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On the modeling of diffusion-controlled growth of primary alpha in heat treatment of two-phase Ti-alloys

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ABSTRACT

Volume fraction of primary alpha is an important microstructure feature and can be changed by controlling its diffusive growth during heat treatment of two-phase Ti-alloys. A model for predicting its growth is urgently needed to realize microstructure control. Classical diffusion model based on additivity rule causes a significant underestimation of volume fraction of primary alpha phase. In present work, a diffusion-controlled growth model is developed to predict the evolution of phase fraction with temperature in the finite beta matrix, by solving the 3-dimensional diffusion equation with moving boundary conditions. By introducing a thermal history-related function and considering soft impingement, the prediction precision of present model is improved notably. Moreover, by considering the effect of secondary alpha precipitation on the far-field matrix composition and thus matrix supersaturation, the maximum error is almost one third of that by classical diffusion model when applied to TA15 and Ti-6Al-4V alloys. The results show that the volume fraction of primary alpha phase is overestimated in the later stage due to the effect of secondary alpha which is not captured by classical model. Combining the calculated length of diffusion field with metallographic analysis, the present model slightly underestimates the volume fraction of primary alpha in the initial stage due to the overestimation of soft impingement.

1. Introduction

Titanium alloys have attracted more and more attentions due to the combination of superior mechanical and physical properties, such as high strength, low density, good thermal stability, biocompatibility and excellent corrosion resistance [1–4]. The mechanical properties of titanium alloys are strongly dependent on the microstructure morphology, i.e. equiaxed, basket-wave, Widmanstaten, bi-modal and tri-modal structures exhibit different strength, ductility and fracture toughness [5–7]. Uniting preferable strength and ductility, equiaxed structure is the desirable microstructure and is usually obtained by numerous hot working and heat treatment steps in bulk forming of titanium alloys [8].

However, the microstructure morphology, viz. volume fraction of primary alpha phase and the characteristics of secondary alpha in transformed beta matrix, is very sensitive to thermal-processing history [9]. Hence, it is crucial to precisely predict the evolution rules of microstructure so as to realize the accurate control of microstructure morphology. One of important processes about microstructure evolution is the diffusive growth of primary alpha in two-phase titanium alloys. However, during its diffusion-controlled growth, the diffusion field around primary alpha particles is usually sensitive to temperature history due to the temperature dependence of the diffusion coefficient. Moreover, the precipitation of secondary alpha has an important effect on its diffusive growth [10]. Therefore, establishing accurate models for predicting the growth of primary alpha particles in complex temperature history condition faces the challenge to realize the microstructure control.

Physically-based internal state variable modeling is an important method to capture the characteristics of microstructure evolution, i.e. diffusion-controlled phase transformation [11]. By now, some investigations have been carried out on the growth of primary alpha during non-isothermal conditions in titanium alloys. Semiatin et al. [10] established the growth kinetics of primary alpha phase in Ti-6Al-4V during continuous cooling process. It was

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suggested that the growth of primary alpha phase was controlled by the diffusion of aluminum/vanadium. From theoretical analysis, the model predictions should be physically larger than measurements due to the precipitation of secondary phase. However, at the high cooling rate (194 °C/min), the volume fraction of primary alpha is underestimated. Zhu et al. [12] quantitatively investigated the effect of the cooling rate on the growth of primary alpha phase of TA15 titanium alloy. It was found that the thermodynamic correction factor for molybdenum is obtained by fitting the experimental data and overestimated. Even so, the model predictions are still lower than experimental measurements at fast cooling rate (165 °C/min). The models proposed by these researchers under non-isothermal transformation were based on additivity rule. This rule has been used widely to predict the kinetics of transformations during continuous cooling condition from isothermal models [13–16]. In fact, as suggested by Ye et al. [17], the real thermal history was not considered in such method and the physical meaning was not clear. The validity of such method depends heavily on whether the instantaneous growth rate was a state function independent of temperature history. Moreover, the effect of secondary alpha on the growth of primary alpha was not considered in these models.

Obviously, as to diffusion-controlled growth of precipitates, the additivity rule is not always valid and the thermal history needs to be considered carefully. Thus, the model predictions based on additivity rule may lead to a deviation from the exact solution. In order to describe this type of growth kinetics, diffusion equations with moving boundary conditions need to be solved [18–23]. From the work of Song et al. [24], with regard to the diffusion-controlled growth of planar boundaries, the diffusion field around precipitates under non-isothermal transformation is close related to the thermal history due to the temperature dependence of the diffusion coefficient and the solute concentration at the interphase boundary. Therefore, the instantaneous growth rate is not a state function and the additivity rule is not applicable. Considering the effect of thermal history on the growth kinetics of precipitates, the model proposed by Song et al. [24] can predict the growth of Si precipitates in Al—Si binary alloys. This method provides a good basis for the present work. In this model, soft impingement is not considered, which is reasonable in the infinite matrix. However, in the finite beta matrix, the impact of soft impingement on the kinetics of primary alpha can be significant and the model needs to be modified for two-phase Ti-alloys.

In the present work, considering the effect of thermal history on the evolution of the diffusion field around precipitates and soft impingement, the model is developed for predicting the three dimensional diffusion-controlled growth of primary alpha in titanium alloys. Finally, the model predictions will be compared with experimental measurements and the effect of secondary alpha on the growth of primary alpha is analyzed carefully.

2. Material and experimental procedure

The material used in this investigation is hot forged TA15 titanium alloy received in rod form with the measured β-transus temperature 985 °C. The chemical compositions (wt%) of this alloy are as follows: Al: 6.69; Mo: 1.77; V: 2.25; Zr: 2.26; Fe: 0.14 and Ti balance, and the initial microstructure is given in Fig. 1. The volume fraction of the primary α phase (α_p) was approximately 50%.

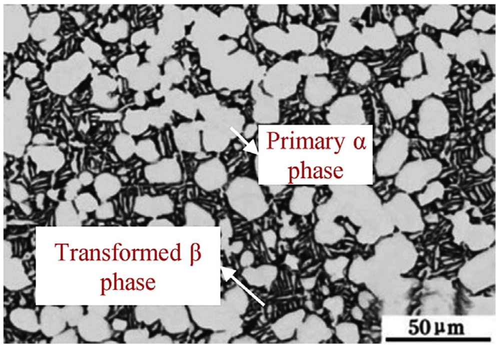

Fig. 1. Original microstructure of the billet.

Cylinder specimens with 10 mm in diameter and 15 mm in height were machined from the as-received bar. The specimens were heated to a peak temperature of 960 °C and held for 30 min, then cooled at a constant rate of 10 °C/min, 26 °C/min or 50 °C/min, and finally water quenched when reaching a prescribed temperature of 930 °C, 870 °C, 810 °C or 750 °C. To obtain equilibrium volume fraction of alpha, the specimens were heated to corresponding temperature ranging from 750 to 950 °C and held for 60min, then water quenched. Metallographic preparation of the specimens was carried out by sectioning perpendicular to the axis at the midlength location, mechanically grinding and polishing, and etching with a solution of 13%HNO_3, 7%HF and 80%H_2O. Micrographs were taken by scanning electron microscopy and examined using quantitative image analysis to acquire the microstructural parameters to validate the developed model.

The compositions of primary α phase at the prescribed quenching temperatures were obtained by electron microprobe analysis on JEOL JXA 8900. The resolution is about 1 μm and much lower than the grain size of primary alpha. So the experimental results are reliable. This will provide a good basis for the model implement.

3. Model description

As stated previously, the additivity rule is often used to predict the kinetics of transformation under non-isothermal conditions from isothermal models. It will be demonstrated in details in Appendix A. As proposed by Christian [13], a sufficient condition for the additivity rule is that the instantaneous rate of phase transformation depends only on the transformed fraction and the temperature. Reactions of this type are called isokinetic. This will be given in more details in Appendix A. The instantaneous transformation rate is independent of the time—temperature path.

The theoretical analysis for diffusion-controlled growth of spherical interface has to conduct the troublesome problem of

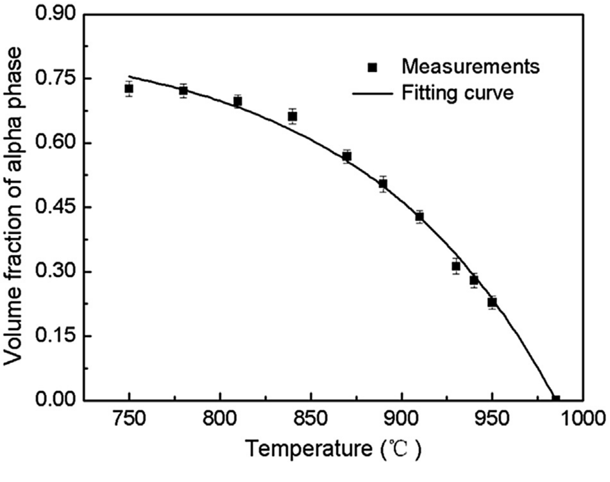

Fig. 2. The equilibrium volume fraction of alpha phase at different temperatures.