Modeling constitutive relationship of Ti17 titanium alloy with lamellar starting microstructure

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A B S T R A C T

The isothermal compression tests of Ti17 titanium alloy with lamellar starting microstructure were conducted on a Gleeble-1500 thermo-mechanical simulator at the deformation temperatures ranging from 780 to 860 °C with an interval of 20 °C and the strain rates of 0.001, 0.01, 0.1, 1.0 and 10.0 s−1 with the height reduction of 40% and 60%. The typical flow curves exhibit softening at all the deformation conditions, even at low strain rate (0.001 s−1), which have been considered that the flow softening results from adiabatic shear bands at high strain rates and lamellar globularization at low strain rates. On the basis of the experimental data, the artificial neural network model was proposed to develop the constitutive relationship of Ti17 alloy with lamellar starting microstructure. In the present investigation, the input parameters of ANN model are strain, strain rate and deformation temperature. The output parameter of ANN model is the flow stress. The comparison of experimental flow stresses with predicted value by ANN model and calculated value by regression model was carried out. It is found that the predicted flow stresses obtained from ANN were in a better agreement with the experimental values, indicating that it is available and novel to establish the constitutive relationship of Ti17 alloy using the technique of artificial neural network.

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1. Introduction

During hot deformation behavior of materials, several interconnect metallurgical phenomena inevitably occur, such as working hardening, flow softening, dynamic recovery (DRV) and dynamic recrystallization (DRX), etc. It is well known that the working hardening and flow softening mechanisms are significantly influenced by a couple of factors (strain, strain rate and deformation temperature), thus it is necessary to understand their effects systematically, which is a difficult task due to their complex nature [1–3]. In addition, the development of constitutive relationship during hot deformation has a great importance for the design of metal forming processes because of its effective role on metal flow pattern as well as the kinetics of metallurgical transformation. In the past few decades, some beneficial efforts have been made to establish the constitutive equations, which would provide a complete mathematical description of the flow stress of materials by phenomenological [4–6] or empirical/semiempirical equations [7–9]. Generally, conventional methods are applied to obtain the materials constants using regression analysis with the experimental results. However, the response of the deformation behaviors of the materials under different temperatures and strain rates presents highly non-linear relationship, which cannot ensure the accuracy of the calculated flow stress by the regression method and thus the applicable range is limited. Especially, when a new experimental data is added, the regression constants need to be recalculated, which costs large amount of time during computation. Therefore, it is quite difficult to deal with the dispersed data through the regression method.

Fortunately, soft computing technique like artificial neural network (ANN) has provided an efficient alternative method in the field of materials science simulation [10–14]. Being different from statistical or numerical methods, the ANN model is able to provide a fundamentally novel approach with materials modeling and processing control techniques. One of the advantages of ANN is that the model can learn from data obtained from experiments and recognizes patterns in a series of inputs and outputs. More important, it is able to predict the flow stress across deformation mechanisms domains, which cannot be carried out using the traditional method. As a result, some helpful research have been conducted regarding the applications of ANN, which has been developed and widely used to study the flow behavior of titanium alloys under isothermal compression [15–17].

Recently, the Ti17 titanium alloy [18–21] has been received much attention in China due to its potential for manufacturing dual-property blisk. Basically, the dual-property blisk [18] should have

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2. Material and experimental procedure

The initial Ti17 alloy used in the present work was β-forged at Baoshan Iron & Steel Co., Ltd. in China to produce a lamellar microstructure. Fig. 1 shows the initial microstructure of Ti-17 alloy. As shown in Fig. 1, the alloy has a typical lamellar microstructure with 400 µm grain size and 15–25 µm length and ~1 µm thick α lamellas. The chemical composition of the Ti17 titanium alloy is listed in Table 1. The beta transus temperature (T_b) of the alloy, as determined by metallographic observations, was approximately 905 °C. The cylindrical compression specimens were machined into cylinders with 8 mm in diameter and 12 mm in height and both ends were grooved for sufficient retention of the glass lubricants during each test so as to reduce the friction.

In order to develop the constitutive relationship and study the hot deformation behavior of Ti17 alloy with initial lamellar microstructure in the α + β phase field, a series of isothermal compression tests were carried out at various deformation temperatures (780, 800, 820, 840 and 860 °C) and different strain rates (0.001, 0.01, 0.1, 1 and 10 s⁻¹) on the Gleeble-1500 thermomechanical simulator. The reductions in height were 40 and 60%. The specimens were heated and held 5 min at each deformation temperature prior to isothermal compression. The true stress–strain curves were recorded automatically during isothermal compression. In addition, all the flow stress curves of Ti17 titanium alloy have been corrected for friction effect by the empirical formula as mentioned in Ref. [22]. Meanwhile, it is well known that the effect of deformation heating on the flow softening is existed during hot compression. The corrected and non-corrected flow curves (at 840 °C and various strain rates) in Fig. 2 provide a convenient means of quantifying the flow softening due to heating effects. As shown in Fig. 2, the flow behaviors exhibited that the data corrected for deformation heating were similar to the measured curves, and obvious flow softening still existed. This implied that the softening in Ti17 alloy was not solely a result of the deformation heating. Furthermore, it can be seen that an obvious degree of flow softening appeared at large strain rate (e.g. 10 s⁻¹) due to near adiabatic conditions, and a negligible difference at strain rate of 0.01 and 0.001 s⁻¹. Therefore, the flow stress curves of Ti17 titanium alloy have not been corrected for adiabatic heating effects. After the compression, the specimens were cooled in water to room temperature. To observe the evolution of microstructure during compression tests, all the tested specimens under different deformation conditions were axially sectioned parallel to the stress axis, and the samples were prepared for scanning electron microscope (SEM).

3. Modeling constitutive relationship of Ti17 titanium alloy using ANN model

Artificial neural networks (ANN) are a large class of parallel processing architectures, which can simulate complex and nonlinear relationships. The feed forward networks are commonly used and consisted of a number of neurons in each layer. The first layer, called an input layer, receives data from outside. The last layer is the output layer, which sends data information out to users. Layers that lie between the input and output layers are called hidden layers and have no direct contact with the environment. The role of the hidden layer, which is a layer contains a systematically determined number of the processing elements, is to provide the necessary complexity for non-linear problems. Basically, it is extremely complicated to choose the number of neurons in hidden layer, which is usually determined according to the experiments or empirical equation. If the architecture is too complicated, it may not converge during training even the trained data may be over fitted. Conversely, the trained network might not have sufficient ability to learn the process correctly with the simple architecture. Their presence is requisite because they can provide complexity to network architecture for modeling non-linear functional relationship [23]. After choosing the network architecture, the network is trained by using...
back-propagation algorithm, which is the most efficient optimization method for minimizing the error through weight adjustment. The training process involves two passes. In the forward pass, the input signals propagate from the network input to the output. In the reverse pass, the calculated error signals propagate backwards through the network where they are used to adjust the weights. Any efficient optimization method can be used for minimizing the error through weight adjustment. If the testing error is much more than the training error, it is considered that the training data is over fitting for the network model. At last, a properly fitted network will give nearly equal training and testing errors. The processing units for computational convenience, like sigmoid functions, are easily differentiable, and are employed in the present model:

\[ y = f(x) = \frac{1}{1 + \exp(-x)} \]  

(1)

where \( y \) is the output of the neuron and \( x \) is the input to the neuron. The process using the experimental outputs to minimize the mean squared error (MSE) iteratively is called as training the network. Once the architecture of network is defined, the learning process starts to be performed, and weights are calculated so as to present the desired output, and can be used later for predicting outputs given a different set of inputs. In the present paper, it is widely recognized that flow stress of materials (\( \sigma \)) is dependent on three independent hot processing parameters \( (\varepsilon, \dot{\varepsilon} \text{ and } T) \) during hot working process. For this reason, the input layer in the present model consists of three neurons representing these parameters. The output layer consists of one neuron representing the flow stress, which is shown as Fig. 3.

Before the training of the network, the input and output datasets must be normalized within the range from 0.1 to 0.9 so that the specific factor can be prevented from dominating the learning for the ANN model [24]. Consequently, the experimental data obtained from the compression tests is unified to make the neural network training more efficient prior to the use of the variables. The inputs variables of the ANN model are strain \( (\varepsilon) \), log strain rate \( (\log \dot{\varepsilon}) \) and deformation temperature \( (T) \) and the output of the model is flow stress \( (\sigma) \). The widely used unification approach is presented as:

\[ X' = 0.1 + 0.8 \times \frac{X - X_{\min}}{X_{\max} - X_{\min}} \]  

(2)

where \( X \) is the original data, \( X_{\min} \) and \( X_{\max} \) are the minimum and maximum value of \( X \), respectively, and \( X' \) is the unified data of the corresponding \( X \). It has to be emphasized that this unification method is not appropriate to directly deal with strain rate \( (\dot{\varepsilon}) \) used in the present study because \( \dot{\varepsilon} \) changes severely. Thus the logarithm method of unification is adopted for the strain rates. It was found the fact that such preprocessing procedure is more efficient for the neural network training. Additionally, the number of hidden-layer neurons determines the complexity of neural network and precision of predicted values. Therefore, in order to decide the appropriate number of hidden layers, the trial-and-error procedure was initialized with two neurons in the hidden layer and further carried out with more neurons. In this study, the values of mean square error (MSE) were used to verify the ability of a particular architecture. It was found that the MSE of ANN model reached the minimum value when the number of neurons was 14. During developing the ANN model, the data set at strain of 0.7 was removed to test the generalization capability of the network and the remaining strains (0.1–0.6 and 0.8) were used to train the network model. Training of the neural network was carried out in MATLAB software with the help of training function ‘TRAINLM’, which is used to update weights and bias values in a back-propagation algorithm on the basis of Levenberg–Marquardt (LM) optimization [25]. Improvement of the generalization has been attempted by means of ‘regularization’ and ‘early stopping with validation’. Finally, the ideal network model was determined for use of future prediction. The optimized model for predicted model of constitutive relationship for Ti17 alloy was 3 input neurons, a single hidden layer with 14 neurons and 1 output neuron with ‘tan sigmoid’ and ‘log sigmoid’ as transfer function. A feed forward back-propagation algorithm is selected to train the network. The setting of other training parameters for neural network is listed in Table 2.

### Table 1

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<th>Name of network parameters</th>
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<td>Training function</td>
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### Table 2

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Fig. 3. The architecture of the BP ANN model in this research.

4. Results and discussions

4.1. Stress–strain behavior

Typical true stress–true strain curves for deformation of Ti17 alloy with lamellar starting microstructure at 780 and 840 °C and various strain rates are shown in Fig. 4, respectively. Similar to other titanium alloys, it can be seen that the flow stress increases rapidly with the increase of strain and reaches a peak, then it decreases to a steady value as the dynamic softening is sufficient to counteract the work hardening of the material in the compression process. It is interesting to note that all the flow curves exhibit a significantly flow softening behavior. However, the flow softening may be attributed to lamellar globularization, dynamic recrystallization, adiabatic shear bands, and so on [26]. As seen from Fig. 4, the predicted curves exhibit a more obvious flow softening at high strain rate (e.g. 10 s–1). In general, Prasad and Seshacharyulu [27] have suggested that titanium materials exhibit flow stress decreasing due to adiabatic shear bands formation at higher strain rates. It is universally acknowledged that adiabatic deformation heat generated during hot working is not conducted because of insufficient time and low thermal conductivity, inducing highly localized flow along the maximum shear stress plane at high strain rates. Thus, the formation of adiabatic shear bands plays a role in the softening
of flow stress for Ti17 alloy at high strain rates, which is coincident with the observation by Wang [28].

In contrast, at the strain rate of 0.001 s⁻¹, the flow stress decreases slowly at 780 °C and does not reach a steady stress level at a large strain (in Fig. 4a). However, the value of flow stress at 840 °C quickly presents steady state at a small strain (approximately 0.5) as shown in Fig. 4b. Such phenomenon of flow softening behavior has been observed in many α + β titanium alloys at lower strain rates and considered as lamellar globulization [28–31]. In other words, these examples indicate that the flow stress level decreases while the lamellar microstructure transform gradually to the globular one [30]. Semiatin et al. [31] suggested that materials with the lamellar microstructure exhibited flow stresses which were slightly higher than (0.1 and 10 s⁻¹) those for the coarser-grain size materials. The metallographic investigation conducted in this work confirms this conclusion (Figs. 5–7). It can be clearly seen from Fig. 5a that the break-up of α lamellas have been lightly observed at 780 °C/0.001 s⁻¹ and strain of 0.51 (the reduction of 40%). With increasing strain, a lamellas broke up more effectively, and a phase of more globular or equiaxed morphology generated at strain of 0.92 (the reduction of 60%) (Fig. 5b). Meanwhile, Fig. 6 represented that the degree of globulization increase noticeably at 840 °C/0.001 s⁻¹ and different strains, which is because diffusion increases with increasing temperature and thus dynamic globulization occurs more easily. Fig. 7 shows the microstructure of compressed specimen deformed at 840 ºC/60% and strain rate of 10 s⁻¹. It can be obviously observed that the degree of globulization at higher strain rate was much less than that at lower strain rate as shown in Figs. 4 and 5. It is because that the material is deformed at high strain rate, there is still not enough time for α phase to transform into equiaxed α phase with the help of diffusion. Correspondingly, the flow stress decreases with increasing deformation temperature, as shown in Fig. 4. These results are agreed with the reported by Wang et al. [32] who suggested that the flow softening are attributed to lamellar globulization and the strains for initiation and completion of dynamic globulization were predicted to be about 0.06–2.4 at 780 ºC/0.001 s⁻¹ and 0.02–1.9 at 840 ºC/0.001 s⁻¹ in Ti17 titanium alloy with lamellar structure during the hot compression. By contrast, in the present investigation, the strains for flow softening and steady stress levels are about 0.03–0.8 at 780 ºC/0.001 s⁻¹ and 0.02–0.5 at 840 ºC/0.001 s⁻¹ in Ti17 titanium alloy, the difference of which is because there are other deformation mechanisms existing. In a word, combined with the flow curves, it suggested that the globulization of lamellas structure is playing an important role on flow softening behavior of Ti17 titanium alloy at low strain rate in this paper.

Based on the analysis above, the effect of the deformation temperature and strain rate on flow stress is significant at different deformation conditions. Therefore, it is necessary to establish the constitutive relationship and characterize the deformation behavior of Ti17 alloy with lamellar starting microstructure.
4.2. Constitutive relationship by regression model

The constitutive relationship between flow stress, strain rate and deformation temperature during hot deformation at a given strain can be usually presented with an equation known as the classical hyperbolic sine relation [33,34] as following:

\[ \dot{\varepsilon} = A[\sinh(\sigma \alpha)]^n \exp \left( -\frac{Q}{RT} \right) \]  

(3)

where \( \dot{\varepsilon} \) is the strain rate (s\(^{-1}\)), \( \sigma \) is the flow stress (MPa), \( A, \alpha \) and \( n \) are the material constants for the particular strain, \( Q \) is the apparent activation energy for deformation, \( R \) is the universal gas constant, \( T \) is the deformation temperature (K) and \( Z \) is known as Zener–Hollomon parameter. Taking log on both sides of Eq. (3) and differentiating with respect to \( \ln \dot{\varepsilon} \) and \( 1/T \), one gets

\[ \ln \dot{\varepsilon} = \ln A - \frac{Q}{RT} + n \ln[\sinh(\alpha \sigma)] \]  

(4)

Then

\[ n = \left. \frac{\partial \ln \dot{\varepsilon}}{\partial \ln[\sinh(\alpha \sigma)]} \right|_T \]  

(5)

In the present study, flow stress, strain rate and temperature data for a strain of 0.7 are fit to Eq. (3) using the non-linear multivariate regression analysis. The plot of \( \ln \dot{\varepsilon} \) versus \( \ln[\sinh(\alpha \sigma)] \) and the plot of \( \ln[\sinh(\alpha \sigma)] \) versus \( 10,000/T \) are shown in Figs. 8 and 9, respectively. Then the four constants of Eq. (3), \( A, \alpha, n \) and \( Q \) obtained for this investigation using regression method have been listed in Table 3. On the basis of regression method, the hyperbolic
sine constitutive relationship equation at the steady state of flow stress of Ti17 alloy is developed as follow:

\[
\dot{\varepsilon} = 7.663 \times 10^{13} \ln \sinh(0.00776 \sigma)]^{3.613} \exp \left( \frac{-320.422}{RT} \right)
\]  

(6)

The temperature compensated strain rate parameter or the Zener–Hollomon parameter is evaluated by Eq. (7) to check the validity of Eq. (6).

\[
Z = \dot{\varepsilon} \exp \left( \frac{Q}{RT} \right) = A[\sinh(\alpha \sigma)]^n
\]  

(7)

Fig. 10 shows the variation plot of flow stress with Zener–Hollomon parameter for Ti17 alloy. It can be seen from Fig. 10 that the correlation coefficient \( R \) for the linear regression of \( \ln Z \) and \( \ln[\sinh(\alpha \sigma)] \) is 0.989. Although these constants of Eq. (3) depending on the material are considered in the fixed condition, they cannot fit the whole data set to one set of equation parameters very well. Moreover, the fit of one equation or a set of equation parameters to the whole strain range does not capture the essence of the specific deformation characteristics. Fortunately, the ANN model can deal with the problems mentioned above effectively.

4.3. Constitutive relationship by ANN model

Training is the process in which the network’s predictions are refined to fit the experimental data. Then the trained network must be tested to show a suitable degree of reliability and accuracy. During the training period, the mean square error decreased with increasing number of iteration. The performance changing of ANN during training stage is shown in Fig. 11. It can be seen that after 316 training cycles, obvious effect on error reduction has not been traced, which indicated that the ANN model has finished the learn process and possessed the relationship between strain, strain rate, deformation temperature and flow stress. The neural network model was tested using the data (at strain of 0.7) which was unused earlier for testing purpose. The prediction capability of the trained network is tested in light of correlation coefficient \( R \) based on the equation:

\[
R = \frac{\sum_{i=1}^{N}(E_i - \bar{E})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{N}(E_i - \bar{E})^2 \sum_{i=1}^{N}(P_i - \bar{P})^2}}
\]  

(8)

where \( P \) is the predicted value obtained from ANN model and \( E \) is the experimental value. \( \bar{P} \) and \( \bar{E} \) are the average values of \( P \) and \( E \), respectively. \( N \) is the total number of data set.

Fig. 12 shows the comparison of the flow stress values between the experimental values and with the predicted flow stress using ANN model at a strain of 0.7 in the hot compression of Ti17 alloy. From this figure, it can be clearly seen that most of the training data points are quite close to the 45° line and the correlation coefficient for the ANN model is 0.998, which is indicated that all of the predicted flow stress of training samples are in a good agreement with the experimental flow stresses. Consequently, the established ANN model is able to predict the flow stress in the isothermal compression of Ti17 titanium alloy. Fig. 13 presents the comparison of experimental value of flow stress and predicted value by ANN model as well as calculated value by Eq. (8) at the strain of 0.7 in the form of percentage error. As indicated from this figure that the average percentage error (2.77%) between predicted value and experimental value is much less than that (7.67%) between
calculated value by Eq. (8) and experimental value. That means the fact that the constitutive relationship developed using ANN is more accurate and appropriate to the present material than the traditional method. In order to verify the prediction capacity of the trained network model, the comparison of predicted flow stress values from ANN model and the experimental values at 780 and 840 °C are carried out. Fig. 14 shows a comparison between the experimental flow stress curves and the predicted flow stress curves using the present ANN model. From Fig. 14, it can be presented that the non-linear relationship between flow stress and strain rate is easily described by the network model for Ti17 alloy. As a result, it can be concluded that the artificial neural network model is a powerful tool to investigate the flow behavior of the present alloy.

5. Conclusions

The hot deformation behavior of Ti17 titanium alloy with lamellar starting microstructure under various hot deformation conditions has been studied systematically based on the method of traditional regression and artificial neural network, respectively. The academic results obtained are summarized as follows:

1. The flow stress curves exhibit flow softening at all the deformation conditions, which are attributed to adiabatic shear bands at high strain rates and lamellar globularization at low strain rates. Based on the non-linear regression and assuming a hyperbolic sine equation among the stress, strain rate and deformation temperature, the constitutive equation was constructed and the average value of deformation activation energy of the alloy was derived as 320.422 kJ/mol at strain of 0.7.

2. The developed ANN model with BP learning algorithm is able to predict the flow stress of Ti17 alloy over the ranges of strain, strain rate and deformation temperature. It is found that the average relative error between the predicted values by ANN model and experimental value is 2.77%, indicating that the proposed ANN model possesses the excellent ability to predict the flow stress of Ti17 alloy. More important, the ANN model can be a much more effective tool to develop the constitutive relationship than the traditional regression method for Ti17 alloy with lamellar starting microstructure.

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