Grain Size Evolution Model of TB6 Titanium Alloys During β Process

Cui Xia, Lu Shi-qiang, Du Hai-ming and Ouyang De-lai

ABSTRACT

Grain size evolution of TB6 titanium alloy during β process, which take into account the static grain growth, strain-induced grain growth and DRX-induced grain refinement, is modeled according to the deformation mechanism and driving forces. The material constants arising in the model has been determined from the experimental data of DRX grain sizes of the alloy deformed at the temperature of 1273K-1373K and strain rate of 0.001s⁻¹-1s⁻¹. Good agreement between the experimental data and the calculated results has been achieved.

INTRODUCTION

TB6 titanium alloy, a kind of near-beta(β) alloy, is widely applied in large aircraft construction owing to its excellent hot workability and very attractive combinations of strength, toughness and fatigue resistance at large cross sections[1-3]. Recently, the β forging process of titanium alloy is developed for fabricating the (α+β) lamellar microstructure, which consisting of lamellar alpha in a transformed β grain, and thus shows a better high temperature creep property, impact toughness and fracture toughness[4-5]. In β forging process, the high diffuse coefficient of titanium atom leads to the rapid growth of the β grains[6]. As a result, the Ti-alloys with the lamellar microstructure have poor ductility due to so-called “β brittleness” and “Structural inheritance”, which limits the application of β processing in greater depth.

Dynamic recrystallization (DRX) is a significant approach on grain refinement of metals through thermomechanical processing. Several investigators have mentioned that DRX occurs in titanium alloy including TB6 titanium alloy during β process[7-10], which suggests hot deformation accompanied by DRX should be a promising method for the β grain refinement of the Ti-alloy, and thus deals with the problem of β grain coarsening. Also several prediction model of DRX gain size evolution has been proposed including classical D-Z model by sellars[11, 12], in which the applications to DRX gain size prediction during hot working have been achieved for steel with a low and middle steady stain which can be reached

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practically. Titanium TB6, however, presents middle steady strains for low strain rates, but large steady strains for high strain rates (e.g., a steady strain $\varepsilon \approx 2.5$ at strain rate of $1s^{-1}$ and deformation temperature of $1050^\circ C$)\textsuperscript{[13]}. Therefore, the classical D-Z model seem to be hardly applicable to the Ti-alloy for, especially for high strain rate.

The present work aims to develop a DRX grain size evolution model of the Ti-alloy with a wide range of deformation conditions. In addition, the genetic algorithm (GA) based objective optimization technique is used to determine the material constants within the model from experimental data of TB6 titanium alloy deformed at $\beta$ phase region.

**MODELING OF GRAIN GROWTH**

**Static Grain Growth**

Grain growth is thermally activated due to “holding time” at a certain temperature during hot working. The driving force is considered to be the reduction in surface energy \textsuperscript{[14]}, the value of which can be determined as

$$p_{surf} = \frac{\sigma_{surf}}{d} \tag{1}$$

where $\sigma_{surf}$ is the grain boundary energy per unit area, $d$ is curvature radius of grain. Thus, assumed the grain to be spherical, the static grain growth rate related to this driving force through a mobility $M$ can be written as

$$\dot{d}_t = \frac{M \sigma_{surf}}{d} \tag{2}$$

where $M$ is the mobility of grain boundaries. The multiplicative factor ($M \sigma_{surf}$) is used as a fitting constant. And hence,

$$d_t^2 - d_0^2 = kt \tag{3}$$

Where $d_t$ is the size of grain at a certain time, $d_0$ is the initial grain size, $t$ is the heat treatment time, $k$ is the temperature-dependent constant, but is independent of grain size.

As a generalization of Eq.(3), the contribution of temperature influence to grain size changes is commonly written as\textsuperscript{[15]}

$$\Delta d_t = d_t - d_0 = \beta_0 \exp(-Q / RT)^n \tag{4}$$

where $Q$ is the activation energy for the process, $T$ is the absolute temperature and $R$ is the gas constant.

**Strain-Induced Gain Growth**

Grain growth during deformation is significantly more rapid than static grain growth. This strain-enhanced grain growth is a widespread phenomenon, being found in both single-phase alloys and in microduplex alloys including titanium alloy\textsuperscript{[16, 17]}. In view of solely strain-enhanced grain growth, the evolution of grain size is dependent on strain, strain rate, and independent on temperature. And the model of strain-enhanced grain growth rate can be taken in the form\textsuperscript{[18, 19]}:

$$\dot{d}_e = \eta \dot{\varepsilon} d_e^{-\beta} \tag{5}$$
where \( \eta \) characterizes the strain rate and temperature dependence, \( \beta_1 \) is material constants. According to eqn.(5), For solely plastic-strain-induced grain growth, the grain size increase, \( \Delta d_{\varepsilon} \), can be modeled to the following:

\[
\Delta d_{\varepsilon} = \left[ (1 - \beta_1 \eta \varepsilon) \right]^{1/\beta_1} \\
\text{where } d_{\varepsilon} = 0 \text{ is assumed at } \varepsilon = 0. \text{ This equation is implicit to strain rate and temperature in parameter } \eta, \text{ and strain rate exponent dependence on strain-induced grain growth is found empirical equation}^{[20, 21]} \text{. So eqn.(6) modified to}
\]

\[
\Delta d_{\varepsilon} = \left[ (1 - \beta_1 Z \beta_2 \varepsilon) \right]^{1/\beta_1} \\
\text{in which } Z \text{ [Zener–Hollomon parameter; } Z = \dot\varepsilon \exp(Q / RT) \] is introduced to characterize the strain rate and temperature dependence, \( \beta_1 \) and \( \beta_2 \) are material constants.

**Recrystallization**

During high temperature deformation of TB6 titanium alloy, new grains nucleate dynamically due to the inhomogeneity deformation which provides high dislocation density and large strain gradient. The driving force of DRX and the nucleation is mainly considered to be reduction of stored strain energy. Since the total grain number increases during DRX, the average grain size decreases. Taking only DRX into account the evolution of the grain size can be modelled as\[^22\]

\[
d_r = -d_r \ast \left( \frac{dS}{dt} \right) \ast \ln N \\
\text{where } N \text{ is the number of new grains per old grain after one cycle of recrystallization, which may be grain size dependent, } S \text{ the number of recrystallization cycles, which can be a non-integer number. According to eqn.(8), lin et al}[^23] \text{carried out the model of grain size evolution due to DRX-induced grain refinement}
\]

\[
d_r = -\beta_3 f \dot{\beta}_4 d_r \beta_5 \\
\text{where } \beta_3, \beta_4 \text{and } \beta_5 \text{ are material constants, } \dot{f} \text{ is the volume fraction rate of DRX. In view of the volume fraction exponent dependence on grain size during dynamic recrystallization}[^24], \text{ the model of DRX-grain refinement is proposed in this paper as}
\]

\[
d_r = -\beta_3 f \dot{\beta}_4 f_\text{DRX} \beta_5 \\
\text{where } f \text{ is the volume fraction of DRX. Thus, the contribution of DRX influence to grain size changes, according to eqn.(10), can be modeled as}
\]

\[
\Delta d_r = -((1 - \beta_5) \beta_{3} f \beta_4 \dot{f} + 1)^{1/(1 - \beta_3)} \\
\text{where } d_r = 0 \text{ is assumed while } f = 0.
\]

**Grain Size Evolution**

Grain size evolution during dynamic recrystallization of TB6 titanium alloy is dependent on the three aspects of competing: static grain growth, strain-induced grain growth, and DRX-induced grain refinement. Considering the influence of them on grain size change, the grain growth may take the form as
\[ d = d_0 + \Delta d_t + \Delta d_c + \Delta d_r = d_0 + \beta_0 \exp(-Q/RT) + \frac{1}{[(1 - \beta_1)Z\beta_2\varepsilon]^{\frac{1}{1 - \beta_1}} - [(1 - \beta_5)\beta_3 f \beta_4 + 1]^{(1 - \beta_5)}} \]  

Obviously, the above constitutive equation developed for the prediction of grain size evolution is a non-linear equation containing six material constants. Optimization techniques should be used for determining the material constants within eqn.(12) from experimental data for application purpose.

APPLICATION OF MODEL TO TB6 TITANIUM ALLOY

Experimental

The chemical composition of TB6 titanium alloy used in the present investigation is given in Table 1. Cylindrical specimens of 8mm diameter and 12mm height were machined to carry out isothermal compression experiments with constant strain rate. The isothermal compression tests were conducted using a THERMEOASTOR-Z simulator for hot working with optical dilatometer. The specimens and compression rams were heated using the high frequency induction heating system under the vacuum condition to avoid oxidation. The testing temperatures ranged in β phase region from 1098K to 1423K at an interval of 50K and at constant true strain rates of 0.001, 0.01, 0.1, 1s\(^{-1}\) at each deformation temperature. The specimens were compressed as 3%, 5%, 8%, 18%, 20%, 30%, 40%, 50%, 60%, 70% of the reduction in height at each combination of the deformation temperatures and the strain rates and subsequently quenched by helium gas.

The specimens were then sectioned parallel to deformation direction, grinded, polished, and etched for further microstructural studies. The dynamically recrystallized average grain size was determined utilizing a powerful image analyzing system, by which the dynamically recrystallized grains could be almost readily distinguished from the pre-existing grains.

| Table 1. Chemical compositions of titanium alloy tb6 (mass fraction, %). |
|---------------------|-----|-----|-----|-----|-----|-----|-----|
| V | Fe | Al | O  | N  | C  | Ti |
| 10.2 | 1.8 | 3.1 | 0.11 | 0.01 | 0.02 | Bal. |

Determination Of Material Constants

A genetic algorithm (GA)-based multiple objective optimization technique has been used for determining material constants within eqn.(14) which is strongly non-linear and non-smooth. The GA-based optimization technique is very effective in solving this kind of problem, which completely overcome the difficulty of choosing correct starting values for the constants in the traditional optimization techniques and provides a better chance to converge to the global minimum\(^{25}\). In this paper, experimental data of DRX grain size at deformation temperature of 1273K ~ 1373K, strain rates of 0.001s\(^{-1}\)~ 1s\(^{-1}\) and strain of 0.03~1.2 were employed as parent samples to determine the material constants arising in the
constitutive equations. The material constants determined using the GA-based objective optimization technique are listed in Table 2.

**Table 2.** Optimized material constants for eqn.(14).

<table>
<thead>
<tr>
<th>$\beta_0$</th>
<th>$\beta_1$</th>
<th>$\beta_2$</th>
<th>$\gamma_0$</th>
<th>$\gamma_1$</th>
<th>$\gamma_2$</th>
<th>$\gamma_3$</th>
<th>$k_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.00016</td>
<td>-0.797</td>
<td>-2.04</td>
<td>2.30</td>
<td>0.8997</td>
<td>1</td>
<td>0.722</td>
<td>-0.01112</td>
</tr>
</tbody>
</table>

**Verification Of Constitutive Equation**

Based on the material constants in Table 2 and, the comparisons of experimental data with computed results are shown in Fig 1. It can be seen that good agreements between the sampled experimental data and the calculated data with the average relative error of 11.3%. It is indicated that eqn.(12) can be used to predict the DRX grain size evolution of TB6 titanium alloy during $\beta$ process very well.

![Figure 1](image.png)

**Figure 1.** Comparison of calculated results with experimental ones of $\beta$ phase grain size.

**CONCLUSIONS**

Considering the influence of static grain growth, strain-induced gain growth and DRX-induced grain refinement on grain size change, the mathematical models describing the grain size evolution of TB6 titanium alloy during $\beta$ process were elaborated. All of the material constants arising in the model were determined using the GA-based objective optimization technique. Through comparing the experimental data with the model computed results, the model was proved to be able to predict the evolution of grain size for $\beta$ process of TB6 titanium alloy.

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