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ARTICLE

Internal-Atate-Variable Based Constitutive Modeling for Near β Ti-7Mo-3Al-3Nb-3Cr Alloy during Hot Deformation Process

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Abstract: A constitutive model using dislocation density rate as an internal state variable has been proposed for hot working of near β titanium alloy. In the constitutive equations, the effects of solution strengthening and dislocation interaction on flow stress were included. Based on the internal-state-variable model, the constitutive relationship of a new near β titanium alloy Ti-7Mo-3Al-3Nb-3Cr (Ti-7333) for high temperature deformation was established. And the model parameters were obtained by the genetic algorithm based objective optimization method. Calculating results show that the average relative difference between the calculated flow stress and the experimental flow stress is about 7.2%. The developed internal-state-variable based constitutive model can efficiently characterize the flow behavior of Ti-7333 alloy.

Key words: near β titanium alloy; hot deformation; constitutive model; flow stress

Near β titanium alloys, such as Ti-10V-2Fe-3Al (Ti-1023) and Ti-5Al-5Mo-5V-3Cr (Ti-5553), have been used for commercial applications in high strength structural components, such as the landing gear assemblies of large airframes, thanks to their advantages of workability and good combination of high strength and ductility [1]. However, up to now, the processing window of the near β Ti alloys has not been clearly understood since the discovery of the alloys due to their inherent complexity, multicomponent and metastability, as well as the microstructure sensitivity [2-5]. For the hot deformation ability, the flow stress of near β titanium alloys are extremely sensitive to processing parameters, such as strain, strain rate and deformation temperature. Therefore, it's necessary to establish an accurate constitutive relationship considering the main processing parameters, in order to understand the deformation behavior and optimize the deformation process.

To date, a lot of work have been done on modeling of hot deformation constitutive relationship. Various approaches have been applied, including the empirical methods [6-8], advanced statistical methods [9-11], and physically-based internal state variable methods [12-19]. Among these approaches, the internal state variable methods have been growing in its influence on modeling the constitutive relationship since the past decade [12], relying on its advantage of describing the underlying mechanism in terms of a small number of internal state variables. It is critical to select the internal state variables for these constitutive models. It is well known that the deformation behavior and mechanical properties of material are affected by microstructural parameters. Therefore, some microstructural state variables have been selected to consider in the constitutive model. In order to modeling the microstructure evolution caused by dynamic recrystallization and grain growth during hot deformation, Busso [13] proposed a viscoplastic constitutive model relying on scalar internal state variables including mean

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dislocation spacing and average grain size. Roters et al. [14] proposed a working-hardening model for heterogeneous cell-forming alloys based on the evolution of mobile dislocations, immobile dislocations in the cell interiors and immobile dislocations in the cell walls, so that the dependence of flow stress on microstructure can be considered. A set of mechanism-based unified viscoplastic constitutive equations for multi-pass hot rolling of C-Mn steel were developed by Lin et al. [15], using dislocation density, recrystallization and grain size as the internal state variables. Many efforts have been done on modeling the high temperature deformation behavior of titanium alloys with this method in recent years, and it has been used in the high temperature deformation of two-phase Ti-6Al-4V alloy [16,17], near α titanium alloy IMI834 [17] and TA15 [18], and β titanium alloy Ti-10V-4.5Fe-1.5Al [19].

A newly developed near β titanium alloy, named Ti-7Mo-3Al-3Nb-3Cr (Ti-7333) was investigated in the present paper, which has promising application in aerospace industry due to its excellent property (with tensile strength ~1350 MPa and strain ~8%). The isothermal compression of Ti-7333 alloy has been conducted at different hot working temperatures, strain rates and strains to characterize the flow deformation process. Based on the above tests, a constitutive model using dislocation density rate as internal state variable has been applied to establish the constitutive relationship in the hot deformation process of Ti-7333 alloy.

1 Experiment

The nominal composition of Ti-7333 alloy is Ti-7Mo-3Al-3Nb-3Cr (wt%). The β transus temperature of the alloy, as measured by metallographic phase disappearing techniques, is approximately 1123 K. The isothermal hot compression tests were carried out on Gleeble-3800 thermal and mechanical simulator using cylindrical samples with 12 mm in height and 8 mm in diameter, at the deformation temperatures of 1068, 1093, 1118, 1143, 1193, 1243 K, strain rate of 0.001, 0.01, 0.1 and 1 s^{-1}, and a height reduction of 70%. The specimens were heated to applied temperature at a rate of 25 K/min and then held for 2 min before the commencement of deformation to ensure homogeneous temperature fields. In order to reduce friction and maintain uniform deformation, two pieces of thin tantalum sheets were placed between the compression specimen and the die. The strain-stress data were recorded automatically in isothermal compression. The original microstructure of Ti-7333 before hot compression is shown in Fig.1a, which consisted of a single β phase. The optical microstructures after deformation under different conditions are shown in Fig.1b~1d. After deformation at the temperature of 1093 K and strain rate of 0.001 s^{-1} (Fig.1b), the initial grains are elongated perpendicularly to the compression axis and few recrystallized grains can be observed. The microstructure deformed at the temperature of 1143 K and strain rate of 0.1 s^{-1} (Fig.1c) is similar to that in Fig.1b, while the serrated boundaries are more obvious. At higher deformation temperature of 1193 K (Fig.1d), more recrystallized grains on grain boundaries can be observed, where there are still a number of elongated grains. Fig.2 shows the TEM image of Ti-7333 after deformation under the same conditions with that in Fig.1b, from which it is clear to see the dislocation structures formed during deformation. The arrangements of dislocation line at different regions vary, for the activated slip systems are different.

2 Constitutive Model

2.1 Internal state variable constitutive modeling for an individual phase

The flow stress σ measured in a polycrystal in terms of the critical resolved shear stress τ in the constituent single crystals can be expressed using a "Taylor factor" M [20]:

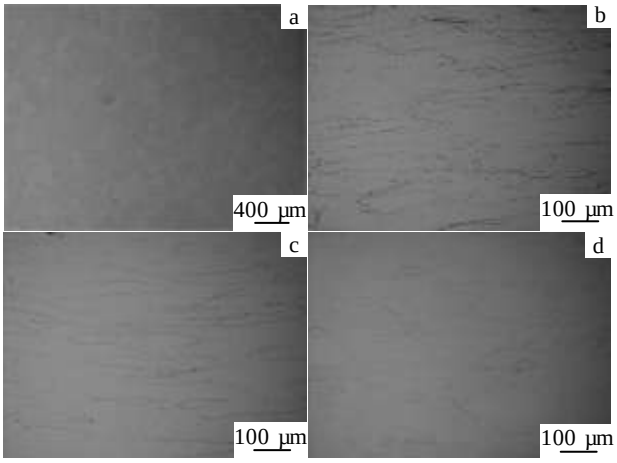

Fig.1 Optical microstructures of Ti-7333 alloy: (a) original undeformed; (b) deformed at 1093 K, 0.001 s^{-1}; (c) deformed at 1143 K, 0.1 s^{-1}; (d) deformed at 1193 K, 0.01 s^{-1}

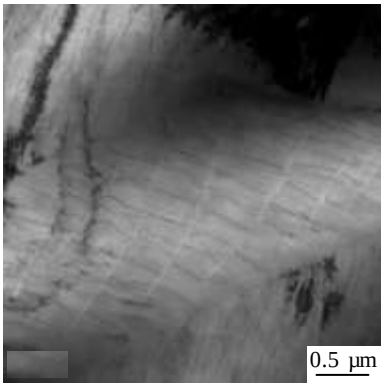

Fig.2 TEM image of Ti-7333 alloy deformed at 1093 K, 0.001 s^{-1}

$$\sigma = M\tau \quad (1)$$

where, M=3.06 for most of the engineering materials [21].

For a rate-dependent material, the critical resolved shear stress can be expressed in the following power law form[17]:

$$\frac{\dot{\gamma}}{\dot{\gamma}_0} = \left(\frac{\tau}{g}\right)^{1/m} \quad (2)$$

where, $\dot{\gamma} = M\dot{\varepsilon}$ is the shear rate, $\dot{\gamma}_0$ is the reference shear rate, g is the slip resistance, and m is the strain rate sensitivity parameter. $\dot{\gamma}_0$ is set to be 3×10^{-3} s^{-1} in the present work. The slip resistance is related to the dislocation structure and microstructure, which can be expressed as follows:

$$g = g_0 + g_f + g_{HP} \quad (3)$$

where, g_0 is the initial slip resistance, g_f represents the working hardening due to dislocation interactions, and g_{HP} represents the barrier effect of grain boundaries. Essentially g_0 is due to the interaction of dislocations with short-range obstacles which depends on temperature, strain rate and solute density of alloying elements [22], including the Peierls stress, point defects such as vacancies and self-interstitials, and other dislocations which intersect the slip plane [23]. The temperature and solution dependence of initial slip resistance can be expressed as follows [24]:

$$g_0 = K\exp(-T/B) \quad (4)$$

where, K is the strength coefficient which links to the solution density of the alloying elements, and B is a material constant.

The slip resistance due to dislocation interactions scales as the square root of average dislocation density ρ can be written using the Taylor relation:

$$g_f = \chi\mu(T)b\sqrt{\rho} \quad (5)$$

where, b is the Burgers vector magnitude (2.86×10^{-10}m), and χ is a material constant. $\mu(T)$ is the temperature-dependent shear modulus, and can be expressed as [25]:

$$\mu(T) = \mu_0 - \frac{e}{\exp(T_r/T)-1} \quad (6)$$

where, e and T_r are the material constants.

The barrier effect of grain boundaries is generally modeled via a Hall-Petch relationship:

$$g_{HP} = K_{HP}d^{-1/2} \quad (7)$$

where, K_{HP} is the Hall-Petch coefficient, and d is the grain size.

During the hot working process, the dislocation density ρ of metals and alloys depends on two competing processes, work hardening and dynamic softening. Plastic deformation leads to the accumulation of dislocations, while dynamic recovery (DRV) annihilates dislocations. Kocks and Mecking [26] developed a phenomenological model to predict the variation of dislocation density with strain which can be expressed as:

$$\frac{d\rho}{d\gamma} = k_1\sqrt{\rho} - k_2\rho \quad (8)$$

where, ρ is the average dislocation density, γ is the plastic strain, k_1 is a material constant characterized the process of athermal dislocation storage. The parameter k_2 describes a thermally activated process of dynamic recovery by dislocation cross-slip or dislocation climb which can be expressed as a function of shear rate and temperature[27]:

$$k_2 = k_{20}\left[\dot{\gamma}\exp(Q_{act}/RT)\right]^{-1/n} \quad (9)$$

where, Q_{act} is the activation energy, R is the gas constant, k_{20} and n are material constants.

2.2 Internal state variable constitutive modeling for near β titanium alloy

For the near β titanium alloy, the globular α phase with small sizes may precipitate from the β matrix when the deformation is taken in (α+β) phase region. However, it has been reported that the precipitation of small globular α phase has little effect on the flow behavior of the alloy [3]. Therefore, only the effect of single β phase on flow stress is to be considered in the constitutive modeling for near β titanium alloy in the present work. The strength coefficient (K) in Eq.(4) can be expressed in terms of alloying elements. Semiatin et al [28] proposed to use equivalent vanadium content, V_{eq}, for the β phase to determine the strength coefficients, and Fan et al.[17] took the expression as follows:

$$\log_{10}(K^\beta/K_0^\beta) = 0.813\log_{10}V_{eq} \quad (10)$$

where, K^β is strength coefficient of β phase, and K_0^β is a referential strength coefficient. Vo et al. [29] suggested that V_{eq} can be calculated by:

$$V_{eq} = V + 0.27Al + 0Sn + 2Mo + 0.30Zr + Cr + 0.4Nb + 13Si \quad (11)$$

where, the elements are measured in wt%. The interstitial elements, O, H and N, are neglected as the strengthening effect of these elements deteriorated rapidly at hot working temperatures.

Because the Hall-Petch phenomena confirmed don't exist in the β phase [30], the constitutive model of near β titanium alloy can be expressed as follows:

$$\begin{aligned}
&\sigma = M\tau\\
&\frac{\dot{\gamma}}{\dot{\gamma}_0} = \left(\frac{\tau}{g}\right)^{1/m}\\
&g = g_0 + g_f\\
&g_0 = K^\beta\exp(-T/B)\\
&\log_{10}(K^\beta/K_0^\beta) = 0.813\log_{10}V_{eq}\\
&g_f = \chi\mu(T)b\sqrt{\rho}\\
&\mu(T) = 49.02 - \frac{5.821}{\exp(181/T)-1}\\
&\frac{d\rho}{d\gamma} = k_1\sqrt{\rho} - k_2\rho\\
&k_2 = k_{20}\left[\dot{\gamma}\exp(Q_{act}/RT)\right]^{-1/n}
\end{aligned} \quad (12)$$

where, Q_{act} is 20 kJ/mol [16]. Besides, the V_{eq} of Ti-7333

alloy calculated by Eq.(11) is 19.31.

3 Constitutive Model of Ti-7333 Titanium Alloy

3.1 Identification of material constants

A genetic algorithm (GA) based objective optimization method developed by Lin and Yang [31] is employed to determine the material parameters. The GA method is a stochastic search method based on some phenomena of evolution and genetics, such as natural selection, cross and mutation. It's an excellent optimization approach to estimate material parameters for complicated and nonlinear constitutive models. Compared to the traditional methods based on gradient search, the GA method provides a better chance to search for the global minimum in the multimodal distribution space.

In the present work, 264 experimental data of the Ti-7333 alloy at deformation temperatures of 1068~1243 K and strain rates of 0.001~1 s^{-1} were chosen to determine the material constants in the constitutive model. The domains of the material constants are listed in Table 1. Moreover, the optimized material constants using the GA based objective optimization technique are listed in Table 2.

3.2 Calculating results

The effect of processing parameters on predicted flow stress is shown in Fig.3. It can be seen from the smooth surface that the predicted flow stress rise with the strain rate increases, while the strain has little effect on the flow stress. It indicates that the evolution law predicted by the internal-state-variable based model is consistent with the experimental results.

Fig.4 shows the calculated and experimental flow stress simultaneously. The solid curve represents the experimental stress-strain curve, and the symbols represent the data calculated by the present constitutive equations using the optimized constants listed in Table 2. As shown in Fig.4, the average relative error between the experimental and the computed flow stress is about 7.2%. Therefore the constitutive model can efficiently characterize the flow behavior of the alloy.

Table 1 Domains of the material constants in the constitutive model of Ti-7333 titanium alloy

$100 \le k_1 \le 1000$	$1 \le k_{20} \le 1000$	$1 \le n \le 200$	$1 \le B \le 1000$
$0.01 \le \chi \le 1$	$0.01 \le m \le 1$	$1 \le K_0^{\beta} \le 150$	

Table 2 Optimized material constants for the constitutive model of Ti-7333 titanium alloy

k_1	k_{20}	n	B	χ	m	K_0^{β}
371.2569	940.7045	15.6720	279.8472	0.7391	0.1911	92.7152

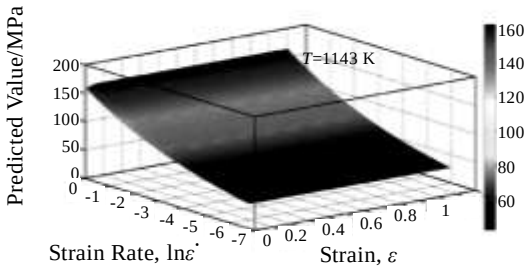

Fig.3 Effects of the different variables on the predicted results

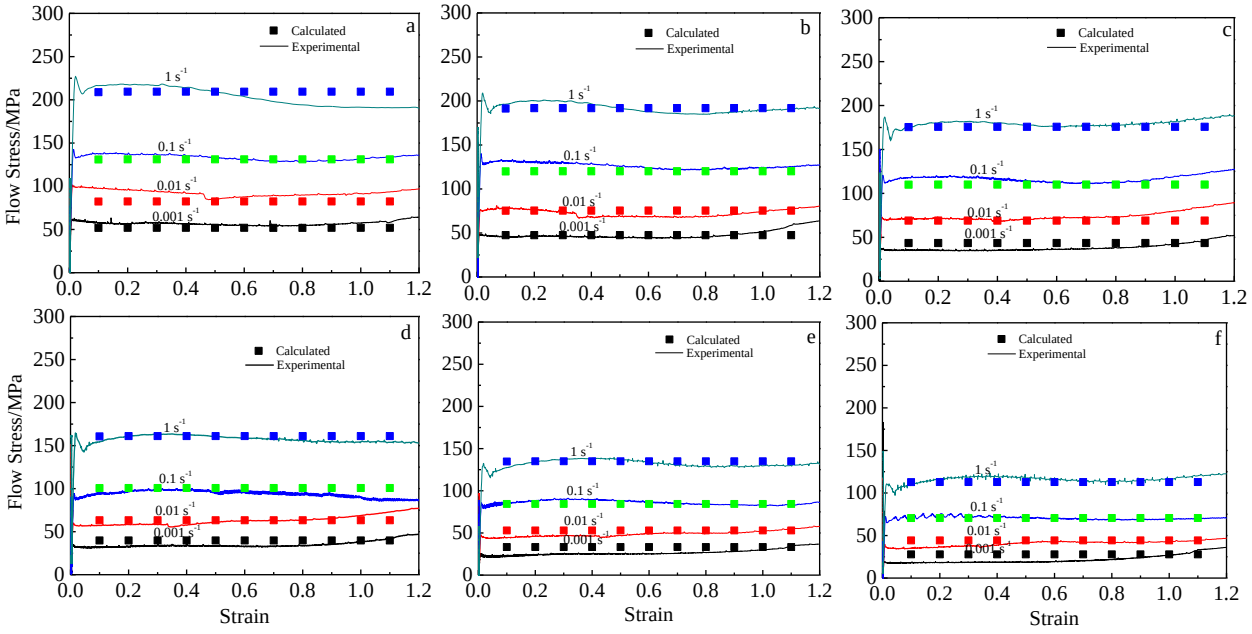

Fig.4 Comparison of the calculated flow stress and the experimental flow stress at different temperatures: (a) 1068 K, (b) 1093 K, (c) 1118 K, (d) 1143 K, (e) 1193, and (f) 1243 K

4 Summary

In the present study, a constitutive model using dislocation density rate as an internal state variable has been proposed for hot working of near β titanium alloy by considering the underlying deformation mechanism. The developed constitutive model considers the effects of solution strengthening and dislocation interaction at the same time. Then, the constitutive relationship of a new near β titanium alloy Ti-7333 during hot deformation process has been established using the internal-state-variable model. Model parameters are determined by the GA based objective optimization method. The average relative difference between the calculated flow stress and the experimental flow stress is about 7.2%, indicating that the constitutive model can efficiently characterize the flow behavior of this kind of alloy.

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基于内变量的近β Ti-7Mo-3Al-3Nb-3Cr 钛合金热变形本构模型

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摘　要：针对近β钛合金提出了一种以位错密度变化率作为内变量的热变形本构模型，该模型同时考虑了溶质元素的固溶强化作用和位错之间的交互作用对流变应力的影响。将该模型应用于一种新型近β钛合金Ti-7Mo-3Al-3Nb-3Cr (Ti-7333)，并采用基于目标优化的遗传算法定量确定了Ti-7333合金的本构模型参数。模型计算的结果表明，利用该热变形本构模型计算出的流变应力与实验数据间的平均相对误差为7.2%，采用基于位错密度变化率的近β钛合金本构模型能够有效地表征Ti-7333合金的流变行为。

关键词：近β钛合金；热变形；本构模型；流变应力

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