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High-temperature behaviors of grain boundary in titanium alloy: Modeling and application to microcrack prediction

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ABSTRACT

Grain boundary (GB) deformation usually occurs during the high-temperature deformation process of titanium alloy, which may result in microcrack initiation and propagation. GB exhibits the characteristics of viscosity softening and rate sensitivity in its deformation, which lead to flow softening, enhanced plasticity and rate sensitive damage of the alloy. In view of the fact that it is extremely hard to directly observe GB deformation in experiments, a cohesive zone model (CZM) of GB has been proposed by taking into account the aforementioned characteristics. The CZM model is then combined with an actual-microstructure-based crystal plasticity finite element model (CPFEM) to include the effect of grain morphology, grain orientation and α and β phases of titanium alloy. The model is applied to study the microcrack initiation and propagation of a near-α titanium alloy. The predicted microcrack initiation and propagation were verified by experimental observations, which proves the reliability of the proposed model. Then, the model is applied to study the fracture rule of GBs, the effects of grain morphology, misorientation and property on the fracture of GBs. The results show that (a) the α-α GBs tend to be the most difficult one to deform, while the β-β GBs are the easiest one; (b) grain morphology affects microcrack initiation and propagation most. The α-β GBs decohesion at triple junctions is the dominant type for crack initiation, then the crack propagates mainly along the straight GBs vertical to tensile axis; (c) the critical strength of GB reaches the minimum at the case that the grains misorientation falls into 45–60°.

1. Introduction

Titanium alloys are widely used in aircrafts, ships, vehicles, and son on due to their light weight and prominently high specific strength, excellent corrosion resistance [1]. Because of the high strength at room temperature, high-temperature forming has become an effective approach for manufacturing complex-structured components of titanium alloys. However, during the high-temperature deformation, microcracks may initiate and propagate in the material, which will result in fracture failure or interior fracture that weakens the fatigue life of the component. Grain boundaries (GBs, including phase interface) contribute much to the microcracks because that GBs become the weakest region during the high temperature deformation, and so the deformation, damage and fracture of GBs may directly cause plasticity enhancement, microcrack initiation and propagation, respectively. That is to say, the plastic deformation and damage of GBs play a key role on the deformation and failure of titanium alloys at high temperature. The investigation on GBs deformation and damage will bring in new insights in understanding the mechanism of the microcrack initiation and propagation of the titanium alloy.

Unlike the behavior of the interface in non-metal material, grain boundary in titanium alloy shows viscoelastoplascity under high temperature deformation. GBs absorb the dislocations caused by the deformation at high temperature, instead of blocking the dislocations at room temperature. Thus, remarkable characteristics of viscosity and rate sensitivity are exhibited [2], and the softening induced by the decrease of GB viscosity seems significant. The viscosity softening and rate sensitivity determine the ability of GBs on their resistances to deformation, damage and fracture, which are crucial for the plastic deformation, microcracks initiation and propagation of the material.

To do study on the deformation and damage of GBs, experiments have been carried out by using nano-indentation with scanning electron microscopy (SEM) [3] or orientation imaging microscopy (OIM) [4]. However, this approach becomes incompetent for refined grains because the indenter is usually larger in size

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than GBs and thus the indentation may destroy GBs. In recent years, numerical modeling and simulation on this topic have been reported. During the early modeling, a transition zone was specified between neighboring grains and was treated as grain boundary to be assigned specified property [5]. Some works used shell element instead of the transition zone [6]. In these works, solid meshes with the given properties similar as that of grains were treated as GBs, which is hard to describe the GBs fracture and has no consideration of the viscosity behavior of GBs. Cohesive zone model (CZM) is an effective method for this purpose [7]. Wei et al. [8], Warner et al. [9] and Jérusalem et al. [10] used a rate-independent CZM to study the viscoelastic sliding-separation response of nano-polycrystalline material. Wu et al. [11] introduced the Chaboche model into a CZM to account for the rate-dependent behavior of grain boundary. Simonovski et al. [12] adopted an embedded bilinear CZM to simulate the GBs deformation of stainless steels. Hosseini et al. [13] adopted the exponential CZM to model damage nucleation and possible debonding of the ferrite-martensite interfaces in dual phase steels. These works bring approaches for modeling the GB behaviors, however, they did not consider the viscoelastoplastic behaviors with viscosity softening at high temperature.

Some recent CZMs have taken into account the hardening or softening during GBs deformation. Xu et al. [14] proposed an elastic–plastic CZM for metal-ceramic interfaces, which accounted for the hardening and softening during the plastic deformation of interface. In this work, the interface does not exhibit the characteristics of viscosity softening and rate sensitivity as those of titanium alloy GBs. In addition, GBs were generally considered to be regular in geometry in the aforementioned works, and thus the effect of grain morphology on GBs deformation and damage was ignored in these works. Although Hosseini et al. [13] established a model based on the actual profile of grains, there was no grain orientations considered.

In view of the above-mentioned facts, a new CZM will be proposed in this work to account for the GB behaviors of viscosity softening and rate sensitivity during the deformation of titanium alloy. To this end, an actual-microstructure-based geometry model together with a crystal plasticity finite element model (CPFEM) will be presented to combine with the proposed CZM in order to account for the effect of grains morphology, orientation and phase property on the deformation of GBs. Then, the model will be applied to study the microcrack initiation and propagation of a two-phase titanium alloy during the high temperature deformation.

2. Modeling procedure

2.1. Viscoelastoplastic constitutive modeling of grain boundary

2.1.1. Elastoplastic deformation of GB

Based on the work carried out by Wei et al. [8] and Xu et al. [14], the elastoplastic model of grain boundary can be described briefly as follows.

By setting $\boldsymbol{\delta}$ as the elastic–plastic displacement jump vector of grain boundary, $\mathbf{t}$ as the traction on grain boundary, and $\mathbf{t}\cdot\dot{\boldsymbol{\delta}}$ as the energy per unit area, there is

$$\boldsymbol{\delta} = \boldsymbol{\delta}^e + \boldsymbol{\delta}^p \tag{1}$$

where $\boldsymbol{\delta}^e$ and $\boldsymbol{\delta}^p$ denote the elastic and plastic portion of $\boldsymbol{\delta}$, respectively. Also, $\boldsymbol{\delta}$ can be additively decomposed as

$$\boldsymbol{\delta} = \boldsymbol{\delta}_n + \boldsymbol{\delta}_t \tag{2}$$

where $\boldsymbol{\delta}_n$ and $\boldsymbol{\delta}_t$, respectively, denote the displacement jump in normal direction and tangential direction.

The free energy per unit undeformed area can be expressed as

$$\varphi = \varphi(\boldsymbol{\delta}^e, k, D) \tag{3}$$

where k is a softening factor describing the GB softening during plastic flow, and D is a damage factor.

Thus, the time derivative of the free energy (Eq. (3)) is given by

$$\dot{\varphi}(\boldsymbol{\delta}^e, k, D) = \frac{\partial\varphi}{\partial\boldsymbol{\delta}^e}(\dot{\boldsymbol{\delta}} - \dot{\boldsymbol{\delta}}^p) + \frac{\partial\varphi}{\partial k}\dot{k} + \frac{\partial\varphi}{\partial D}\dot{D} \tag{4}$$

Based on the local energy imbalance that represents the first two laws of thermodynamics under isothermal conditions,

$$\dot{\varphi} \leqslant \mathbf{t}\cdot\dot{\boldsymbol{\delta}} \tag{5}$$

Eq. (5) implies a general elastic and dissipative law form as

$$\left(\mathbf{t} - \frac{\partial\varphi}{\partial\boldsymbol{\delta}^e}\right)\dot{\boldsymbol{\delta}} = 0 \tag{6}$$

$$\frac{\partial\varphi}{\partial\boldsymbol{\delta}^e}\dot{\boldsymbol{\delta}}^p - \frac{\partial\varphi}{\partial k}\dot{k} - \frac{\partial\varphi}{\partial D}\dot{D} \geqslant 0 \tag{7}$$

Hence, the free energy can be expressed in following form in order to keep consistent with Eqs. (6) and (7), as

$$\varphi = \frac{1}{2}((1-D)(\boldsymbol{\delta} - \boldsymbol{\delta}^p)\cdot\mathbf{K}\cdot(\boldsymbol{\delta} - \boldsymbol{\delta}^p) + Hk^2) \tag{8}$$

where H is the softening modulus, $\mathbf{K}$ denote the elastic stiffness tensor of grain boundary which can be decomposed into a normal portion K_n and a tangential portion K_t as

$$\mathbf{K} = K_n\mathbf{n}\otimes\mathbf{n} + K_t(1 - \mathbf{n}\otimes\mathbf{n}) \tag{9}$$

According to Eqs. (6) and (8), the local traction $\mathbf{t}$ can be derived from φ in the form as

$$\mathbf{t} = \frac{\partial\varphi}{\partial\boldsymbol{\delta}^e} = (1-D)\mathbf{K}\cdot(\boldsymbol{\delta} - \boldsymbol{\delta}^p) = \mathbf{t}_n + \mathbf{t}_t \tag{10}$$

$$\mathbf{t}_n = (\mathbf{n}\otimes\mathbf{n})\mathbf{t}, \mathbf{t}_t = (1 - \mathbf{n}\otimes\mathbf{n})\mathbf{t} \tag{11}$$

where $\mathbf{t}_n$ and $\mathbf{t}_t$ are the normal and the tangential portion of traction $\mathbf{t}$, respectively.

Then the traction after initial yield companied by softening can be expressed as

$$\tau = -\frac{\partial\varphi}{\partial k} = -Hk \tag{12}$$

here, H is the softening modulus.

In order to prevent the penetration of two adjacent boundaries, a scalar valued yield function is proposed as

$$\psi = \bar{t} + \mu\langle t_n\rangle - \tau - \mathrm{t}_0 \tag{13}$$

where $\bar{t}$ is the effective tangential traction, $\bar{t} = \sqrt{\mathbf{t}_t\cdot\mathbf{t}_t}$ and $\langle t_n\rangle = \frac{1}{2}(t_n + |t_n|)$, t_0 is the reference critical strength, and μ is the friction coefficient for capturing the frictional sliding between cohesive boundaries.

2.1.2. Viscosity softening and rate sensitivity of GB deformation

In order to account for the viscosity softening behavior due to the decrease of the viscosity of grain boundary, the viscosity plastic flow rule [14] is introduced, as expressed as

$$\dot{\boldsymbol{\delta}}^p = \dot{\alpha}\mathbf{n}_2 \tag{14}$$

where $\dot{\alpha}$ is the plastic multiplier and $\mathbf{n}_2$ is the unit flow vector defined in terms of the cohesive plastic yield function as

$$\mathbf{n}_2 = \frac{\partial\psi}{\partial\mathbf{t}}\left(\left|\frac{\partial\psi}{\partial\mathbf{t}}\right|\right)^{-1} = \frac{1}{\sqrt{1+\mu^2}}\left(\frac{\mathbf{t}_t}{\bar{t}} + \mu\mathbf{n}\right) \tag{15}$$