Constitutive model and microstructural evolution of hot deformation of investment-cast Ti-4Al-0.005B alloy

Zong Xuewen1,2,∗, Zhang Jian1,2,∗, and Lu Bingheng1

1 School of Mechanical Engineering, Xi’an University of Science and Technology, Xi’an, People’s Republic of China
2 Institute of Additive Manufacturing Technology, Xi’an University of Science and Technology, Xi’an, People’s Republic of China

∗ Authors to whom any correspondence should be addressed.
E-mail: zjvan@qq.com

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Abstract
Hot compression tests of investment-cast Ti-4Al-0.005B (TA5) alloy were conducted over a wide temperature range of 750 °C–850 °C at strain rates of 0.01–1 s⁻¹. Based on the flow stress curve and dynamic material model, a constitutive equation is established. The thermal deformation behavior and microstructural evolution of investment-cast TA5 alloy at high temperatures is systematically analyzed. The results show that the Zener–Hollomon parameter’s formula calculates the apparent activation energy of TA5 as 469893 J · mol⁻¹, α is 0.0032, and the apparent value of n is 12.34. The peak flow stress decreases with increasing deformation temperature and decreasing strain rate. At high strain rates, the grains appear nonuniform and exhibit microcracks. Thus, high temperature and low-strain rate are beneficial to the occurrence of slip. Under these conditions, grain boundaries can sufficiently migrate, the microstructure remains compact and stable, and dynamic recrystallization grains distribution is more uniform. Therefore, the high-temperature and low-strain zone is most suitable for processing TA5 alloy.

Introduction

Because of its high strength, good corrosion resistance, and excellent impact resistance, titanium alloys are widely used in aerospace, shipbuilding, and other fields [1–3]. TA5 is an all-α titanium alloy. It exhibits medium strength, high plasticity, and good thermal stability. It is also widely used in shipbuilding because of its excellent casting and welding properties [4, 5].

The constitutive model of a metal alloy is the key to predicting its deformation behavior during processing [6]. Many researchers have studied the hot deformation behavior of titanium alloys by constructing constitutive models in the form of equations. A constitutive model can predict the dynamic recovery (DRV) and dynamic recrystallization (DRX) of titanium alloys during high-temperature deformation. In practical applications, the hot deformation behavior and microstructure of a titanium alloy significantly affect the product quality. In general, thermal deformation behavior is primarily affected by temperature and strain rate, among other factors [7–11]. Among these, strain rate is an important process parameter affecting the hot deformation behavior of titanium alloys. Bobbili et al [12] conducted hot compression tests of Ti-10-2-3 alloy over a temperature range of 900 °C–1050 °C and strain rates of 0.001–1 s⁻¹. They found that the flow stress of titanium alloy was indeed significantly influenced by the temperature, strain, and strain rate. Sadeghpour et al [13] studied the effect of strain on the hot deformation behavior of β-Ti alloys at strain rates of 7 × 10⁻⁵–7 × 10⁻² s⁻¹ to compress the specimen. They found that yield strength of the alloys increased while its sensitivity to strain rate decreased as β phase stability increased. Hot deformation behavior has been studied not only for traditionally processed titanium alloys but also for additive-manufactured titanium alloys. Saboori et al [14] studied the hot working behavior of Ti6Al4V alloy over a temperature range of 1000 °C–1200 °C and strain rates of 0.001–1 s⁻¹. Their results indicated that the porosity of electron beam-melted parts significantly decreased, whereas the flow

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softening curve of the single β zone remained approximately constant. However, with the exceptions of common Ti6Al4V and β-Ti alloys, a constitutive model has not been developed to predict the work hardening before peak strain and flow softening behavior of most titanium alloys. Little research has been published on TA5 titanium alloy, and no study has yet investigated its hot deformation behavior. Therefore, we aim to establish a constitutive model for TA5 titanium alloy and study its hot deformation behavior and microstructural evolution.

The present study analyzes the hot deformation behavior of TA5 alloy during investment casting. The effects of deformation temperature and strain rate on the flow stress in TA5 alloy were analyzed, and a constitutive equation was constructed according to the peak flow stress in the true stress–true strain curve. The microstructures of deformed samples were characterized, and the effects of temperature and strain rate on the mechanisms of the microstructural evolution of TA5 alloy were systematically determined. This investigation aimed to provide evidence-based support for the theoretical design of a hot deformation forming process for TA5 alloy.

**Experimental procedure**

The experimental material was investment casting TA5 alloy provided by Luoyang Shuangrui Precision Casting Titanium Co., Ltd., a subsidiary company of the 725 Research Institute. To improve the material properties and reduce internal defects, the original test bar was hot-isostatic-pressed (HIP) and annealed. The process parameters for HIP were 920 °C, 130 MPa, and 2 h, whereas the process parameters for the heat treatment were 5 °C·min⁻¹, increasing the temperature to 800 °C, and holding at that temperature for 1 h. The test bar was wire-cut into 8 × 12 mm² compressed samples. The hot compression experiment was conducted on a Gleeble-3500 thermal simulation testing machine whose deformation conditions included three deformation temperatures (750 °C, 800 °C, and 850 °C) and three strain rates (0.01, 0.1, and 1 s⁻¹). As shown in figure 1, the single-pass compression strain was 60%. The sample was heated to the preset deformation temperature at a rate of 10 °C·s⁻¹, kept at that temperature for 5 min while compressed in a vacuum environment, and thereafter immediately quenched with water to retain the hot deformed structure. Each sample was cut into two halves along the compression direction. This was followed by mechanical grinding and polishing. Subsequently, etching was performed with an etching solution of 10% HF + 40% HNO₃ + 50% H₂O, and the microstructure under thermal deformation was characterized by optical microscopy.

**Results and discussion**

**Flow stress curve**

The process of hot compression is divided into three stages—work hardening, softening, and stabilization [15]. In the first stage, the density of internal defects such as dislocations increases with increasing strain and increase in applied stress leads to enhanced dislocation movement per unit time and increased resistance to macroscopic deformation. When the dislocation density reaches a certain threshold, grains with higher distortion energy
recover and recrystallize. At that point, the softening effect cannot balance the hot working effect. With further increase in thermal deformation, dislocation density increases, distorsion energy gradually increases and DRX occurs; thereafter, the recrystallization softening effect exceeds the work hardening effect, and the flow stress slowly decreases with increasing strain. Furthermore, the softening and work hardening effects are in a state of dynamic equilibrium that characterizes the stable deformation stage.

Figure 2 shows the true stress-strain curves of TA5 alloy samples under various deformation conditions. Work hardening, DRV, and DRX occurred during hot working deformation. Work hardening appeared at the initial stages of compression deformation. The flow stress sharply increased with increasing strain, reaching its peak value at a small strain. At deformation temperatures of 800 °C and 850 °C, under each of the three strain rates, the flow stress reached a peak value, and the curve then quickly entered the fluctuation state and remained stable at a particular level. It also has the same characteristics at 750 °C and 0.01 s⁻¹. At that point, the deformation process overcame dislocation winding and accumulation [16], and the work hardening and DRV softening effects (including DRV and DRX) attained a dynamic balance. However, at a deformation temperature of 750 °C and at strain rates of 0.1 and 1 s⁻¹, after the flow stress reached its peak, the curve gradually stabilized after a short slow decline.

Almost all the observed curves exhibited typical DRX characteristics, and the peak stress decreased with increasing deformation temperature and decreasing strain rate. This behavior can be explained as follows: higher temperature leads to stronger thermal activation of the material, which implies higher atomic kinetic energy. This higher atomic kinetic energy reduces the critical shear stress of slip between the grains, facilitating dislocation movement and grain boundary slip in the material, thereby reducing the flow stress. When the temperature increased from 750 °C to 850 °C at a strain rate of 1 s⁻¹, the peak flow stress decreased by 73.10 MPa. For a similar increase in temperature at a strain rate of 0.1 s⁻¹, the peak flow stress decreased by 76.63 MPa, whereas at a strain rate of 0.01 s⁻¹, the peak flow stress decreased by 113.20 MPa. Therefore, during the process of increase in temperature, the degree of reduction of the peak flow stress was higher at lower strain rates. TA5 alloy is sensitive to deformation temperature and strain rate, and the deformation resistance fluctuates during hot working, leading to uneven deformation and thereby reducing the dimensional accuracy and microstructural uniformity of its parts. For these reasons, finding suitable hot working conditions is particularly important.

**Constitutive equation**

Figure 2 reflects the variation of the flow stress (σ) for TA5 alloy with deformation temperature (t) and strain rate (ético). The equation established by the constitutive model can quantitatively describe the relationship of the influence of temperature and strain rate on rheological stress according to the Arrhenius equation, which is expressed as follows:

\[
\dot{\varepsilon} = A_1 \sigma^{n_1} \exp(-Q/RT), \quad \alpha \sigma < 0.8, \quad (1)
\]

\[
\dot{\varepsilon} = A_2 \sigma \exp(\beta \sigma) \exp(-Q/RT), \quad \alpha \sigma > 1.2, \quad (2)
\]

\[
\dot{\varepsilon} = A [\sinh(\alpha \sigma)]^{n_1} \exp(-Q/RT), \quad \text{for all } \sigma. \quad (3)
\]

Here, ˙\varepsilon is the strain rate, n and n_1 are stress indices, σ is the flow stress under the given strain conditions, Q is the activation energy, R is the molar gas constant (8.314 J · mol⁻¹ · K⁻¹), and T is the thermodynamic temperature. A_1, A_2, n, n_1, and β are constants, which are obtained by fitting related parameters and σ is the peak stress [20]. α is expressed as follows:

\[
\alpha = \frac{\beta}{n_1}. \quad (4)
\]

Equations (1) and (2) are applicable for low- and high-pressure states, respectively [21]. Therefore, the hyperbolic sine equation (equation (3)) proposed by Sellars et al [22] is more suitable for establishing the constitutive model.

The influence of ˙\varepsilon and T on σ can be expressed using the Zener–Hollomon parameter [23], combined with a hyperbolic sine function as follows:

\[
Z = \dot{\varepsilon} \exp(Q/RT) = A [\sinh(\alpha \sigma)]^{n_1}. \quad (5)
\]

For a given ˙\varepsilon, equation (5) can be transformed to express Q as follows:

\[
Q = R \left[ \frac{\partial \ln \dot{\varepsilon}}{\partial \ln [\sinh(\alpha \sigma)]} \right]_T \left[ \frac{\partial \ln [\sinh(\alpha \sigma)]}{\partial (1000/T)} \right]_\dot{\varepsilon} = Rnb, \quad (6)
\]
where $b$ is a constant expressed as follows:

$$b = \left[ \frac{\partial \ln \left[ \sinh \left( \alpha \sigma \right) \right]}{\partial (1000/T)} \right] \dot{\varepsilon}. \quad (7)$$

The peak stress is used to simulate the hot deformation behavior of TA5 alloy. By taking logarithms of equations (1) and (2), the linear fitting curve of $\ln \dot{\varepsilon} - \ln \sigma$ can be derived as shown in figure 3, thereby

**Figure 2.** True stress–true strain curves and strain rates at (a) 750 °C, (b) 800 °C, and (c) 850 °C.
providing values of $n$, and $\beta$, respectively. Thereafter, $\alpha$ can be calculated using equation (4). According to equation (6), $n$ can be obtained from $\ln \dot{\varepsilon} - \ln [\sinh (\alpha \sigma)]$, and $b$ can be obtained from $\ln [\sinh (\alpha \sigma)] - (1000 / T)$. The fitting curve is shown in figure 4. Thereafter, $Q$ can be found according to equation (6). If lattice self-diffusion activation energy is used in constitutive equation analysis, the hot deformation mechanism of alloy is controlled by the glide and climb of dislocations [24–26]. According to linear regression fitting, $Q$ is 469.893 KJ \cdot \text{mol}^{-1}, which is significantly higher than the reported value that the lattice self-diffusion activation energy of titanium is about 242 KJ \cdot \text{mol}^{-1} [27]. Since the $Q$ value is obtained under the condition that the microstructure remains constant, this is usually called apparent activation energy [28].

Taking the logarithm of equation (5) to obtain the following equation:

$$ \ln Z = \ln A + n \ln [\sinh (\alpha \sigma)]. $$

The linear regression curve of $\ln Z - \ln [\sinh (\alpha \sigma)]$ can be drawn as shown in figure 5. The value of $\ln A$ is obtained by fitting the intercept of the curve using equation (8).

The constitutive equation for TA5 alloy is obtained by substituting the above material parameters into equation (3) as follows:

$$ \dot{\varepsilon} = 4.15 \times 10^{21} [\sinh (0.0032 \sigma_p)]^{2.34} \exp \left( \frac{-469893}{8.314T} \right). $$

To verify the accuracy of the constitutive equation, the peak stress under various deformation conditions was calculated at different temperatures and strain rates using equation (9). The curves indicating the comparison of the experimental and calculated values are shown in figure 6. It can be concluded from figure 6 that the error
Figure 4. Linear relation of (a) $\ln(\dot{\varepsilon}) - \ln[\sinh(\alpha\sigma)]$ and (b) $\ln[\sinh(\alpha\sigma)] - (1000/T)$.

Figure 5. Linear relation of $\ln Z - \ln[\sinh(\alpha\sigma)]$. 
between the calculated and experimental values is less than 8%; this shows that the hyperbolic sine constitutive equation can be used to effectively describe the deformation behavior of TA5 alloy during hot deformation and provide insights for the design of a hot forming process for this alloy.

Microstructural evolution
TA5 alloy is an α-type alloy, and its microstructure is composed of serrated α+flaky α in HIP and annealed states. Figure 7 shows the microstructure of TA5 alloy under various hot deformation conditions, with evaluation of the machinability of the microstructure of each TA5 alloy after compression. It can be seen that the grains of the original structure extend along the direction perpendicular to the compression, since the original α structure was axially compressed, thereby elongating the grains. Deformation primarily occurred by dislocation slip along the slip planes. When the stress applied in the sliding direction exceeded the required minimum stress, dislocation movement occurred. In addition, the force required for dislocation movement is closely related to the temperature and strain rate [29]. Higher temperatures are beneficial to sliding, but elevated strain rates reduce the sliding effect. Therefore, at high strain rate and low temperature, stress concentration caused by reduction of the slip leads to instability and internal defects [30].

At 750 °C, sheetlike α phase slipped under axial compression, producing fibrous deformation structure. As the strain rate increased, the grain became uneven, as shown in figure 7(c), and the stress concentration caused by the reduction of the slip resulted in obvious microcracks. This behavior can be explained as follows: although DRX and DRV are produced at high strain rates, minimal dislocation movement provides DRX grains with insufficient time to grow. Therefore, stress gradually accumulates in the interior, resulting in stress concentration and microcracks. At a given temperature, the greater the strain rate, the lower the DRX level. At 800 °C and 850 °C, a jagged α phase gradually becomes obvious, as shown in figures 7(d), (e), (h), and (i), illustrating the internal instability of TA5 alloy during casting. The uneven distribution of the flaky α phase is shown in figure 7(f). A gradual increase in temperature and decrease in strain rate is beneficial to the occurrence of the slip. Under such conditions, the high diffusion speeds and long diffusion times of metal atoms allows the grain boundaries to fully migrate, and grains grow and coarsen visibly, as shown in figure 7(g). At this point, the microstructure is compact and stable, no microcrack defects are observed, and DRX grains are substantially uniform. Therefore, the high-temperature and low-strain zone is most suitable for processing TA5 alloys.

Conclusions
1. The peak flow stress decreases with increasing deformation temperature and decreasing strain rate. With increase in temperature, the degree of reduction of the peak flow stress increases with decreasing strain rate. At strain rates of 1, 0.1, and 0.01 s⁻¹, the peak flow stress decreases by 73.10, 76.63, and 113.20 MPa, respectively, as the temperature increases from 750 °C to 850 °C. At higher temperatures, the thermal
activation of the material is higher; hence, the critical shear stress of slip between the grains is lower, thereby facilitating dislocation movement and grain boundary slip in the material and reducing the flow stress.

2. Based on processing and analysis of the experimental data of stress and strain, the constitutive equation of TA5 alloy is expressed by equation (9).

   The average error between the calculated and experimental values is less than 8%.

3. At 750 °C, sheetlike α phase slips under axial compression, producing fibrous deformation structure. Moreover, at high strain rates, the grain becomes uneven, and stress concentration caused by the reduction of the slip phenomenon causes visible microcracks. At 800 °C and 850 °C, an internally unstable sawtooth α phase gradually becomes obvious.

4. High temperature and low-strain rate are beneficial to the occurrence of slip. Under such conditions, the high diffusion speeds and long diffusion time of metal atoms allow grain boundaries to fully migrate, microstructure remains compact and stable, and DRX grain uniformity is high. Thus, the high-temperature and low-strain zone is most suitable for processing TA5 alloys.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.
ORCID iDs

Zhang Jian  
https://orcid.org/0000-0003-3809-923X

References

[1] Guo K, Wang T S, Meng K, Yao C and Wang Q 2020 Influence of cold rolling deformation on mechanical properties and corrosion behavior of Ti-6Al-3Nb-2Zr-1Mo alloy Mater. Res. Express 7 066531
[2] Chuan Y B, Yu S H, Semiatin S L and Hwang S K 2005 Effect of deformation twinning on microstructure and texture evolution during cold rolling of CP-titanium Mater. Sci. Eng. A 398 209–19
[3] Boyer R R 1996 An overview on the use of titanium in the aerospace industry Mater. Sci. Eng. A 213 103–14
[4] Zhou Y B 2000 The Conceptus of Titanium Castings 1th ed. (Beijing, China: Aviation Industry Press)
[5] Li Q Y 1987 Handbook of Rare Metal Materials Processing 1th ed. (Beijing, China: Metallurgical Industry Press)
[6] Huang X M, Zang Y and Guan B 2021 Constitutive models and microstructure evolution of Ti-6Al-4V alloy during the hot compressive process Mater. Res. Express 8 016534
[7] Zang Q, Yu H, Lee Y S, Kim M S and Kim H W 2019 Effects of initial microstructure on hot deformation behavior of Al-7.9Zn-2.7Mg-2.0Cu (wt%) alloy Mater. Sci. Charact. 151 404–13
[8] Sahoo B N and Panigrahi S K 2019 Deformation behavior and processing map development of AZ91 Mg alloy with and without addition of hybrid in situ TiC + TiB2 reinforcement J. Alloys Compd. 776 865–81
[9] Wen D X, Lin Y C, Bin L H, Chen X M, Deng J and Li L T 2014 Hot deformation behavior and processing map of a typical Ni-based superalloy Mater. Sci. Eng. A 591 183–92
[10] Li L X, Rao K P, Lou Y and Peng D S 2003 Hot deformation characteristics of Ti-6Al-4V International Journal of Materials Research 94 1006–11
[11] Dong Q and Zhang J S 2019 Constitutive modeling for high temperature compressive deformation of non-oriented electrical steel Mater. Test. 61 204–8
[12] Bobbili R, Ramudu B V and Madhu V 2017 A physically-based constitutive model for hot deformation of Ti-10-2-3 alloy J. Alloys Compd. 696 295–303
[13]Sadeghpour S, Javaherib V, Bruschi S, Komi J and Karjalainen P 2020 Strain rate and mechanical stability in determining deformation behavior of beta Ti alloys Mater. Sci. Eng. A 798 139852
[14]Saboobi A, Abdi A, Fatemi S A, Marchese G, Biamino S and Mirzadeh H 2020 Hot deformation behavior and flow stress modeling of Ti–6Al–4V alloy produced via electron beam melting additive manufacturing technology in single β-phase field Mater. Sci. Eng. A 792 139822
[15]Chen X, Lin Y, Chen M, Li H, Wen D, Zhang J and He M 2015 Microstructural evolution of a nickel-based superalloy during hot deformation Mater. Des. 77 41–9
[16]Ghasemi E, Zarei-Hanzaki A, Farabi E, Tesaf K, Jäger A and Rezaee M 2017 Flow softening and dynamic recrystallization behavior of BT9 titanium alloy: a study using process map development J. Alloys Compd. 695 1706–18
[17]Sellars C M 1990 Modelling microstructural development during hot rolling Mater. Sci. Technol. 11 1072–81
[18]Bruni C, Forcelluse A and Gabrielli F 2002 Hot workability and models for flow stress of NIMONIC 115 Ni-base superalloy J. Mater. Process. Technol. 125-126 242–7
[19]Askariani S A and Fishbin S M H 2016 Hot deformation behavior of Mg-4Li-1Al alloy via hot compression tests Journal of Alloys & Compounds 688 1058–65
[20]Liu D F, Qin J, Zhang Y H, Wang Z G and Nie J C 2020 Effect of yttrium addition on the hot deformation behavior of Fe–6.5 wt%Si alloy Mater. Sci. Eng. A 797 140238
[21]Wang G, Bian D W, Kou L Y and Zhu X J 2019 Hot deformation behavior and processing map of 6063 aluminum alloy Mater. Res. Express 6 96527
[22]Sellars C M and McTeague W J 1966 On the mechanism of hot deformation Acta Metall. 14 1136–8
[23]Zener C and Hollomon J H 1949 Effect of strain rate upon plastic flow of steel J. Appl. Phys. 15 22–32
[24]Mizrahi H 2015 Simple physically-based constitutive equations for hot deformation of 2024 and 7075 aluminum alloys Transactions of Nonferrous Metals Society of China 25 1614–8
[25]Mizrahi H 2016 Quantification of the strengthening effect of rare earth elements during hot deformation of Mg–Gd–Y–Zr magnesium alloy at elevated temperatures J. Alloys Compd. 713 1–4
[26]Barezbani M H, Mirzadeh H, Roumina R and Mahmudi R 2019 Constitutive analysis of wrought Mg–Gd magnesium alloys during hot compression at elevated temperatures J. Alloys Compd. 791 1200–6
[27]Conrad H 1981 Effect of interstitial solutes on the strength and ductility of titanium Prog. Mater. Sci. 26 342
[28]Mizrahi H 2015 Constitutive description of 7075 aluminum alloy during hot deformation by apparent and physically-based approaches J. Mater. Eng. Perform. 24 1095–9
[29]Rollett A, Humphreys F J, Rohrer G S and Hatherly M 2004 Recrystallization and related annealing phenomena 2nd ed. (Britain: Pergamon)
[30]Jiang D and Wang C 2003 Influence of microstructure on deformation behavior and fracture mode of Al–Mg–Si alloys Mater. Sci. Eng. A 352 29–33