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A unified growth model of the secondary grain boundary α phase in TA15 Ti-alloy

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ABSTRACT

The growth mechanisms of the flat, zig-zag and mixed secondary grain boundary α (α_{GB}) phase in TA15 Ti-alloy were investigated through heat treat experiment (cooled from β-phase field at a constant rate combined with interrupted water quenching). A unified growth model was proposed by introducing the relationship between the critical length of flat α_{GB} (*Lc*) and β grain boundary (GB) length. The *Lc* is related to the characteristic and energy of the host GB, possible variants and habit plane of α_{GB}, and chemical driving force. α_{GB} preferentially nucleates at a triple junction (TJ) and extends on one side of β GB to form the flat morphology. Deviated growth of the heterogeneously and separately nucleated α_{GB} on a high-angle grain boundary results in zia-zag morphology. The driving force and time available for α_{GB} growth on the undecorated β GB determines its type, connected or unconnected. The flat and zig-zag α_{GB} showed a competitive growth, and if α_{GB} nucleated at the TJs and in the middle of the β GB simultaneously, the mixed α_{GB} would appear.

1. Introduction

TA15 (Ti-6Al-2Zr-1Mo-1V) alloy, a near-α Ti-alloy of high aluminum, has been widely used in the aeronautical industries owing to its high-strength, low-density, and high-temperature properties [1]. The microstructure of the near-α Ti-alloy typically consists of a primary α phase (α_p), a secondary α phase (α_s), and a transformed β matrix [2]. The secondary α phase includes grain boundary α (α_{GB}) and intra-granular α (α_{WI}). They act as barriers to dislocation slip and crack propagation, and determine the fracture toughness, creep properties, and fatigue crack propagation behavior [3,4]. When an α/β Ti-alloy is cooled from the β region or a higher temperature of the α/β region at a cooling rate that is lower than the critical rate for the martensite phase transformation, the secondary α_{GB} phase preferentially precipitates from the super-saturated β phase to decorate the pre-existing β grain boundaries (GBs) in diverse morphologies. However, it's not easy to identify the formation of α_{GB} due to intricate GB structures [5], diverse variants and morphologies, and growth or decomposition during thermal processing [6]. In most cases, the α_{GB} has the Burgers orientation relationship (BOR), i.e., $\{0\,0\,0\,1\}_\alpha//\{1\,1\,0\}_\beta$ and $\langle 1\,1\,\bar{2}\,0\rangle_\alpha//\langle 1\,1\,1\rangle_\beta$ [7], with one of the two adjacent β grains. There are 12 crystallographically equivalent orientation variants available for the α_{GB} if it develops BOR with only one of the β grains. However, only a limited number of α_{GB} variants are observed on most β grain boundaries [4,8–10]. It was pointed out that the variant selected among all 12 possible variants by a prior β GB during nucleation should arrange itself to have the minimum interfacial energy and elastic strain energy with the two contacting β grains [11]. Diverse morphologies of α_{GB}, the flat α_{GB}, zig-zag α_{GB}, and a mix of flat and zig-zag α_{GB}, have been observed [12–16].

Xu et al. [17] investigated the formation processes of precipitated phases relative to α_{GB} and grain boundary Widmanstätten α_{WGB} under different cooling rates when material was cooled down from the β phase region and the α/β region. Yang and Shao et al. [18,15] found that morphologies of both α_{GB} and α_{WGB} were dependent on cooling rates, for the specimen subjected to furnace cooling zig-zag and smooth α_{GB} appeared. α_{GB} of different morphologies precipitated on one β GB and it was considered that such a morphological difference may arise from the change in the orientation relationship between the α precipitates and the β matrices [19]. The competitive character of the β to α_m transformation relative to diffusional α formation was confirmed at slower cooling rates, i.e. <20 °C/s, and heterogeneous nucleation of

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a grain boundary α layer was observed, zig-zaged appearance [20].

Different growth models have been proposed for flat and zig-zag α_{GB}. For flat α_{GB}, D. Qiu et al. [21]validated that when the habit plane of a variant was parallel to the grain boundary plane (GBP), it would have the maximum growth rate in the GBP and evolved into flat α_{GB} via a three-dimensional phase field model. Appolaire et al. [12] suggested that α_{GB} nucleated heterogeneously on one side of a β GB and the α_{GB} nucleus having the same orientation grew in directions normal to the GB and merged to form the flat morphology. However, electron backscattering diffraction (EBSD) orientation mapping of the Ti-17 microstructure after 920°C/30min→800°C/1 h/water quenched (WQ) showed that α_{GB} precipitating from one β GB had the different orientations [14]. The precipitated α_{GB} of different orientations on one β GB were also found in Refs. [9,11,22]. Salib et al. [14] investigated the competitive growth of α_{GB} and grain boundary Widmanstätten α_{WGB} under different phase transformation temperatures and pointed out that the α_{GB} initially nucleated at the triple junction (TJ) and then grew straight along a high energy β GB. The inverse pole figure (IPF) map of Ti-4.3Fe-6.7Mo-1.5Al after 900°C/10min→780°C/18 h/WQ showed that α_{GB} grew on one side of the β GB [13]. While different positions for nucleation and growth of α_{GB} have been reported, there is not currently a unified understanding of the growth mechanism of the flat α_{GB}.

Koyama et al. [23] observed zig-zag morphology of GB cementite using a situ scanning electron microscopy. They proposed that zig-zag morphology was caused by heterogeneously deformation of the grain boundaries, which resulted in a change to the grain boundary shape from smooth to a zig-zag. For the Ti-29Nb-13Ta-4.6Zr alloy, Narita et al. [24] proposed that separately nucleated Widmanstätten α-laths (α_1 and α_2) grew into the adjacent β grains (β_1 and β_2, respectively), to form the zig-zag morphology. Angelier et al. [25] proposed that the zig-zag morphology was caused by the so-called "pucker" mechanism [26], i.e., in order to have a specific BOR between α_{GB} and one of the β grains, the β GB bent and α_{GB} grew within the opposite β grain to form the zig-zag structure. Sharma et al. [13] proposed a modified pucker mechanism and suggested that after initial growth along β GBs, branching of α grains (with some branches growing inside the β grain) and bending of β GB took place, which resulted in the zig-zag morphology. It was considered that bending of the β GB occurred before the nucleation of a zig-zag α_{GB} [13,25]. However, the models proposed in the literatures are inconsistent and cannot explain the experimentally observed phenomena.

The mixed morphology of flat and zig-zag α_{GB} has been observed in experiments, but it has not been explained. Why does α_{GB} show different morphologies? All morphologies belong to the α_{GB} phase, therefore, there should be some type of relationship between the morphologies, their growth mechanisms, and the thermal processing conditions.

Variant selection (VS) of α_{GB} arises from differences in orientation relationships of α_{GB} with respect to both adjacent β grains and in habit plane orientations of α_{GB} relative to the grain boundary inclination among all 12 candidate α_{GB} variants [27]. Van Bohemen et al. [10], M. Salib et al. [14], Shi et al. [11,9], Qiu et al. [28,21], and Furuhara et al. [29] studied the VS of grain boundary α in titanium alloys through experiments, phase-field simulations, etc. Shi et al. [11] developed a crystallographic model based on the BOR between α_{GB} and one of the two β grains to investigate how such a special prior β GB contributed to VS of α_{GB}. Shi et al. [9] assessed systematically the applicability of current empirical rules for VS of α_{GB} at prior β GBs using experimental characterization of GB misorientation, boundary plane inclination, and orientation relationships between the α_{GB} and adjacent β grains in Ti-5553. Qiu et al. [28] discussed the effect of dislocations on VS and subsequent development of transformation texture during α precipitation in α/β titanium alloys through three-dimensional phase-field simulations and found that the elastic interaction between α precipitates and dislocations dominated VS during the nucleation stage, whereas the habit plane orientations of α precipitates relative to the dislocation lines played an important role in VS during the growth stage. Qiu et al. [21] established a three phase field model considering discreteness of internal GB structures and pointed out that the degree of VS of a given variant was not only determined by the strength of its elastic interaction with the GB dislocations, but also number of other variants sharing the same preferred nucleation sites as well as preponderant growth direction relative to the GB dislocation line directions. All these works are important to reveal the orientations and VS for α_{GB}, however the formation and growth of α_{GB} with different morphologies are still lack of understanding.

In this study the growth mechanisms of the grain boundary α_{GB} in the TA15 Ti-alloy were investigated through cooling experiment, and a unified model was proposed to describe growth behavior of the flat, zig-zag, and mixed α_{GB}.

2. Materials and experimental method

2.1. Goal and starting point of experiment

The purpose of the experiments is to investigate the formation process and mechanisms of grain boundary α_{GB} with different morphologies, the flat, zig-zag, and mixed, and the possible relation among them. For a Ti-alloy when cooled from temperatures above T_β the phase transformation process (such as β→α phase transformation) will happen. As a thermodynamics and kinetics process, the type, morphology, quantity, and size of the precipitated α phase should be related to the chemical driving force (cooling rate, transformation temperature, duration time, alloy chemical composition, etc).

When cooled from temperatures above T_β at a high cooling rate, a martensitic reaction can occur. At relatively slow cooling rates, during which the main alloying elements can partition between β and α phases, grain boundary α (α_{GB}) is preferentially formed [15]. The formation of α_{GB} includes nucleation and growth, its morphology relies to the nucleation mode and site, growth pattern, and VS frequency of α phase. For a given Ti-alloy the different morphologies of α_{GB} will be observed by changing the cooling rates, transformation temperatures and durations.

It was found that α_{GB} formed in distinctly different morphologies [10,30]. Cooled at the rates of 0.5 °C/min [25], 0.18 °C/min, 1.8 °C/min, 18 °C/min [31], 13.8 °C/min [32], and 50 °C/min [16], the α_{GB} was observed and showed different morphologies. This is because the cooling rate will affect the phase transformation driving force and further affects the formation and VS of α_{GB}. Based on this a low cooling rate of 0.5 °C/min and an intermediate cooling rate of 20 °C/min were selected in this study which were beneficial to obtain diverse morphologies of α_{GB} for TA15 Ti-alloy.

In order to analyze the formation process of α_{GB}, the beginning temperature of α-phase precipitation should be determined first. It was found that the beginning temperature of α-phase precipitation in Ti-alloys varied when cooled at different rates [25]. Based on this for TA15 alloy involved in this paper it was about T_β-(30–50 °C) at a rate of 0.5 °C/min and T_β-(50–90 °C) at 20 °C/min.

At a given cooling rate, to what temperature the specimen is cooled, will affect the phase transformation degree, and will further affect morphology and size of α_{GB}. Meanwhile cooled to a certain temperature and held, here the isothermal phase transformation occurs, the duration (holding time) for which will have an impact on the diffusion of solute elements and precipitation α phase. It was found the duration also had an effect on the VS frequency of α_{GB} [10,11,14]. Therefore by changing the temperature cooled to and the