}^n(t) + \eta\delta_i^n S_j^{n-1} + \alpha[W_{ij}^n(t) - W_{ij}^n(t-1)] \qquad (5)$$

$$Q_i^n(t+1) = Q_i^n(t) + \eta\delta_i^n \qquad (6)$$

where t is the number of weight updates, η is a learning rate, α is a smoothing parameter, and δ_i^n is the error gradient of the ith unit on the nth layer.

For the output layer

$$\delta_i^n = (S_i^* - S_i^N)P'(E_i^n) \qquad (7)$$

and for the hidden layer

$$\delta_i^n = P'(E_i^n)\sum_{j=1}^{n+1} \delta_j^{n+1} W_{ij}^{n+1} \qquad (8)$$

$$P'(E_i^n) = \delta_i^n(1-\delta_i^n) \qquad (9)$$

where $P'(E_i^n)$ is the first derivative of the function.

Task 8

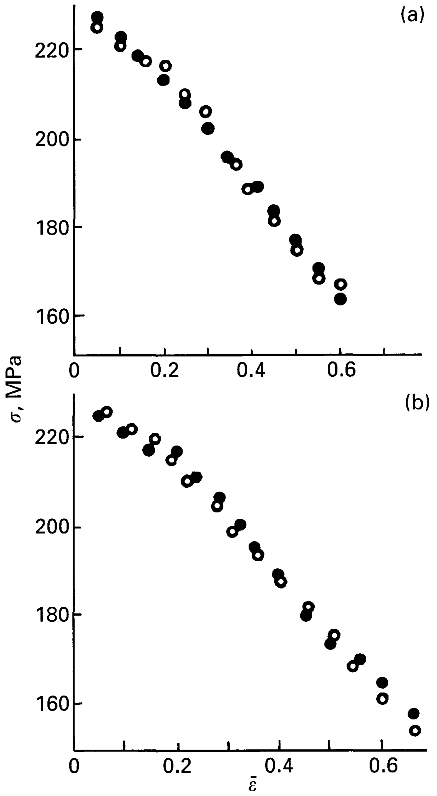
The process then returned to Task 4. After the weights and thresholds have been adjusted for one set of training data, additional training sets can be used to further adjust all the weights and thresholds.

Results and discussion

In establishing the neural network model for the constitutive relationships of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy, deformation temperature T, equivalent strain rate $\dot{\varepsilon}$, and

Table 1 Chemical compositions of experimental alloy, wt-%

Al	Sn	Zr	Cr	Mo	Fe	Si	C	N	H	O	Ti
4·6	1·72	1·91	3·81	4·01	<0·1	<0·1	0·023	0·011	0·0056	0·137	Bal.



○ experimental results; ● predicted results
a 1138 K, 10 s^{-1}; *b* 1078 K, 10 s^{-1}

3 Comparison of ANN predicted flow stress with experimental results

equivalent strain $\bar{\varepsilon}$ were taken as the inputs, flow stress σ (MPa) was taken as the output, and three neurons were used in the hidden layer. The neural network became stable after 32 500 repetitions in training.

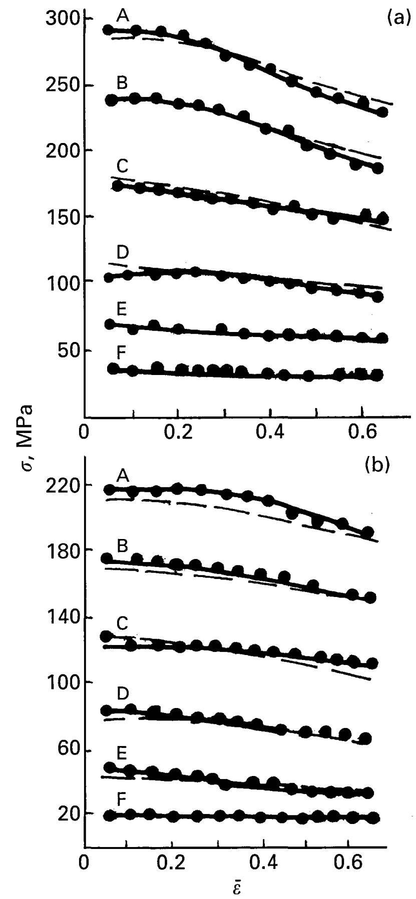
Figure 3 shows comparisons of the experimental flow stress results of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy with predicted flow stress using ANNs, from which it can be seen that the difference between the predicted and experimental data is generally within $\pm 5\%$, indicating reasonably good precision. Also illustrated in Fig. 3*b* are results from outside the training data area, the differences between the predicted stress and the experimental stress results are within the same degree of error ($\pm 5\%$), giving evidence of good generalisation of the present neural network model.

Table 2 shows the effect of the number of training samples on the flow stress predicted by ANNs with a deformation temperature of 1138 K and an equivalent strain rate of 0·1 s^{-1}. It can be seen that as the number of samples increases, so does the predicted flow stress, leading to greater precision.

A comparison of the precision of the neural network methods in predicting the flow stress of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy with those using regression analysis[4] is shown in Fig. 4. The non-linearity of the neural network is better suited to the present data.

Table 2 Comparisons of measured flow stress with that predicted

Equivalent strain, s^{-1}	Measured flow stress, MPa	Predicted flow stress, MPa		
		6 samples	8 samples	10 samples
0·25	103·030	100·360	101·020	101·11
0·35	99·141	97·701	98·147	98·221
0·45	95·107	95·114	95·351	95·401
0·55	92·256	92·606	92·636	92·657
0·65	88·845	90·185	90·014	90·001



A: 0·001 s^{-1}; B: 0·01 s^{-1}; C: 0·1 s^{-1}; D: 1 s^{-1}; E: 10 s^{-1}; F: 80 s^{-1}
—— ANN predicted flow stress; ---- flow stress calculated by regression method; ● experimental results
a 1118 K; *b* 1198 K

4 Comparison of measured flow stress with those calculated using regression methods at given deformation temperatures

Conclusions

Artificial neural network models have been established to predict the constitutive relationships of the Ti–5Al–2Sn–2Zr–4Cr–4Mo alloy and exhibit good learning precision and good generalisation, the neural network method shows much better agreement with the experimental data than earlier methods, and has the advantage when treating noisy data or data with strong non-linear relationships.

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