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Mechanical study of crystalline orientation distribution in Ti-6Al-4V: An assessment of micro-texture induced load partitioning

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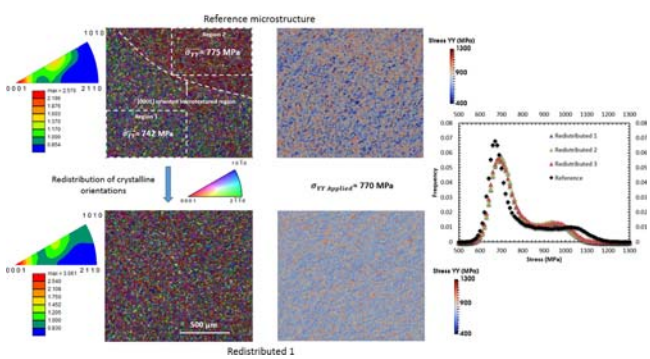
HIGHLIGHTS

- Fast Fourier Transform-based simulations of the elastic stress field were performed on real and synthetic microstructures
- A crystalline orientation redistribution procedure was proposed
- The load partitioning between microtextured regions was assessed in relation with elastic anisotropy
- Stress fields analysis reveals a non-local influence of microtextured regions on the stress field

GRAPHICAL ABSTRACT



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ABSTRACT

Microtextured regions are known to have a detrimental effect on the fatigue performance of near α and α/β titanium alloys. Due to the elastic anisotropy of α titanium, stress heterogeneities are expected to result from such microstructural features. The present work is an assessment of their influence on the elastic stress field, using Fast Fourier Transform-based computations on a 2D extruded aggregate built from a real microstructure. The contribution of the microtextured regions was then isolated by comparing simulations obtained on a synthetic aggregate with similar grain morphology and texture but removed microtextured regions through a redistribution of crystalline orientations. The analysis of the computed fields revealed that the average stress experienced by α grains is only weakly affected by the neighborhood and mostly determined by the elastic anisotropy of α titanium. Nevertheless, complex mechanical interactions between microtextured regions were evidenced. Indeed, load partitioning and non-local influence on the stress field were found to result from the presence of microtextured regions. The implications on fatigue crack initiation are discussed in light of these results.

1. Introduction

Titanium alloys are increasingly employed in the aerospace industry due to their high strength to weight ratio, corrosion resistance, fracture toughness and fatigue performance. As a consequence, their properties have been extensively characterized and some microstructural features have been identified as impairing their mechanical properties. For instance, ageing or prolonged use at high temperature leads to a reduced ductility [1,2]. The texture resulting from the processing steps also have a significant influence on mechanical properties under monotonic [3,4] and cyclic [5,6] loadings. In particular, α/β processing steps imply the formation of millimeter long clusters of α grains with sharp local texture [7,8]. Experimental studies evidenced an adverse influence of

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such microtextured regions, called macrozones, on the dwell-fatigue [9,10], low-cycle fatigue [11,12] and high-cycle fatigue life of components [13]. As fatigue performance is a critical concern, the design of the components is significantly impacted, since failure issues are especially critical in the aerospace industry.

Microtextured regions were found to influence both fatigue crack initiation [11,12,14] and propagation stages [13,15,16]. Nevertheless, as initiation is usually considered to account for most of the fatigue life of titanium alloys [17], it has been an intense field of research over the last decades. Although secondary cracks may initiate on prismatic slip bands, fatal crack nucleation is reported to proceed from quasi-cleavage facets associated with basal slip [12,18,19]. Similar to the Stroh or Fatemi-Socie criteria for instance [20,21,22], a combination of a high resolved shear stress to activate basal slip and a high normal stress to enable the quasi-cleavage process appear as mandatory requirements [12,13,23]. Although an agreement is found about an early crack initiation and a fast propagation related to the promotion of basal slip rather than prismatic slip in [0001] oriented micro-textured regions [11,12,13], the root cause of the deleterious effect of microtextured regions has not been clearly identified yet. Pioneering work by Le Biavant et al. suggested crack coalescence plays a role, due to a high density of tiny cracks noticed in macrozones [11]. Indeed, [0001] oriented microtextured regions gather a high fraction of nodules well oriented for basal slip and quasi-cleavage facet formation. Therefore, crystallographic aspects might appear as the controlling parameter. Nevertheless, the previous observations contrast with those of Bridier and his co-workers who reported a low number of secondary cracks under slightly different loading conditions [12]. They rather attributed the early crack initiation to the elastic anisotropy of α titanium hexagonal closed packed lattice (HCP). Actually, the [0001] direction exhibits the highest stiffness and [0001] oriented microtextured regions are reported as preferential crack nucleation locations. High stiffness crystallites are more likely to experience high magnitude stresses, thus promoting both an early activation of plastic slip and a high normal stress [12,13]. Finally, more recent studies reported crack initiation at the interfacial region of neighboring microtextured regions due to the presence of specific microstructural arrangements [14,23]. The proposed mechanism involves dislocations originating in a soft region and accumulating at the interface with a hard region. The resulting stress concentration is likely to enable the nucleation of quasi-cleavage facets characteristic of basal slip related crack initiation.

The parameters previously evidenced are either related to specific microstructural arrangements or to a heterogeneous stress field. Several studies have been conducted in order to identify the role of macrozones on the deformation and damage processes. Plastic strain heterogeneities were noticed under monotonic tensile loading at the microtextured region scale by Lunt and colleagues using digital image correlation of Ti-6Al-4V containing macrozones [24]. An early yield onset was evidenced in macrozones while the overall behavior is controlled by the texture in the specimen. Therefore, the apparent elastic behavior of specimens tested under fatigue loading may hinder plastic strain restricted to macrozones. Echlin and his co-workers confirmed this hypothesis using high resolution digital image correlation on Ti-6Al-4V as well [25]. An early onset of plastic slip is noticed in [0001] oriented microtextured regions. Nevertheless, crystalline orientations favorable to the onset of plastic slip can be found outside of macrozones as well. Hence, this may suggest the role of stress field heterogeneities related to the elastic anisotropy of α titanium. Morris showed that crystallites with similar orientations but embedded in a stiff or compliant sheet experience a significantly different stress (i.e. driven by crystallographic texture of neighboring grains) [26]. Therefore, non-negligible elastic stress heterogeneities might be due to the presence of microtextured regions. Spatially resolved experimental assessment of the stress field is still difficult. Alternatively, numerical modeling might provide useful indications about the resulting stress heterogeneities. Interestingly, a recent study revealed significant stress heterogeneities at the macrozone (i.e. mm) scale in the elastic regime [27]. To the author's knowledge, no thorough mechanical study considering such large regions has been conducted yet.

The aim of the present work is to assess the influence of microtextured regions on the mechanical fields in a realistic microstructure. The multiscale character of the microstructure of titanium alloys implies to employ an efficient computation method to account for both crystallographic and morphological aspects of the microstructure over a sufficiently large area. Fast Fourier Transform-based computations (FFT) were thus used in the present work using a realistic aggregate built from electron backscattered diffraction (EBSD) data. Alternative methods were applied in the past such as cellular automaton [28], which neglects crystal morphology, or finite element modeling [29,30,31], which limits the volume considered. To the author's knowledge, this is the first time both are considered simultaneously. As a first step, the stress field resulting from a reference microstructure containing microtextured regions was analyzed. Regions with different textures were identified and used to evidence load partitioning inside a specimen. An order of magnitude of the stress heterogeneities at this scale could thus be obtained from the computations. The contribution of local textures and grain clusters with preferential orientations could then be isolated through the use of synthetic aggregates with redistributed crystalline orientations to avoid any sharp local texture while retaining textures and grain morphologies. Average stress distributions at the grain scale were also studied depending on the realistic or random orientation distributions to evaluate the influence of the neighbors from a statistical point of view. Since microtextured regions are known to have a detrimental influence on fatigue performance, the potential influence of the resulting stress field on crack initiation processes is finally discussed.

2. Method

2.1. Reference microstructure

The material studied in this work is Ti-6Al-4V with a bimodal microstructure. Its duplex structure is composed of about a 45% volume fraction of equiaxed α_P nodules and a 55% volume fraction of lamellar α_S plates (thickness $\approx$ 1 μm) embedded in a β matrix. The average α_P nodule size is about 16 μm. Typical yield stress, tensile strength and elongation are 924 MPa, 998 MPa and 13.4% respectively. The microstructure morphology and local crystalline orientations are obtained using the electron backscattered diffraction technique. EBSD characterization of a 1313 μm × 1475 μm region was thus performed with a step of 1 μm using a JEOL 6100 scanning electron microscope equipped with an orientation imaging system provided by EDAX. This step size was applied to obtain a good compromise between the calculation time and an accurate description of the microstructure since the nodule size is about 16 μm and the microtextured regions reach several millimeters in length. Post-processing of the EBSD data was performed using the OIM analysis software. A neighbor confidence index correlation step was applied with a 0.2 criterion to eliminate low confidence index pixels. Finally, to facilitate grain identification, the orientation was averaged inside single grains defined with a 5° misorientation criterion. The β phase was neglected in the present analysis as it is reported to be about 3% [32] and falls below 0.05% after the cleaning steps previously described. Since the average mechanical fields were studied, a minor influence was expected.

The resulting inverse pole figure (IPF) map coded with respect to the Y axis superimposed with the image quality map (IQ) is shown in Fig. 1. A [0001] microtextured region is delimited with a dashed