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Original Research Article

Application of the Digital Material Representation to strain localization prediction in the two phase titanium alloys for aerospace applications

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ABSTRACT

In the present work Digital Material Representation (DMR) approach was utilized to simulate the deformation behavior of the two phase Ti-6Al-4V alloy. DMR models of the two phase structure, containing different morphologies of alpha grains within a beta matrix – lamellar and equiaxed, were created. Each phase was then separated and different mechanical properties were assigned. Subsequently, their response to loading was tested using simple shear numerical simulations with special focus on strain inhomogeneities, as the main driving force for spheroidization is considered to be the formation of intense shearing within alpha lamellae. The proposed modeling approach combining Finite Element Method (FEM) with DMR allowed for much more detailed numerical analysis of deformation behavior of two phase titanium alloys at the micro scale and provided information such as strain localization and stress distributions within the alpha and beta phases. It was showed that presented model offers a new and powerful tool to study the physical bases of microstructure evolution processes such as spheroidization or recrystallization of Ti alloys. It shows good potential in simulation of deformation processes of complex two-phase morphologies that is a crucial step towards optimization of process parameters during hot forming of Ti-6Al-4V alloys.

1. Introduction

The continuous drive to save weight in the aerospace industry has led to increase use of titanium alloys, particularly in jet engine components but more recently also in landing gear and fuselage sections. The main mechanical property requirements that have to be fulfilled by two phase alpha/beta Ti alloys designed for aforementioned applications include high ductility at room temperature as well as high fracture-crack-initiation resistance. Obtaining a highly formable microstructure during primary hot working that is suitable for secondary

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hot working processes, is usually achieved by the process known as spheroidization [1,2]. During this process, a fine grained two-phase microstructure is developed through the breakdown of the as-cast large grained lamella microstructure. The main mechanism of spheroidization is formation of high energy alpha/alpha interfaces (as an effect of alpha lamella kinking due to deformation) in contact with beta platelets, which give rise to surface-tension-driven penetration of the alpha plates by the beta phase. It has also been shown that spheroidization – similarly to recrystallization in steels – is strongly dependent on the applied strain, strain path and temperature [3,4], suggesting that optimization of process routes to maximize spheroidization could lead to a substantial cost reduction in widely used alpha/beta alloy systems.

Nowadays, optimization of manufacturing cycle is most effectively performed with the aid of computer modeling tools that support experimental analysis. Additionally, the continuous advancement in computing power has opened new fields of application for computer simulation software and has allowed more detailed models to be developed and implemented into industrial practice. A good example is the Digital Materials Representation (DMR) approach that offers quite a powerful tool to predict the deformation behavior of various types of microstructure morphologies taking into account its local heterogeneities [5,6].

Thus, in the present research, the DMR concept was applied to investigate local inhomogeneities occurring across complex two phase Ti alloy microstructures, and to evaluate their influence on obtained properties during material processing.

Proposed idea of utilization of exact representation of the two phase microstructure for prediction of the deformation behavior of two phase Ti alloys provides more insight into possible interactions between various alpha and beta morphologies under deformation conditions. Understanding of this problem is crucial as strain localization at lower deformation temperatures may lead to shear band crossing of the alpha/beta lamellae or shear band cracking. It may also lead to shear-induced kinks forming in alpha/beta lamellae and eventually to fragmentation/spheroidization of the alpha/beta lamella [7]. Kinking and complete reorientation of α laths are due to tension and shear stresses respectively. However the break up of the β-phase is mainly attributed to the shear stresses and partial transformation of beta into alpha phase [8].

So far however, the modeling of deformation behavior of two phase Ti alloys has been limited to conventional empirical models where microstructure morphology was neglected e.g. prediction of spheroidization kinetics in [9]. In the present work, DMR approach, described in the following section, was used to simulate behavior of the two phase Ti-6Al-4V alloy. It allowed for very detailed local information from the microstructural level for evaluation of material behavior under deformation. The DMR of the two phase structure, containing different morphologies of alpha grains within beta structure matrix – lamellar and equiaxed, were created on the basis of real images of microstructures. Each phase was then separated and different mechanical properties were assigned. Subsequently, after finite element discretization their response to loading was investigated by simple shear numerical simulations, with special attention placed on strain inhomogeneities, which could lead to formation of intense shearing within alpha lamellae that cause onset of spheroidization. The DMR concept as well as experimental procedure used to provide the images for subsequent DMR model development is described in the following sections.

2. General concept of the Digital Material Representation

In the scientific literature the DMR is generally defined as a material description based on measurable quantities that provides the necessary link between simulation and experiment [10]. The digital material model is composed of three main components: explicit representation of microstructure features, properties assigned to these features and appropriate discretization allowing subsequent numerical simulations as schematically shown in Fig. 1.

Thus, first of all the key to the success of development of a DMR model is creation of an accurate digital representation of microstructure morphology under consideration, with its features represented explicitly to match the real microstructure morphology. Clearly, the more detailed the reconstructed morphology is applied, the more realistic results of calculations regarding material behavior will be. Consequently, they are most often created as exact replicas based on post-processing of real microstructure images (optical or electron) both in 2D and 3D spaces. However, applications of various numerical methods to provide statistically representative morphologies can also be found in scientific literature – see author's previous works e.g. [11]. As mentioned, another crucial aspect is evaluation of local material properties that will be assigned to particular features of the digital microstructure morphology. There are several approaches that can be used to determine such local material behavior, see e.g. [5,12–14]. When microstructure morphology is filled with properties, then the last stage is application of discretization procedures that are strictly related to numerical methods that are used to solve a direct problem model e.g. finite element method, boundary element method, cellular automata method, etc. When all three stages are combined then a Digital Material Representation model can be created and used for micro or multiscale applications [15–19].

3. Experimental

In order to generate initial microstructures with various morphologies of alpha/beta phases isothermal torsion tests were conducted on a commercially produced α/β titanium alloy, Ti-6Al-4V provided by TIMET UK Ltd. The material with chemical composition (in wt. pct.) being 6.6Al/4.1V/0.2O/0.06C/0.07N/0.004H was received as a hot-rolled, 30-mm-diameter bar, which had been mill annealed at 700 °C for 2 h, resulting in a microstructure comprising of equiaxed-alpha and transformed beta structure. In the present work, prior to mechanical testing, a special multi-stage heat treatment procedure was carried out in order to produce an initial microstructure that is typical of an as-cast microstructure of heat-treated ingots, which is then subjected to primary hot working routes. This