Research on Constitutive Relation of TC11 Titanium Alloy Based on PSO-LSSVM

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Abstract. In order to accurately predict the flow behavior of the TC11 titanium, the uniaxial compressive tests of TC11 titanium alloy were carried out by Gleelbe-1500 thermal simulator with the temperature in the range of 900~1050℃, and the strain rate of 0.1~10s\textsuperscript{-1}. Then the particle swarm optimization (PSO) was used to optimize the parameters of the least square support vector machine (LSSVM) model, and a high-temperature constitutive model of TC11 titanium alloy based on PSO-LSSVM was established, and the average relative error between the predicted value and the experimental value of the established constitutive model based on PSO-LSSVM is 1.51%, and the correlation coefficient is 0.997. The established constitutive model can accurately predict the high temperature flow behavior of TC11 titanium alloy. This indicated that a new method for establishing the constitutive model is provided.

1. Introduction
TC11 titanium alloy is one of the typical α+β phase titanium alloy, and the chemical composition (wt.%) is Ti-6.5Al-3.5Mo-1.5Zr-0.3Si. Because of its high specific strength, excellent thermal strength performance, corrosion resistance and other excellent performance, it is widely used in aerospace, defense and military fields [1], such as the turbine disks, blade disks and blades of TC11 titanium alloys which work in high temperature, high pressure, strong heat shock and high corrosion environments [2]. It is also considered to be a difficult-to-deform metal because of its high strength and high deformation resistance at room temperature. According to the law of elevated temperatures can bring the softening effect during metal plastic forming, the parts of TC11 titanium alloy are generally obtained by thermoforming. However, the corresponding temperature effect also brings about the evolution of complex thermal coupling and phase change, dynamic recrystallization and other micro-organizations. The above reasons lead to many problems in the thermoplastic forming process of TC11 titanium alloy, such as the forming performances are sensitive to temperature and forming process parameters, result in the forming mechanism is complex. Therefore, the study and prediction of TC11 titanium alloy flow behavior is the key to obtain a reasonable forming process.

At present, the researchers have done a lot of research on high temperature constitutive models that characterize and predict the TC11 titanium alloy flow behavior. Such as the physical constitutive models (Arrhenius model [3], Zerilli-Armstrong model [4] and dislocation density based constitutive model [5], etc.), the phenomenological constitutive models (Johnson-Cook model [6], Khan-Huang-Liang (KHL) model [7], etc.) and other methods of constitutive models such as artificial neural networks [8]. All of
the above constitutive models have obtained a good prediction effect. At present, intelligent algorithm as a prediction method of big data well in application. LSSVM is a kind of intelligent algorithm which is widely used in data analysis, regression fitting and linear classification. Its essence is to establish the optimal decision function through the mapping relationship between the input and output spaces, and mapping the data to high-dimensional space in order to achieve linear separation through the kernel function \[9,10\]. As the application of using LSSVM to establish constitutive model, only Mo et al. used fruit fly optimization algorithm (FOA) to optimize the parameters of LSSVM model, and established a FOA-LSSVM-based constitutive prediction model of 9Ni steel with good prediction accuracy \[11\].

As an exploration of the establishment of constitutive model based on intelligent algorithm, in this study, the PSO algorithm was used to optimize the LSSVM model parameters. A high temperature constitutive model of TC11 titanium alloy based on PSO-LSSVM with high prediction accuracy is established. It provides theoretical support for the study of thermoplastic forming performance of TC11 titanium alloy, and also provides a new method for the prediction of flow behavior of metal material.

2. Experiments of TC11 titanium alloy

The TC11 titanium alloy of composition (wt.%) Ti-6.5Al-3.5Mo-1.5Zr-0.3Si was researched in this study, and the experiments were performed on the Gleeble-1500 thermal simulation machine. The samples were machined by wire cutting with a diameter of 8mm and a height of 12mm. The TC11 titanium alloy \((\alpha+\beta)/\beta\) phase transition temperature is around 1008\(^\circ\)C \[12\], and recrystallization temperature range is 900~980\(^\circ\)C. Therefore, considering the two temperature ranges, the experimental temperatures were selected as 900\(^\circ\)C, 950\(^\circ\)C, 1000\(^\circ\)C and 1050\(^\circ\)C, the strain rates were 0.1s\(^{-1}\), 1s\(^{-1}\) and 10s\(^{-1}\), each sample deformation was not less than 60% of the height. In order to avoid uneven heating of the sample due to the low thermal conductivity of the titanium alloy, The heating scheme was designed as show in Figure 1, rapidly heated to the experimental temperature at a heating rate of 10 \(^\circ\)C/s, held for 5 minutes to equalize the temperature of the sample, and then started to compress. After the sample deformation reached, stopped the compression and rapidly water quench the sample to retain its high temperature deformation microstructure for the future study of the microstructure evolution.

![Figure 1. Heating scheme of samples of uniaxial compression.](image)

3. TC11 titanium alloy flow behavior analysis

The Figure 2 shows the true stress-true strain curves of TC11 titanium alloy at the temperatures of 900~1050\(^\circ\)C and the strain rates of 0.1~10s\(^{-1}\). From the Figure 2, it can be observed that under the action of temperature, the flow stress curves of TC11 titanium alloy present three distinct stages. They are work hardening (WH), dynamic recovery (DRV), and dynamic recrystallization (DRX) softening dominates, respectively. In the initial stage of deformation, WH predominates, which shows that the flow stress increases sharply with the increase of strain. The reason for this stage is that the dislocations multiply rapidly with the deformation of the material, resulting in dislocation pile-up, difficult to deform and increased deformation resistance. Then velocity of the flow stress curve increases slowly before reaching the peak and slowly decreases after peak. At this stage dominates by the DRV. This is mainly due to the amount of deformation increases, the dislocation annihilation caused by DRV in the sample is greater than the proliferation of dislocations. In this stage the softening effect is presented. After the above two stages, there is a trend that the flow stresses show a steady or slow decline with the increase
of strain. This is mainly due to the dominant position of DRX. In this stage, WH, DRV and DRX are coexisting and competing with each other, but the softening caused by DRX dominates, and the stress decreases steadily or slowly with strain.

From the Figure 2, It can be observed that under a certain strain rate condition, when the temperature increases, the deformation resistance of the material decreases, and the metal plasticity increases, so that the flow stress decreases. This is because the increasing of temperate bring four main effects. Firstly, as the deformation temperature increases, the thermal activation of the material and the average kinetic energy of the atoms increasing, at the same time the critical shear stress for the slip of the crystal decreasing. Secondly, as the temperature increases, DRX and DRV are also easier to perform, which reduces the dislocation density and produces softening effect for plastic deformation. Thirdly, as the temperature increases, the diffusion creep effect is strengthened, which not only plays an active role in plastic deformation, but also coordinated deformation, result in the plasticity of metal is enhanced. In addition, the increasing of the temperature can enhance the phase transformation which lead to the proportion of the β-phase with good plasticity increases, result in the deformation resistance to decrease.

(a) \( \dot{\varepsilon} = 0.1 / s \)

(b) \( \dot{\varepsilon} = 1 / s \)

(c) \( \dot{\varepsilon} = 10 / s \)

Figure 2. True stress-true strain curve of TC11 titanium alloy.

4. Construction and analysis of constitutive model based on PSO-LSSVM

The essence of LSSVM is to convert the samples from \( R^n \) space to the feature space through the method of nonlinear mapping, that is, convert the nonlinear regression problem to a linear regression problem of high-dimensional feature space, and construct a linear decision function in the feature space. For a given training sample set \((x_i, y_i), i = 1, 2, \cdots, N, x_i \in R^n, y_i \in R, x_i \) is the input vector and \( y_i \) is the output vector. According to the structure of high-temperature constitutive model of \( y_i = f(T, \varepsilon, \dot{\varepsilon}) \), the input vector of \( x_i \) is defined as temperature \( T \), strain \( \varepsilon \) and strain rate \( \dot{\varepsilon} \), and the output vector of \( y_i \) is defined as stress \( \sigma \). According to the basic theory of LSSVM, the following optimization problems are defined as:

\[
\min_{w, b, \lambda} J(w, \lambda) = \frac{1}{2} \mu w^T w + \frac{1}{2} c \sum_{i=1}^{N} \lambda_i^2 \\
\text{s.t.:} \quad y_i = w^T \phi(x_i) + b + \lambda_i \quad i = 1, 2, 3 \cdots N
\]

In equation (1), \( \phi(x_i) \) is a non-linear transformation mapping function; \( w \) is a weight vector; \( b \) is an offset; \( \lambda_i \) is a relaxation factor, \( \lambda_i \in R^+ \); \( c \) is a penalty parameter, \( c > 0, c \in N \), it’s purpose is to comprehensively consider the empirical risk and confidence range; \( \mu \) is an adjustable parameter. In order to solve the above functions, the following Lagrange multiplier was introduce.

\[
L(w, b, \lambda, \alpha) = J(w, \lambda) - \sum_{i=1}^{N} \alpha_i (w^T \phi(x_i) + b + \lambda_i - y_i)
\]

In equation (2), \( \alpha_i \) is the Lagrange multiplier. The partial derivative of equation (2) can be obtained as equation (3).
Eliminating the variables of w and $\lambda_i$ of equation (3), the equation (4) can be got.

$$\frac{\partial L}{\partial w} = 0 \rightarrow w = \sum_{i=1}^{N} \alpha_i \phi(x_i)$$

$$\frac{\partial L}{\partial b} = 0 \rightarrow \sum_{i=1}^{N} \alpha_i = 0$$

$$\frac{\partial L}{\partial \lambda_i} = 0 \rightarrow \alpha_i = c \lambda_i$$

$$\frac{\partial L}{\partial \alpha_i} = 0 \rightarrow w^T \phi(x_i) + b + \lambda_i - y_i = 0$$

(3)

In equation (4), $\Omega = \phi(x_i)^T \phi(x_j) = K(x_i, x_j)$, $e = [1, \ldots, 1]^T$, $K(x_i, x_j)$ is a kernel function that meets Mercer's conditions; $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_N]^T$, $y = [y_1, y_2, \ldots, y_N]^T$ and $E$ is the unit matrix of order $N$.

The regression model of TC11 high-temperature constitutive relationship based on LSSVM can be obtained as the following equation (5) when the $\alpha$ and $b$ of equation (4) were solved.

$$f(x) = \sum_{i=1}^{N} \alpha_i K(x_i, x_j) + b$$

(5)

From the equation (5), It can be observed that the kernel function $K(x_i, x_j)$ is the key to the LSSVM prediction algorithm, which can directly affect the prediction performance, and Linear kernel function of $K(x_i, x_j) = x_i^T x_j$, Polynomial kernel function of $K(x_i, x_j) = (\gamma x_i^T x_j + r)^p$, $\gamma > 0$ and Radial Basis Function (RBF) in Gaussian kernel function of $K(x_i, x_j) = \exp\left(-\frac{||x_i - x_j||^2}{2\sigma^2}\right)$ ($\sigma$ is the width of the kernel function) are the commonest kernel functions. And the Gaussian kernel function has better learning performance in practical pattern recognition and regression prediction, and the generalization ability of the RBF kernel function is the best. Therefore, in this paper, the RBF kernel function was selected as the kernel function.

In the LSSVM prediction model, the value of penalty parameters of $c$ and the width of kernel function of $\sigma$ will have great influence on the model's learning and generalization ability. Therefore, the optimization of these two parameters can balance the generalization ability and fitting accuracy of the regression function. The traditional way to obtain the optimal value of the two parameters is trial and error, manually. Result in different training samples obtain different values of $c$ and $\sigma$, and the prediction accuracy are very bad.

Particle Swarm Optimization (PSO) is from bird foraging behavior, its essence is the optimal solution can be obtained through collaboration and information sharing [16]. The PSO algorithm is used to automatically optimize the parameters of the LSSVM prediction model, therefore, it can reduce manual intervention. The update method of particle swarm speed and position of PSO algorithm are shown in equation (6).

$$\min f(c, \sigma) = \frac{1}{n} \sum_{i=1}^{n} \left| T_i - Y_i \right|$$

s.t. $c \in [c_{\text{min}}, c_{\text{max}}], \sigma \in [\sigma_{\text{min}}, \sigma_{\text{max}}]$  

(6)

In equation (6), $Y_i$ and $T_i$ are the $i$-th predicted value and actual value, respectively; $n$ is the number of predicted samples. The optimization process of parameter of LSSVM constitutive model by PSO algorithm is shown in Figure 3.
Sample pretreatment

Initialize the particle position and velocity in the population, set the search range of \( c \) and \( \sigma \)

Calculate the fitness value of each particle

Update particle position and velocity

Meet the optimization conditions

Yes

No

Update particle individual optimal and global optimal

Output the optimal combination \((c, \sigma)\), establish the LSSVM model

Figure 3. The optimization process of parameters of \( c \) and \( \sigma \)

According to the structure of high-temperature constitutive model, the three factors of temperature \( T \), strain rate \( \dot{\varepsilon} \) and strain \( \varepsilon \) as the input of the model, and the flow stress \( \sigma \) as the output. The selection of the training samples and the test samples are shown in Table 1, where ‘Test’ represents the test sample and ‘Train’ represents the train sample. The comparison between the test values of the samples in the uniaxial compression of TC11 titanium alloy and the predicted values of the high-temperature constitutive model based on PSO-LSSVM are shown in Figure 4. From Figure 4, it can be observed that the predicted values are in good agreement with the test values. It indicate that the high-temperature constitutive model based on PSO-LSSVM can well predict the stress and strain under different temperatures and strain rates, and the whole dynamic mechanical behavior of TC11 titanium alloy can be accurately described.

Table 1. The selection of TC11 titanium alloy samples.

| Strain rate/s\(^{-1}\) | Temperature/°C | 900 | 950 |
|------------------------|----------------|-----|-----|
|                        | 0.1            | Train | Test  |
|                        | 1              | Test  | Train |
|                        | 10             | Train | Test  |

![Test values](image1.png) ![Predicted values](image2.png)

(a) \( \dot{\varepsilon} = 0.1 / s \)  
(b) \( \dot{\varepsilon} = 1 / s \)  
(c) \( \dot{\varepsilon} = 10 / s \)

Figure 4. Comparison of test values and predicted values of LSSVM model.

In order to quantitatively describe the accuracy of the constitutive model of TC11 titanium alloy based on PSO-LSSVM, the average relative error \( MRE \) and correlation \( R \) were used to evaluate the prediction effect of the established constitutive model. The results show that the maximum average relative error is 4.68%, the minimum average relative error is 0.4%, the total average relative error is 1.51%, and the correlation coefficients \( R \) are all more than 0.98. This shows that the constitutive model based on PSO-LSSVM has good prediction accuracy.

5. Conclusion
The true stress-true strain curve of TC11 titanium alloy at a temperature of 900~1050℃ and a strain rate of 0.1~10s⁻¹ decreases with increasing temperature and decreasing strain rate, and it is sensitive to deformation temperature and strain rate.

(2) The essence of constitutive model based on PSO-LSSVM is the mapping relationship between input and output, and as a way of machine learning, which solves the nonlinear problem of model construction well and can obtain results with high prediction accuracy, moreover, the prediction accuracy will increases with the number of experimental samples increasing.

(3) The average relative error of the high-temperature constitutive model of the TC11 titanium alloy based on PSO-LSSVM reached 1.51%, which has a high prediction accuracy. It provides a new method for the prediction of the flow behavior of metal materials, and the application scope of SVM is extended to the field of intelligent prediction of material properties.

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