Constitutive models and microstructure evolution of Ti-6Al-4V alloy during the hot compressive process

Xiaomin Huang1,2, Yong Zang1,2 and Ben Guan1,2

1 School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, People’s Republic of China
2 Beijing Key Laboratory of Lightweight Metal Forming, Beijing 100083, People’s Republic of China
E-mail: yzang@ustb.edu.cn

Keywords: Ti-6Al-4V, Arrhenius equations, artificial neural network, microstructure evolution

Abstract
Using the Gleeble-1500D thermal simulation machine, and the Ti-6Al-4V titanium alloy was subjected to isothermal compression test under the conditions of deformation temperature of 1023 K–1323 K, strain rate of 0.01 s⁻¹–10 s⁻¹ and maximum deformation degree of 60% (the true strain is 0.916), and the stress and strain data under different deformation conditions were obtained. Based on the stress and strain data, the Arrhenius model and Back-Propagation Artificial Neural Network (BP-ANN) model were obtained. The results show that the BP-ANN model has higher accuracy than Arrhenius model, its correlation coefficient is as high as 0.99959, and the average absolute relative error is only 3.0935%. The Ti-6Al-4V titanium alloy model can make up for the lack of prediction accuracy of the constitutive model, and can predict the flow stress in all deformation ranges. Finally, the influence of different deformation temperature, deformation rate and deformation amount on microstructure is analyzed.

1. Introduction
In recent years, with the rapid growth of air transportation mileage, the shortage of resources and the increasing pressure of energy saving and emission reduction, the urgent need to reduce costs and improve the weight-to-weight ratio, there is more and more research on high-performance lightweight materials [1, 2]. Ti-6Al-4V titanium alloy is a general purpose high Al equivalent nearly α alloy, which is widely used in aerospace industry [3–5]. Special working environment and high safety require excellent mechanical properties, and the macroscopic mechanical behavior and properties of materials are always determined by the microscopic structure. As a bi-phase polycrystalline material, Ti-6Al-4V usually has different grain structure and mechanical properties [6]. Therefore, the interaction mechanism of the two phases during plastic processing deformation is complex, and the interaction between uniform and coordinated deformation is limited. In polycrystalline materials due to the grain morphology, distribution, crystal orientation, the factors of interaction between adjacent grain is different, the response of the different grain size on the macroscopic mechanical behavior are different, which can lead to local stress and strain concentration is easy to appear, uneven plastic deformation ability is reduced, which serious influence its plastic shaping and service performance.

Constitutive model is an equation to describe the relationship between force and deformation in material deformation [7–9]. It is very important for the accuracy of finite element simulation. A large number of experimental results of hot forming of aluminum [10, 11], magnesium [12–14], titanium [15, 16] and other metals [17, 18] and related studies show that: the change of flow stress is mainly affected by deformation temperature, deformation amount, deformation rate, internal structure and alloying credit. It is an idea to obtain the experimental data through basic experiments and then combine the experimental data with different constitutive models to establish the stress constitutive equation of materials. Different constitutive models have great influence on the description of different machining processes, so the proper constitutive relation should be selected according to the processing technology of material properties [19, 20]. The constitutive models of thermal deformation of titanium alloys have been studied by different scholars and some results have been.
obtained. Porntadawit et al. [21] based on hyperbolic sine equation, Cinggara equation, Shafie and Ebrahimi equation established a constitutive model considering the influence of work hardening and dynamic recrystallization on the deformation behavior of Ti-6Al-4V. The model can accurately calculate the flow stress. Babu et al. [22] based on the constitutive model of immovable dislocation density and hole concentration, which can describe the plastic flow in a wide range of temperature and deformation rate, including the main deformation mechanism of the alloy. The model can describe the flow softening and stress relaxation of Ti-6Al-4V well and can be used to simulate the forming and heat treatment process. Sun et al. [23] established the thermal deformation constitutive model of Ti-6Al-4V titanium alloy by using artificial neural network method, and trained the model by using thermal simulation compression test data in the range of 800 °C ~ 1050 °C, 0.01 s^{-1} ~ 10 s^{-1}. The predicted results of the model were in good agreement with the experimental data. Fan et al. [24] established a constitutive model based on internal variables and self-consistent constitutive theory. The constitutive relationship of each phase is coupled with physical mechanisms such as solid solution strengthening, Hall-Petch effect, dislocation interaction and dynamic recrystallization. Finally, the constitutive relationship of the two phases is unified by means self-consistent theory to calculate the macroscopic stress and strain of the material. Gao et al. [25, 26] established a set of constitutive models for coupled microstructure evolution to predict the flow stress and spheroidization behavior of two-phase titanium alloys with lamellar initial microstructure during thermal deformation. The model consists of two parts: flow stress model and microstructure evolution equation. The flow stress is decomposed into the stress related to thermal activation process and the stress independent of temperature. The microstructure model includes dislocation density evolution equation, structure spheroidization evolution equation and Hhall-Petch strengthening equation. Gao [27, 28] used Ti-6Al-4V and the test data to verify the model, and the predicted results of the model were in good agreement with the test data. Bai et al. [29, 30] developed a constitutive model for the main mechanism of plastic flow softening of Ti-6Al-4V titanium alloy on the basis of the unified viscoplastic constitutive framework proposed by Lin. In this model, the plastic flow law of α phase and β phase is considered respectively. Reuss simplified criterion is used to assume that the flow stress of the two phases are equal, and the macroscopic plastic strain rate is the volume average of the plastic strain rate of the two phases. The model combines the information of dislocation density, phase transformation and secondary phase spheroidization, which can not only accurately predict the flow stress, but also reflect the microstructure evolution during the material deformation process. The Arrhenius constitutive model [31–33] is widely used in the construction of various metal materials.
and has a high prediction accuracy. Therefore, the mathematical relationship can be calculated based on the true stress-true strain curve obtained from the experiment. BP-ANN model \cite{34–36} is a multi-layer feedforward network trained according to the error reverse propagation algorithm, which is composed of an input layer, one or more hidden layers, and one output layer.

At the same time, there is no related literature to describe the plastic flow behavior of Ti-6Al-4V through Arrhenius constitutive equation and ANN model. In this paper, the strain rate is \(0.01 \text{s}^{-1}–10 \text{s}^{-1}\), and the deformation temperature is 1123 K, 1173 K, 1223 K, 1273 K and 1323 K through thermal simulation experiments. The prediction effects of the two constitutive models of the Arrhenius constitutive equation and the ANN model are compared. Finally, the influence of different deformation temperature, deformation rate and deformation amount on microstructure is analyzed. The study found that the microstructure is very different at the phase transition point. When the deformation temperature is below the phase transition point, the primary equiaxed \(\alpha\) phase grows up, a small amount is elongated, and the content of acicular \(\beta\) phase increases; The \(\beta\)-phase grains become coarse and flat sub-crystals appear when the phase transition point is above. When the deformation temperature is above the phase transition point, the \(\beta\)-phase grains become coarse and the sub-crystals with straight boundaries appear, and finally pass through the polygon realization of equiaxed grains.

### 2. Experimental process

The experimental material is forged annealed Ti-6Al-4V titanium alloy. The initial structure of the alloy is shown in figure 1. It is composed of \(\alpha\) phase (dark region) and \(\beta\) phase (bright region), and mainly consists of \(\alpha\) phase. The size of Ti-6Al-4V used in the experiment is Ø8 × 15. It’s shown in figure 2, and the main components are shown in table 1.

![Figure 2. Experimental material specifications.](image)

| Component | Ti  | Al  | V  | Mo | Zr | Fe | Si | C | N | H | O |
|-----------|-----|-----|----|----|----|----|----|---|---|---|---|
| W% allowance | 6.8 | 2.2 | 1.7 | 2.0 | 0.07 | <0.04 | 0.01 | 0.001 | 0.002 | 0.13 |

![Figure 3. Schematic diagram of the thermal compression heating process.](image)
In the thermal simulation experiment conducted on the Gleeble-1500D thermal simulation, the strain rate is $0.01 \text{s}^{-1}$, $0.1 \text{s}^{-1}$, $1 \text{s}^{-1}$, $10 \text{s}^{-1}$, the deformation temperature is 1123 K, 1173 K, 1223 K, 1273 K, 1323 K, and the maximum deformation degree is 60% (the true strain is 0.916). The experiment uses thermocouple heating, and the experimental data is collected by the computer system. During the experiment, the sample is heated to a predetermined temperature at a temperature increase rate of $10^\circ\text{C}$/s and stored for 3 min. Then, isothermal compression is performed at a constant strain rate. Immediately after the experiment is completed, water cooling is performed. It's shown in figure 3.

Figure 4. True stress - strain curves of Ti-6Al-4V obtained by isothermal compression test: (a) 1123 K; (b) 1173 K; (c) 1223 K; (d) 1273 K; (e) 1323 K.
3. Results and discussion

According to the results of thermal simulation test, the obtained stress-strain data are derived and the stress-strain curves under different deformation temperatures and strain rates are drawn, as shown in figure 4.

The hot working behavior of Ti-6Al-4V titanium alloy is more complicated. Among them, the flow stress is mainly affected by work hardening, dynamic recovery and dynamic recrystallization. Flow stress can be divided into dynamic recovery type and recrystallization type. Through the analysis of figure 4, it can be seen that at a given deformation temperature, as the strain rate increases, the flow stress of Ti-6Al-4V increases significantly. When the temperature is different, under a given strain rate, the true stress-strain of Ti-6Al-4V behaves significantly different. As the temperature increases, the peak stress decreases significantly. It can be concluded that the flow stress of Ti-6Al-4V is very sensitive to the temperature changes, and the flow stress decreases as the deformation temperature increases. The reason is that:

1. The increased temperature can reduce deformation resistance and improve its plastic ductility. Higher temperature provides higher mobility for energy accumulation. In addition, the probability of dynamic recovery and dynamic recrystallization of Ti-6Al-4V varies with the deformation temperature. Increased and increased, the dynamic recovery and dynamic recrystallization can eliminate work hardening, so by increasing the temperature, the flow stress of the titanium alloy can be reduced.

2. The temperature increases, the slip system of Ti-6Al-4V increases, and the critical shear stress decreases. A slip system consists of a slip surface and a slip direction. The more slip systems the metal material has, the greater the possibility of metal slippage.

3.1. Arrhenius constitutive model

The Arrhenius constitutive equation, established by Sellers and Tegart, can be used to describe the relationship between the strain rate, deformation temperature and strain of metals and alloys during high-temperature deformation [37–41]. There are usually three forms of expression:

\[ \dot{\varepsilon} = A \sigma^m \exp \left( -\frac{Q}{RT} \right) \quad (\alpha \sigma < 0.8) \]  

\[ \dot{\varepsilon} = B \exp(\beta \sigma) \exp \left( -\frac{Q}{RT} \right) \quad (\alpha \sigma > 1.2) \]  

\[ \dot{\varepsilon} = C \sinh(\alpha \sigma)^n \exp \left( -\frac{Q}{RT} \right) \quad (\text{For all } \sigma) \]  

Where: \( \dot{\varepsilon} \)—strain rate, \( s^{-1} \); A, B, C—temperature-independent material constants, \( s^{-1} \); \( \sigma \)—true stress, MPa; \( R \)—gas friction constant, 8.3145 J mol\(^{-1}\) K\(^{-1}\); \( Q \)—deformation activation energy, J mol\(^{-1}\); \( T \)—absolute temperature, K; \( m \); \( n \)—stress exponent; \( \alpha \), \( \beta \)—stress level parameters independent of temperature.

Among them, the Z parameter can be introduced to represent the relationship between the deformation activation energy \( Q \), strain rate and deformation temperature of the metal during the deformation process:
Combination equation (5):

\[ Z = \dot{\varepsilon} \exp \left( \frac{Q}{RT} \right) \]  

(5)

\[ \sigma = \frac{1}{\alpha} \ln \left\{ \left( \frac{Z}{C} \right)^{\frac{1}{n}} + \left[ \left( \frac{Z}{C} \right)^{\frac{1}{2n}} + 1 \right]^{n/2} \right\} \]  

(6)

Take the stress under different deformation conditions when the strain is 0.5 as an example to calculate the material constant:

Take the logarithm of both sides of equations (1) and (2) respectively to get:

\[ \ln \dot{\varepsilon} = m \ln \sigma + \ln A - \frac{Q}{RT} \]  

(7)

\[ \ln \dot{\varepsilon} = \beta \sigma + \ln B - \frac{Q}{RT} \]  

(8)

The stress under different deformation temperatures (1123 K, 1173 K, 1223 K, 1273 K, 1323 K) and different strain rates (0.01 s\(^{-1}\), 0.1 s\(^{-1}\), 1 s\(^{-1}\), 10 s\(^{-1}\)) are brought into equations (7) and (8). The equations (7) and (8) are fitted to obtain the fitting curves of \( \ln \dot{\varepsilon} - \ln \sigma \) and \( \ln \dot{\varepsilon} - \sigma \), as shown in figure 5.

From equations (7) and (8), it can be seen that \( m \) and \( \beta \) are the slopes of the fitted curve, which can be obtained by calculation: \( m = 5.046 \), \( \beta = 0.6621 \). The value of \( \alpha \) can be calculated by equation (4): \( \alpha = 0.01312 \).

Take the logarithm of both sides of equation (3) to get:

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

(9)

It can be seen from equation (9) that when the deformation temperature and strain rate are determined separately, the constant \( n \) can get:

\[ n = \frac{\partial \ln \dot{\varepsilon}}{\partial \ln [\sinh(\alpha \sigma)]} \]  

(10)

\[ \frac{Q}{R_n} = \left[ \frac{\partial \ln [\sinh(\alpha \sigma)]}{\partial \left( \frac{1}{T} \right)} \right] \]  

(11)

The \( \alpha \) value obtained above is brought into equations (10) and (11), the equations (10) and (11) under different deformation conditions are fitted to obtain the fitting curves of \( \ln \dot{\varepsilon} - \ln[\sinh(\alpha \sigma)] \) and \( \ln[\sinh(\alpha \sigma)] - 1000/T \), as shown in figure 6. It can be seen from equations (10) and (11) that \( n \) and \( Q/(R_n) \) are the slopes of the fitted curve respectively, and can be obtained by calculation: \( n = 3.234 \), \( Q/(R_n) = 22098.94 \).

Usually, the value of \( R \) is 8.3145 J mol\(^{-1}\) K\(^{-1}\). Through calculation, the deformation activation energy of Ti-6Al-4V at a strain of 0.5 can be obtained: \( Q = 594.220 \) kJ mol\(^{-1}\).

Putting the obtained \( Q \) value into equation (5), the \( Z \) value of different strain rates and deformation temperatures can be obtained when the strain is 0.5. Incorporating equation (3) into equation (5), and taking the logarithm of both sides of the equation, the constant \( Z \) can get:
From equation (12), it can be seen that lnZ and ln[sinh(ασ)] are linear, and lnC is the slope of the curve. Fitting lnZ and ln[sinh(ασ)] under different deformation conditions, as shown in figure 7. Through calculation: lnC = 53.0007, C = 1.042 × 10^{23}.

Put the obtained α, C, n, and Q into equation (6) to obtain the Arrhenius constitutive model of Ti-6Al-4V titanium alloy when the strain is 0.5:

\[
\ln Z = \ln C + n \ln [\sinh(\alpha\sigma)]
\]  

(12)
Figure 8. Relationship between constitutive equation parameters and strain in different temperature range.

Table 4. Fitting results of polynomial coefficients for m, β, α, n, Q, lnC.

| m   | β    | α    | n    | Q     | lnC   |
|-----|------|------|------|-------|-------|
| $A_0$ | $B_0$ | $C_0$ | $D_0$ | $E_0$ | $F_0$ |
| 6.39 | 0.085 | 0.0229 | 3.541 | 6.52547E5 | 65.922 |
| $A_1$ | $B_1$ | $C_1$ | $D_1$ | $E_1$ | $F_1$ |
| -16.74 | -0.212 | -0.12217 | -1.723 | 6.49799E5 | 16.253 |
| $A_2$ | $B_2$ | $C_2$ | $D_2$ | $E_2$ | $F_2$ |
| 101.24 | 1.084 | 0.6277 | 3.76789 | -6.05912E6 | -377.424 |
| $A_3$ | $B_3$ | $C_3$ | $D_3$ | $E_3$ | $F_3$ |
| -334.04 | -3.284 | -1.64334 | -6.739 | 1.79533E7 | 1325.681 |
| $A_4$ | $B_4$ | $C_4$ | $D_4$ | $E_4$ | $F_4$ |
| 600.68 | 5.943 | 2.35459 | 13.901 | -2.42924E7 | 2042.978 |
| $A_5$ | $B_5$ | $C_5$ | $D_5$ | $E_5$ | $F_5$ |
| -548.63 | -5.716 | -1.76124 | -17.232 | 1.416E7 | 1403.889 |
| $A_6$ | $B_6$ | $C_6$ | $D_6$ | $E_6$ | $F_6$ |
| 197.41 | 2.185 | 0.53741 | 7.870 | -2.4748E6 | -341.852 |
The stress values of 0.5 strain under different deformation temperatures and strain rates can be obtained by equation (13), as shown in table 2.

Similarly, the parameters of Arrehnius model under different strains can be calculated by the above method, as shown in table 3, and the fitting curve is shown in figure 8.
The above curves are fitted by the sixth degree polynomial shown in equation (14), and the coefficients obtained are shown in table 4.

\[
\begin{align*}
\alpha &= C_0 + C_1 \varepsilon + C_2 \varepsilon^2 + C_3 \varepsilon^3 + C_4 \varepsilon^4 + C_5 \varepsilon^5 + C_6 \varepsilon^6 \\
\beta &= B_0 + B_1 \varepsilon + B_2 \varepsilon^2 + B_3 \varepsilon^3 + B_4 \varepsilon^4 + B_5 \varepsilon^5 + B_6 \varepsilon^6 \\
m &= D_0 + D_1 \varepsilon + D_2 \varepsilon^2 + D_3 \varepsilon^3 + D_4 \varepsilon^4 + D_5 \varepsilon^5 + D_6 \varepsilon^6 \\
Q &= E_0 + E_1 \varepsilon + E_2 \varepsilon^2 + E_3 \varepsilon^3 + E_4 \varepsilon^4 + E_5 \varepsilon^5 + E_6 \varepsilon^6 \\
\ln C &= F_0 + F_1 \varepsilon + F_2 \varepsilon^2 + F_3 \varepsilon^3 + F_4 \varepsilon^4 + F_5 \varepsilon^5 + F_6 \varepsilon^6 \\
\end{align*}
\]

The predicted value of Arrhenius constitutive model obtained by calculation is shown in figure 9. It can be found that the prediction accuracy of Arrhenius constitutive model is relatively low.

### 3.2. Back-propagation artificial neural network model

BP-ANN model is a multi-layer feedforward network trained according to the error reverse propagation algorithm, which is composed of an input layer, one or more hidden layers, and one output layer. Its schematic diagram is shown in figure 10. The working process includes the forward transmission of information and the back propagation of the error, that is, the information is input from the input layer through the transfer function, propagated in the forward direction, and output by the output layer. When the error between the output information and the expected information exceeds the normal range, the error signal will return in the original way (that is the back propagation of the error), and the weight of each layer of neurons will be modified through the training network, and thus repeat until the output information error reaches a reasonable range, the training is completed.

The selection of the number of hidden layer neurons usually depends on the experience of the designer and the trial and error of multiple experiments. There is no ideal formula to derive its number. If the number of hidden layer neurons is too small, the network will not be able to adapt, too much will lead to too long learning time, and will lead to reduced fault tolerance, resulting in excessive adaptation of the network. Therefore, to choose the best hidden layer, which can refer to the following equation (15):

\[
n_h = \sqrt{n + m + a}
\]

In the equation (15), \(n_h\) is the number of nodes in the hidden layer; \(n\) is the neuron in the input layer; \(m\) is the neuron in the output layer; \(a\) is a constant between 1 and 10, and it is found through repeated trials and comparisons that the optimal situation is a total of 18 double hidden layer.

In this paper, the MATLAB software is used for programming calculation, and the BP neural network is trained by using the normalized data. The TRAINLM function is selected as the training function, the.
LEANNGD function is the learning function, the activation function of the input layer to the hidden layer is the SIGMOID function, the activation function of the hidden layer to the output layer is the PURELIN function. The output $O_{pj}$ of the $p$-th training sample $j$ from the input layer to the hidden layer is shown in equation (16):

$$O_{pj} = f(Net_j) = \frac{1}{1 + \exp\left(-\left(\sum W_{ij}X_j + \theta_j\right)\right)}$$  \hspace{1cm} (16)

In the equation (16), $Net_j$ is the input of the $j$th neuron in the hidden layer; $W_{ij}$ is the connection weight between the input layer and the hidden layer; $\theta_j$ is the threshold from the input layer to the hidden layer.

By adjusting the connection weight of the threshold between the network layer and the neuron, the modeling of nonlinear objects can be achieved. If the initial weights of the network are randomly selected, then when the input mode is $p$, the error between the network output and the expected output is $E_p$. The error objective function $E$ for network training is (equation 17).

$$E = \sum_{p} E_p = \frac{1}{2} \sum_{p=1}^{m_2} \sum_{j=1}^{n_2} (O'_{pj} - y_{pj})^2 = E(W_{ij}, W_{jk}, \theta_j, \theta_k)$$  \hspace{1cm} (17)

In the equation (17), $O'_{pj}$ is the actual output of the network; $y_{pj}$ is the corresponding expected output; $m_2$ is the number of training samples; $n_2$ is the number of network output nodes; and $W_{jk}$ is the initial weight.

The 3 layers of $3 \times 9 \times 1$ are selected. The neural network structure is trained and the error target is located $10^{-4}$. The training results are shown in figure 11. As can be seen from the figure, after 235 iterations of the neural network model, the training results reach the minimum error, and the constructed neural network model converges rapidly and the training is completed.

Figure 12 shows the flow stress data under different deformation conditions obtained by the BP-ANN model. It can be seen from the figure that the flow stress calculated by the BP-ANN model basically falls on the experimental stress-strain curve, indicating that the established model can predict the high temperature rheological behavior of Ti-6Al-4V titanium alloy.

4. Comparison of the Arrhenius-type and ANN models

In order to further verify the accuracy of the established Arrhenius model and BP-ANN model, the correlation coefficient (R) and the mean absolute relative error (AARE) were introduced to evaluate the accuracy of the model. The expression is as follows. Figure 13 shows the correlation between experimental values and predictions. The calculations of equations (18) and (19) can be obtained: $R = 0.99204$, AARE = 0.053521. And in ANN model: $R = 0.99959$, AARE = 0.030935. The results show that the established model has a fairly high...
Figure 12. Comparison of experimental and predicted values of BP-ANN model under different deformation conditions: (a) 1123 K; (b) 1173 K; (c) 1223 K; (d) 1273 K; (e) 1323 K.

precision and can accurately predicted the high temperature rheological behavior of Ti-6Al-4V.

$$AARE(\%) = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{E_i - P_i}{E_i} \right| \times 100\%$$  \hspace{1cm} (18)

$$R = \frac{\sum_{i=1}^{n} (E_i - \bar{E})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n} (E_i - \bar{E})^2(P_i - \bar{P})^2}}$$  \hspace{1cm} (19)
4.1. Microstructural analysis

4.1.1. The influence of deformation temperature

When the degree of deformation is 60% and the strain rate is $0.01 \, s^{-1}$, the deformed structure of Ti-6Al-4V alloy under different deformation temperature conditions is shown in figure 14. It can be seen that the deformed structure of Ti-6Al-4V will be very different because of the different deformation temperature. Ti-6Al-4V is a
temperature-sensitive alloy. The diffusion capacity of the $\alpha$ phase will increase as the temperature rises. It will continuously absorb the small $\alpha$ grains nearby, resulting in a decrease in the number of $\alpha$ grains and an increase in the size of the grains. By comparing and observing the sample structure in this temperature range, it can be found that the content of $\beta$ phase increases with the increase of deformation temperature. The content of acicular martensite in the quenched structure gradually increases with the increase of the deformation temperature. Below the transformation point, water cooling ($T = 1223$ K) is carried out after thermal deformation in the ($\alpha + \beta$) two-phase zone, and a martensitic transformation occurs, resulting in a dual-state structure—martensite $\alpha'$ and part of the primary $\alpha$ phase; Above the transformation point and at a deformation temperature of 1273 K, after the compression-deformed alloy is water-cooled, martensite transformation occurs, resulting in a quenched structure acicular martensite phase $\alpha'$. There are two reasons for this phenomenon: one is that the alloy undergoes rapid cooling after deformation; the other is that after the phase transformation occurs, the ($\alpha + \beta$) two-phase region transitions to the $\beta$-phase region.

In figure 14(a), when the deformation temperature of the titanium alloy is 1123 K and the strain rate is 0.01 s$^{-1}$, the primary $\alpha$-phase grains appear mainly in an equiaxed shape, with a few being elongated. From figure 14(b), it can be seen that the structure has undergone $\alpha \rightarrow \beta$ phase transformation, there are a large number of $\beta$ transformation structures, the grain boundary $\alpha$ phase is distributed at the boundary of the $\beta$ phase, and the $\beta$ phase has basically become the main structure of the thermally deformed structure; Because the $\beta$-phase has a body-centered cubic structure, it has high fault energy and is easy to slip and climb, that is, the ability of dynamic recovery will increase, and the ability of dynamic recrystallization will decrease. The decrease of the flow stress of the material will weaken with the decrease of the flow stress curve. When the deformation temperature is near or above the phase transformation point, the softening mechanism of the alloy is mainly dynamic recovery. When the deformation temperature rises to 1273 K, all $\alpha$ phases are converted to $\beta$ phases. In figure 14(c), we can clearly see the $\beta$ grain boundaries in the microstructure. Many layered structures in the $\beta$ grains in the microstructure are arranged in a specific direction and exhibit more obvious aggregation characteristics. It can be concluded that at this temperature, dynamic recovery occurs completely. Due to the lower strain rate conditions, the sub-crystals produced by dynamic recovery tend to grow, and dynamic recovery is the most important softening mechanism at this time.

It can be seen from the above analysis that the size of the crystal grains gradually increases with the increase of the deformation temperature. With the occurrence of $\alpha \rightarrow \beta$ phase transition, the softening changes from the phase transition point (1268 K), which also determines the transition from dynamic recrystallization to dynamic recovery below and above the phase transition point and the characteristics of the flow stress curve. The recrystallization process is an active process. The higher the temperature, the easier it is to crystallize. When the temperature is too high, the recrystallized grains may aggregate and grow, causing them to become coarse. In the process of thermal deformation, keeping the structure uniform and small is beneficial to improve the properties of Ti-6Al-4V alloy, such as strength, plasticity and fatigue properties. Therefore, the proper heat distortion temperature is essential to obtain the ideal microstructure.

4.1.2. The effect of deformation rate

Figure 15 is the metallographic photograph of the Ti-6Al-4V sample after the thermal compression experiment under different deformation rates when the deformation is 60%. It can be seen from figure 5 that the $\alpha$-phase grains have an obvious growth trend when the strain rate decreases. This is mainly due to the fact that the
distortion energy deforms faster at a larger strain rate, and the energy required for dynamic recrystallization is sufficient, grain refinement and equiaxialization are easier to achieve. If the deformation is slow, the deformation time is long and the crystal grains are easy to grow.

Below the transformation point, when the deformation temperature is 1223 K, the size of the primary \( \alpha \) phase and the martensitic \( \alpha' \) phase will grow with the decrease of the strain rate. When the phase transition temperature is 1223 K and the strain rate is \( 1 \text{ s}^{-1} \), the microstructure is composed of a large number of recrystallized \( \alpha \) grains, equiaxed primary \( \alpha \) grains and lamellar secondary \( \alpha \) phases, as shown in figure 15(b). The structure begins to be uniform, the primary \( \alpha \) phase undergoes dynamic recrystallization, and the content of needle-like \( \beta \) phase increases. The first-born equiaxed \( \alpha \) phase has grown, the number has decreased, and a small amount is elongated. When the temperature is 1223 K and the strain rate is 0.1 \( \text{s}^{-1} \), the microstructure is shown in figure 15(a). Its microstructure is composed of obviously grown recrystallized \( \alpha \) grains, equiaxed primary \( \alpha \) grains and acicular martensite \( \alpha' \) with a large aspect ratio. In addition, the content of acicular martensite \( \alpha' \) phase is higher after water-cooling quenching, and the arrangement is relatively regular, showing certain clustering characteristics.

When the deformation temperature is 1323 K (shown in figure 16), the microstructure changes with the increase of the strain rate, and the microstructure changes from the lamellar structure to the basket structure. This is mainly because at high strain rates, the deformation time is short, the \( \beta \) grain boundary is destroyed during the deformation process, and the dispersed granular grain boundary \( \alpha \) does not exist. The \( \alpha \) phase in the original \( \beta \) grains becomes shorter, the size of the \( \alpha \) clusters becomes smaller, and they are staggered like a woven basket. Therefore, the thermal deformation process affects the microstructure and grain size of the near-\( \alpha \) titanium alloy.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure16.png}
\caption{Metallographic structure of different strain rates at 1323 K.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure17.png}
\caption{Metallographic photos of different deformations under 1223 K compression.}
\end{figure}
Under the condition of low strain rate, the metal material has enough time to recrystallize and form nuclei along the grain boundaries of the deformed structure. The deformation energy storage will increase under the condition of a higher deformation rate, but when the strain is the same, the deformation time is short, the atom diffusion is insufficient, the recrystallization is too slow, the dislocations are too late to be eliminated and continue to occur, which increases the dislocation density and the flow stress. Therefore, increasing the deformation rate helps maintain the uncrystallized structure with too high dislocation density. If the deformation rate is too high, the grain growth time will be insufficient, and the deformed grains will be slightly finer. The relationship between the deformation rate and the grain size is that the larger the deformation rate, the smaller the grain size. In other words, the grain refinement can be achieved by increasing the deformation rate. Therefore, when formulating the thermal deformation process, factors such as temperature, strain rate and deformation degree must be considered comprehensively.

4.1.3. The effect of deformation

The driving force for recrystallization is provided by the distortion energy inside the alloy, and the amount of deformation affects the amount of distortion energy inside the alloy. The driving force for recrystallization is affected by the amount of deformation and is positively correlated. Therefore, when formulating the thermal deformation process, factors such as temperature, strain rate and deformation degree must be considered comprehensively.

5. Conclusions

1. The established BP-ANN model of Ti-6Al-4V titanium alloy has a fairly high precision, and its correlation coefficient is as high as 0.99959, and the average absolute relative error is only 3.0935%, which indicates that the established model can accurately predict the high temperature rheological behavior of Ti-6Al-4V titanium alloy.

2. The Ti-6Al-4V titanium alloy model can make up for the shortcomings of the phenomenological constitutive model in predicting accuracy, and can predict the flow stress in all deformation ranges.

3. Ti-6Al-4V alloy undergoes martensitic transformation after hot deformation and water cooling near the \((\alpha + \beta)/\beta\) transformation point. Acicular martensite phase \(\alpha'\) and primary \(\alpha\) phase appear in the quenched structure. With the increase of deformation temperature, acicular martensite \(\alpha\) in the quenched structure increases. During high-temperature thermal deformation, dynamic recrystallization and dynamic recovery are the main softening mechanisms of Ti-6Al-4V in the \((\alpha + \beta)\) two-phase region and \(\beta\)-phase region, respectively.

4. The microstructure is very different at the phase transition point. When the deformation temperature is below the phase transition point, the primary equiaxed \(\alpha\) phase grows, a small amount is elongated, and the content of needle-like \(\beta\) phase increases; The \(\beta\)-phase crystal grains become coarse and flat sub-crystals appear when they are above the phase transition point, and finally equiaxed crystals are realized.

5. When the deformation temperature is 1223 K, the size of the primary \(\alpha\) phase and the martensite \(\alpha'\) phase will grow with the decrease of the strain rate; When the deformation temperature is 1323 K, the microstructure changes with the increase of strain rate, and transforms from lamellar structure to mesh basket structure.
Acknowledgments

This work is supported by the National Natural Science Foundation of China (51805024), this work is also supported by the Tangshan talent foundation innovation team (20130204D) and funded by S&P Program of Hebei (Grant No.19012204Z).

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Compliance with ethical standard

The authors declare no conflict of interest.

Author’s Contribution

Xiaomin Huang: Conceptualization, Investigation, Writing - original draft. Yong Zang: Project administration, conceptualization Project administration, Ben Guan: Review & editing. Investigation.

ORCID iDs

Xiaomin Huang https://orcid.org/0000-0003-2662-3196

References

[1] Yuan L et al 2020 Effect of annealing temperature on texture and residual stress of Ti-6Al-4V alloy seamless tubing processed by cold rotary swaging Vacuum 177 109359
[2] Shen M et al 2020 Comparison of two constitutive modelling methods in application of TC16 alloy at the elevated deformation temperature Materials Today Communications 24 101053
[3] Ji H et al 2020 Constitutive equation and hot processing map of TA15 titanium alloy Mater. Res. Express 7 46508
[4] Pal S et al 2020 Evolution of the metallurgical properties of Ti-6Al-4V, produced with different laser processing parameters, at constant energy density in selective laser melting Results in Physics 17 103186
[5] Benmessaoud F et al 2020 Role of grain size and crystallographic texture on tensile behavior induced by sliding mechanism in Ti-6Al-4V alloy Mater. Sci. Eng. A 774 138835
[6] Xiong W et al 2020 High temperature creep behavior of hydrogenated Ti-6Al-4V alloy International Journal of Lightweight Materials and Manufacture 3 298–304
[7] Qiao L et al 2020 Modelling and prediction of thermal deformation behaviors in a pearlitic steel Materials Today Communications 25 101134
[8] Wang H et al 2020 New method to develop High temperature constitutive model of metal based on the Arrhenius-type model Materials Today Communications 24 101000
[9] Qiao L et al 2020 A comparative study on arrhenius equations and BP neural network models to predict hot deformation behaviors of a hypereutectoid steel IEEE Access 8 68083–90
[10] Liu L et al 2019 Modification of constitutive model and evolution of activation energy on 2219 aluminum alloy during warm deformation process Transactions of Nonferrous Metals Society of China 29 448–59
[11] Li P et al 2017 Characterization of hot deformation behavior of AA2014 forging aluminum alloy using processing map Transactions of Nonferrous Metals Society of China 27 1677–88
[12] Chen X et al 2019 A constitutive relation of AZ80 magnesium alloy during hot deformation based on Arrhenius and Johnson–Cook model Journal of Materials Research and Technology 8 1859–69
[13] Cai Y et al 2017 Hot deformation characteristics of AZ80 magnesium alloy: work hardening effect and processing parameter sensitivities Mater. Sci. Eng. A 687 113–22
[14] Mei R et al 2018 Simulation of the flow behavior of AZ91 magnesium alloys at high deformation temperatures using a piecewise function of constitutive equations Mech. Mater. 125 110–20
[15] Sirvin Q et al 2019 Mechanical behaviour modelling and finite element simulation of simple part of Ti-6Al-4V sheet under hot/warm stamping conditions J. Manuf. Processes 38 472–82
[16] Quan G et al 2013 Prediction of flow stress in a wide temperature range involving phase transformation for as-cast Ti–6Al–2Zr–1Mo–1V alloy by artificial neural network Mater. Des. 50 51–61
[17] Cai Z et al 2019 Hot workability, constitutive model and processing map of 3Cr23Ni8Mn3N heat resistant steel Vacuum 165 324–36
[18] Murugesan M and Jung D W 2019 Two flow stress models for describing hot deformation behavior of AISI-1045 medium carbon steel at elevated temperatures Helijyn S5 e1547
[19] Lin Y C et al 2013 A new phenomenological constitutive model for hot tensile deformation behaviors of a typical Al–Cu–Mg alloy Mater. Des. (1980–2015) 52 118–27
[20] Lin Y C et al 2012 A phenomenological constitutive model for high temperature flow stress prediction of Al–Cu–Mg alloy Mater. Sci. Eng. A 534 654–62
[21] Fornladawit J, Uthaissangsuk V and Chounghong P 2014 Modeling of flow behavior of Ti–6Al–4V alloy at elevated temperatures Mater. Sci. Eng. A 599 212–22

17
Bai Q, Bai Q, Gao P F, Guo J, Han Y, Xiao X, Ma Z, Zhu Y, Fan X G and Yang H 2011 Internal-state-variable based self-consistent constitutive modeling for hot working of two-phase titanium alloys: a review Mater. Sci. Eng. A 528 8051–9

Bai Q et al 2015 A study of direct forging process for powder superalloys Mater. Sci. Eng. A 621 68–75

Bai Q et al 2012 An efficient closed-form method for determining interfacial heat transfer coefficient in metal forming Int. J. Mach. Tools Manuf 56 102–10

Zhang X, Zhao Y and Zeng W 2019 Constitutive relationship during isothermal compression of Ti-6Al-4V alloy sheet Mater. Lett. 255 126504

Sani S A et al 2018 Deformation behavior and microstructure evolution of titanium alloys with lamellar microstructure in hot working process: a review Journal of Materials Science & Technology 39 56–73

Bai Q et al 2020 A comparative study on Arrhenius-type constitutive equations and artificial neural network models for predicting high-temperature deformation behavior and processing map of 33Cr23Ni8Mn3N based on an artificial neural network Mater. Sci. Eng. A 753 134–141

Peng W et al 2013 Optimization the working parameters of as-forged 42CrMo steel by constitutive equation–dynamic recrystallization equation and processing maps Journal of Materials Research and Technology 2 689–96

Li Y et al 2015 Arrhenius-type constitutive model and dynamic recrystallization behavior of V–5Cr–5Ti alloy during hot compression Transactions of Nonferrous Metals Society of China 25 1041–6

Ji H et al 2020 Deformation behavior and microstructure evolution of titanium alloys considering microstructure evolution in thermomechanical processes J. Alloys Compd. 767 34–45

Guo J et al 2018 Unified modeling of work hardening and flow softening in two-phase titanium alloys considering microstructure evolution in thermomechanical processes J. Alloys Compd. 767 34–45

Babu B and Lindgren I 2013 Dislocation density based model for plastic deformation and globularization of Ti-6Al-4V Int. J. Plast. 50 94–108

Sun Y et al 2012 Intelligent method to develop constitutive relationship of Ti–6Al–2Zr–1Mo–1V alloy Transactions of Nonferrous Metals Society of China 22 1457–61

Fan X G and Yang H 2011 Internal-state-variable based self-consistent constitutive modeling for hot working of two-phase titanium alloys coupling microstructure evolution Int. J. Plast. 27 1833–52

Gao P et al 2017 Hot deformation behavior and microstructure evolution of TA15 titanium alloy with nonuniform microstructure Mater. Sci. Eng. A 689 243–51

Guo J et al 2018 Unified modeling of work hardening and flow softening in two-phase titanium alloys considering microstructure evolution in thermomechanical processes J. Alloys Compd. 767 34–45

Gao P F et al 2020 Microstructure and damage based constitutive modelling of hot deformation of titanium alloys J. Alloys Compd. 831 154851

Gao P et al 2020 Deformation behavior and microstructure evolution of titanium alloys with lamellar microstructure in hot working process: a review Journal of Materials Science & Technology 39 56–73

Bai Q et al 2015 A study of direct forging process for powder superalloys Mater. Sci. Eng. A 621 68–75

Bai Q et al 2012 An efficient closed-form method for determining interfacial heat transfer coefficient in metal forming Int. J. Mach. Tools Manuf 56 102–10

Zhang X, Zhao Y and Zeng W 2019 Constitutive relationship during isothermal compression of Ti-6Al-4V alloy sheet Mater. Lett. 255 126504

Sani S A et al 2018 Modeling of hot deformation behavior and prediction of flow stress in a magnesium alloy using constitutive equation and artificial neural network (ANN) model Journal of Magnesium and Alloys 6 134–44

Quan G et al 2011 Constitutive modeling for the dynamic recrystallization evolution of AZ80 magnesium alloy based on stress–strain data Mater. Sci. Eng. A 528 8051–9

Chithirai Pon Selvan M et al 2020 A mathematical modelling of Abrasive Waterjet Machining on Ti-6Al-4V using artificial neural network Materials Today: Proceedings 28 538–44

Cai Z et al 2020 An Investigation into the dynamic recrystallization (DRX) behavior and processing map of 33Cr23Ni8Mn3N based on an artificial neural network (ANN) Materials 13 1282

Peng W et al 2013 Comparative study on constitutive relationship of as-cast Ti60 titanium alloy during hot deformation based on Arrhenius-type and artificial neural network models Mater. Des. 51 95–104

Li Y et al 2015 Arrhenius-type constitutive model and dynamic recrystallization behavior of V–5Cr–5Ti alloy during hot compression Transactions of Nonferrous Metals Society of China 25 1889–900

Ji G et al 2011 A comparative study on Arrhenius-type constitutive model and artificial neural network model to predict high-temperature deformation behaviour in Aermet100 steel Mater. Sci. Eng. A 528 4774–82

Ma Z et al 2020 Constitutive equation and hot processing map of Mg-16Al magnesium alloy bars Materials 13 3107

Wei Z et al 2019 Hot tensile deformation mechanism and constitutive equation of AZ61Ce magnesium alloy sheets Mater. Res. Express 6 116517

Ji H et al 2020 Optimization the working parameters of as-forged 42CrMo steel by constitutive equation–dynamic recrystallization equation and processing maps Journal of Materials Research and Technology 9 7210–24

Li Y et al 2019 Comparative study on constitutive models for 21–4N heat resistant steel during high temperature deformation Materials 12 1893

Xiao X et al 2012 A comparative study on Arrhenius-type constitutive equations and artificial neural network model to predict high-temperature deformation behaviour in 12Cr3WV steel Comput. Mater. Sci. 62 227–34

Han Y et al 2013 A comparative study on constitutive relationship of as-cast 904L austenitic stainless steel during hot deformation based on Arrhenius-type and artificial neural network models Comput. Mater. Sci. 67 93–103

Zhu Y et al 2020 Dynamic behavior and modified artificial neural network model for predicting flow stress during hot deformation of Alloy 925 Materials Today Communications 25 101329