The Mechanistic Link between Macrozones and Dwell Fatigue in Titanium Alloys

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Abstract

This paper addresses the role of macrozone crystallography and morphology in dwell fatigue in titanium alloy Ti-6Al-4V. Until now, the relationship between macrozones and dwell fatigue damage has remained mechanistically uncertain, but this paper establishes a mechanistic link between macrozones and dwell fatigue damage, and explains the preference for dwell facets to be sub-surface. It also outlines the criteria which are important in a potential definition of a macrozone (or microtextured region). High aspect ratio ($>\sim 4$) macrozones are particularly damaging when their long-axes are orientated near-normal to the principal loading direction, such that their basal planes are oriented to within ~ 15 degrees to the principal stress direction. These criteria may be useful in guiding the development of a diagnostic experimental measurement tool (based on EBSD or ultrasonics for example) for macrozone detection in components.

1. Introduction

The fatigue and cold dwell fatigue lifetimes of titanium alloy-based aero-engine components depend on chemistry, processing and the resulting microstructure, and particularly crystallographic texture. Processing techniques including ingot hot-working and rolling need to be designed to produce appropriate microstructures for the different components and their respective applications. Cold dwell fatigue failure is associated with highly stressed components (notably discs) within gas turbine engines which undergo stress holds (the dwell periods) within the fatigue cycle at low temperature (e.g. $T < 0.4T_m$). The early failure resulting from the dwell period compared with conventional fatigue life is known as the dwell debit, and has been recognised since the 1970s [1–3].

Under dwell fatigue loading, facet nucleation may be triggered and is often argued to be associated with clusters of neighboring grains that have similar crystallographic orientations in an unfavorable alignment with respect to the loading direction. The latter are referred to as macrozones, microtextured regions (MTRs) or effective structural units. In service, the required failure rate for aircraft discs is typically less than one in 10^8 flight cycles [4] and the detected defect ratio should be less than one per 500-ton weight melted [4]. In passing, it is noted that cyclic and pure creep deformations can also lead to facet nucleation.

Macrozones, in contrast to the microstructure observed by optical microscopy, are argued to be particularly important with respect to crack nucleation and resulting lifetime reduction under dwell fatigue. The formation of macrozones has been suggested to be caused by variant selection and the resulting crystallographic relationship maintained between HCP α (secondary α_s or primary α_p) and BCC β grains during phase transformation in the processing route [4–6]. These local texture heterogeneities are widely observed in α and $\alpha + \beta$ titanium alloys including Ti-6Al-4V [7–9], Ti-6242 [10], Ti-7Al [11], and IMI-834 [12]. The crystallographic and morphological features of the macrozone are distinct from the apparent microstructure. Macrozones often have one or more very large morphological length scales ~ 1 to 5 mm and sometimes up to 10 mm as shown in Figure

1, compared with an apparent average grain size of ~ 20 to $100\ \mu\text{m}$. During manufacture, macrozone c-axes may preferentially orient perpendicular to the rolling direction, whereas the neighboring regions have very different crystallographic orientation, as shown in Figure 1 (c) and (d). This means that for a given loading direction, the neighboring region of the macrozone may be well aligned for slip (and hence a soft region) whereas the macrozone is unfavorably aligned for slip with respect to the loading direction (and hence a hard region). The resulting “hard” and “soft” neighboring regions potentially allow more significant load shedding and higher stress magnitudes during dwell fatigue, which potentially trigger facet failure in the hard macrozone. Quasi-cleavage facets have been reported on near-basal planes within hard macrozone regions of IMI-834 and Ti-6242 under cold dwell fatigue [12,13]. A mismatch between the dwell fatigue facet plane and the basal plane has been reported in multiple near- α titanium alloys [13–15]. A detailed study on Ti-6242 of cold dwell debit has been reported for samples with differing area fractions of macrozones [16]. Loaded with a dwell time of two minutes, a strongly macrozoned sample exhibited a dwell debit of 18 when loaded to 95% of the yield stress whereas a debit of only six was observed for a weakly macrozoned sample [17]. However, the intrinsic mechanistic basis by which macrozones influence dwell facet nucleation and increasing dwell debit is not clear and in addition, a working definition of a macrozone (or MTR) has yet to be established.

Figure 1 Experimentally observed (a) macrozone free, intermediate and strong macrozone microstructures from top to bottom within Ti-6Al-4V [18]; (b) large-scale macrozones within Ti-6Al-2Sn-4Zr-2Mo [10]; (c) crack nucleation site within a macrozone in IMI 834 [12]; (d) clear neighboring macrozones with different crystallographic orientations in Ti-6Al-4V [8].

Much work has been carried out to understand the mechanistic basis of the load shedding phenomenon from soft to hard grains in titanium alloys under cold dwell fatigue. Creep in the soft

grain was found to cause the redistribution of stress onto the hard grain (termed load shedding) during the dwell period [19]. Discrete dislocation studies have shown this local creep behavior results in high grain boundary stresses [20] which may induce the subsequent crack nucleation. Experimental techniques [13,21] have been utilized to verify the prismatic slip accumulation within soft grains, which induces the basal stress concentration at the hard grain and potentially the subsequent crack nucleation within the hard grain. Modelling studies of both quasi-2D and 3D primary α phase polycrystals [22–26] have been carried out to investigate the local stress development during dwell fatigue loading, and to include crack nucleation criteria. Homogenization methods employing crystal plasticity have been applied to predict the lifetime of Ti-7Al [11] and Ti-6242 [27] during fatigue and dwell fatigue loading.

Recent experimental and modelling studies have begun to address explicitly the role of macrozones in fatigue and dwell fatigue and in particular, to investigate macrozone effects on slip initiation and accumulation of slip at hard-soft macrozone boundaries [10,18,28–31]. Here, true 3D geometries of macrozones (MTRs) in alloy Ti-6Al-4V were extracted through combined laser ablation and EBSD, which were then explicitly modelled using crystal plasticity [29]. However, these studies have focused on the interesting question of slip initiation but have not considered the strain rate sensitivity and corresponding creep accumulation in the soft macrozone. In recent work, the strain rate sensitivity has been examined with applied load for differing titanium alloys, and demonstrates the key role of microstructure on the variation of strain rate sensitivity [32]. Further, a mechanistic explanation of hard macrozone morphology and size in dwell fatigue has yet to be fully agreed, and it is argued that this is also necessary in order to provide a useful definition of a macrozone (MTR) which both captures its key properties in influencing dwell fatigue and provides the key parameters to facilitate non-destructive detection using, for example, ultrasonic NDE methods. Hence in this paper, we address the morphology and size of macrozones and in particular show that macrozone geometry and crystallography also plays a definitive role in controlling the redistribution of stress from soft to hard macrozones through creep, and the magnitude of the load shedding on to the hard macrozone. The local stress *states* established by macrozone morphology are shown to be really important in determining hard macrozone stress levels during stress redistribution. High aspect ratio macrozones commonly observed in the literature, generating plane-strain-like conditions, are shown to be particularly damaging in dwell fatigue. The aspect ratio above which the load shedding exceeds a damaging level is quantified for alloy Ti-6Al-4V. As a consequence of the studies on macrozone size and aspect ratio, it has been possible to introduce a definition of a macrozone which can inform ultrasonic methods for their detection non-destructively in, for example, disc components.

In what follows, section 2 presents a study and comparison of stress redistribution which occurs as a consequence of macrozone morphology, and notably aspect ratio, demonstrating the importance of local stress state. Section 3 then presents systematic analyses of macrozone (MTR) morphological and crystallographic features under dwell fatigue leading to the determination of the worst case macrozone and its specification. Section 4 addresses how to define a macrozone and suggests that the two critical features are the hard macrozone c-axis misorientation threshold and the highest macrozone aspect ratio, which are investigated with respect to experimental EBSD scans. Section 5 presents conclusions.

2. Modelling Macrozones in Titanium Alloy Ti-6Al-4V

The crystal plasticity methodology is firstly outlined for alloy Ti-6Al-4V and the necessary property determination presented for this alloy. A model polycrystal containing a hard-soft grain combination is developed which in 3D gives an approximately equiaxed microstructure. A quasi-2D slice is extracted, which contains the hard-soft grain combination, and which is subjected to plane strain (displacement constrained) conditions. The latter is therefore representative of very high aspect ratio macrozones. The 3D and 2D plane strain models are subjected to dwell fatigue loading and a comparison is then presented of the effect of stress state established on the stress redistribution on to the hard grain resulting from soft grain creep. These results motivate the subsequent study in section 3 which systematically analyses the effect of macrozone morphology on dwell fatigue.

2.1 Crystal plasticity model and property extraction

Strain-rate sensitive crystal plasticity is needed for titanium alloy Ti-6Al-4V to capture the creep and stress redistribution during dwell fatigue. The properties for this alloy are obtained by crystal plasticity modelling utilising an homogenised α HCP microstructure and crystal slip rule detailed in [22], which has the ability to capture strain rate sensitivity (i.e. creep behaviour) and the load shedding under dwell loading. The multiplicative decomposition of current deformation gradient $\mathbf{F}$ is given by

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (1)$$

The time derivative of the plastic deformation gradient $\mathbf{F}^p$ is

$$\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p. \quad (2)$$

Based on planar slip occurring through dislocation glide, pinning and thermally-activated release, the plastic velocity gradient $\mathbf{L}^p$ is given by

$$\mathbf{L}^p = \sum_{\kappa} \rho_m b^2 v \exp\left(-\frac{\Delta F}{kT}\right) \sinh\left(\frac{(\tau^{\kappa} - \tau_c^{\kappa})\Delta V}{kT}\right) \mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa} \quad (3)$$

where ρ_m is the initial mobile dislocation density, ΔF the activation energy associated with thermally-activated escape, ΔV the related activation volume, defined by $\gamma_0 b^2 / \sqrt{\rho_0}$ where ρ_0 is the overall dislocation density (γ_0 the representative shear strain magnitude), b the Burger's vector magnitude, v the frequency of dislocation jumps, k the Boltzmann constant and T is the Kelvin temperature. τ^{κ} and τ_c^{κ} are the resolved and critical resolved shear stresses on κ^{th} slip system; $\mathbf{s}^{\kappa}$ and $\mathbf{n}^{\kappa}$ are the direction and normal vectors associated with the κ^{th} slip system. Further details on the incremental stress update, lattice rotation and the finite element implementation have been given in previous work [22,33].

A polycrystal shown in Figure 2 (a-b) containing 125 grains of random orientation is utilized as a representative volume element (RVE) to extract single HCP crystal Ti-6Al-4V property data using the experimental data taken from NASA [34]. The resulting comparison of behaviour from model and experiment over the strain rates and temperatures given is shown in Figure 2 (c). The grain morphology is not known from [34], and since studies suggest that the texture is predominant in equiaxed polycrystals, the simplified grain representation shown is used. The resulting crystal properties are shown in .

Table 1. The experimental stress-strain curves are captured well using this single set of properties for all temperatures and strain rates considered.

Figure 2 CP model and experimental strain rate and temperature sensitivity in Ti-6Al-4V showing (a) the polycrystalline model setup with 125 grains; (b) initial random orientation distribution of the polycrystal; (c) computational and experimental [34] stress-strain curves.

Table 1 material properties for Ti-6Al-4V at 20°C (elastic properties from NASA [34]; critical resolved shear stress $\tau_{c,basal}^{\alpha} = 1.125 \tau_{c,prism}^{\alpha}$; $\tau_{c,pyramidal}^{\alpha} = 3.01 \tau_{c,prism}^{\alpha}$).

Parameters at 20°C		Units	Quantities
Elastic	E_1	MPa	115302
	E_3	MPa	146100
	G_{13}	MPa	35419
	ν_{12}		0.4611
	ν_{13}		0.2191
Plastic	ρ_m	μm^{-2}	5.0
	ρ_0	μm^{-2}	0.01
	ν	Hz	1.0×10^{11}
	b	μm	2.95×10^{-4}
	k	$J \cdot K^{-1}$	1.381×10^{-23}
	ΔV	b^3	27.12
	τ_c^α	MPa	314
	ΔF^α	eV	0.94

2.2 Same section comparison between 3D RVE and quasi-2D plane strain conditions

Texture and morphology data for alloy Ti-6Al-4V have been provided by [35] and are shown in Figure 3 (a). A representative volume element incorporating grain morphology and texture is established using DREAM.3D [36] in a model 3D polycrystal reconstruction from the experimental data which includes i) the crystallographic orientation distribution, ii) the misorientation distribution, iii) the grain size and iv) the grain shape distribution shown in Figure 3 (a). The reconstructed 3D equiaxed grain morphology is shown in Figure 3 (b).

A truncated section is chosen from the 3D RVE to construct an equivalent quasi-2D model for direct comparison and is shown in Figure 3 (c). The 2D model is based on the truncated plane of the full 3D model also shown in Figure 3 (c). The loading applied to both 2D and 3D models is representative of a dwell fatigue cycle which is shown in Figure 3 (a(v)). For the 2D model, the plane-strain condition is applied such that Z-direction displacements are constrained to be zero on the front and back planes. The resulting predicted σ_{22} stress distribution at a soft-hard-soft grain combination immediately after the applied stress hold and σ_{22} stresses along path O-O' are shown in Figure 3 (d).

Stress concentration occurs at the soft-hard grain boundaries for both the 2D and 3D models. However, the stress redistributions, labelled $\Delta\sigma_2$, for the 2D plane-strain case is seen to be substantially higher than that, $\Delta\sigma_1$, for the 3D case in Figure 3 (d). In the former, the constraint imposed by adjacent grains which would otherwise exist in a 3D polycrystal in front and behind those modelled in the 2D case in Figure 3 (c) has been removed but replaced with a simple plane strain constraint. In the latter, however, a full 3D representation is modelled for which the stress redistribution is markedly reduced confirming that the adjacent grain constraint in 3D is

considerably less than that generated by the 2D plane strain condition. In addition, the plane strain constraint imposed on a hard-soft grain combination under dwell stress loading leads to substantially higher stress redistribution on to the hard grain resulting from soft grain creep. This is a simple result that has not been reported before (to the knowledge of the authors) and suggests that local stress state governed by grain or macrozone morphology is potentially important in driving the magnitude of the load shedding on to the hard grain. This indicates that the anecdotal evidence for the damaging effect of macrozones in dwell fatigue may result from particular aspects of macrozone morphology as opposed simply to macrozone size. That is, plane strain conditions have been shown to lead to much higher load shedding suggesting that highly elongated macrozones, that is, those with high aspect ratio, are potentially much more damaging than simply large equiaxed macrozones. Experimental studies suggest that many, if not all, macrozones have high aspect ratios, sometimes of ~ 100 or greater (see Figure 1 for some examples). Hence, we are motivated to examine the stress redistributions and basal stress development in macrozones during dwell fatigue as a function of macrozone aspect ratio, particularly because of the plane strain result discussed above. In the next section, the results of a systematic study are presented.

Figure 3 shows (a) experimental data for a representative forged rotor grade Ti-6Al-4V alloy provided by [35], (b) 3D grain morphology reconstruction, (c) the 2D reconstruction from 3D truncated surface shown and (d) predicted load shedding resulting during the load hold shown in (a) for fully 3D and quasi-2D plane strain analyses. Note that the 3D microstructure is truncated for clarity such that the 2D slice is, in fact, subsurface in the 3D model. In quasi-2D plane strain,

the z-axis displacements of front and back surfaces are constrained to approximate a sub-surface condition.

3. Macrozone Aspect Ratio Affects in Dwell Fatigue

Many experimental investigations have linked macrozones (MTRs) with short dwell fatigue lives but there has so far not been established any causal mechanistic link between the presence of macrozones and the dwell fatigue debit. In this section, we provide evidence that the high aspect ratios associated with macrozone morphologies drive local constraint to approach that of plane strain conditions which transpire to exacerbate the stress redistribution on to grains badly aligned for slip resulting from creep in an adjacent soft grain. The resulting substantially higher hard grain stresses potentially lead to earlier facet nucleation and shorter fatigue lives.

Figure 4 (a) shows a model configuration of a polycrystal which contains an embedded macrozone. Each colour within the polycrystal represents crystallographic orientation. The Z-direction length of the embedded macrozone is varied such that aspect ratios from 1 to 12 are considered. The macrozone itself is depicted in Figure 4 (b) and (c) and comprises, as is often experimentally observed, grains with parallel c-axes interspersed with grains of differing (soft) crystallographic orientation (angle θ of the soft macrozones shown is 10.5°) which is chosen to replicate the worst case scenario for dwell fatigue [20]. Here, the grains with parallel c-axes are prescribed to have their c-axes orientated parallel to the remote loading direction and within the macrozone, alternate with soft oriented grains. The grains not contained within the macrozone, and shown in Figure 4 (a), are assigned arbitrary, random orientations. The model surfaces intersecting the origin are prescribed to have zero normal displacement as shown in Figure 4 (b). A dwell fatigue cycle of loading is imposed in the Y-direction on the top surface of the polycrystal and normal to the long axis of the macrozone with peak stress hold 862 MPa and load hold time of 120 seconds as shown in Figure 4 (d).

The macrozone (Z-direction) length is varied from one cyclic analysis to the next to examine the effect of its aspect ratio on the stress redistribution which results during the applied stress dwell. The macrozone aspect ratio r is defined as the length of the macrozone L_n divided by the grain size a ,

$$r_n = \frac{L_n}{a} \quad (4)$$

where the macrozone length L_n is changed from $L_1 = a$ to L_{max} (giving aspect ratios of 1 to 12).

Quasi-2D polycrystal configurations under both plane strain and plane stress conditions are also analysed for comparison and are shown in Figure 5 (a-b) (constraint-free front surface for plane stress conditions), and subjected to the same stress loading. Crystallographic orientations are set to be the same as the mid-section of the 3D polycrystalline material with embedded macrozone. The plane strain model provides the extreme case approached by the 3D macrozone model as the macrozone aspect ratio becomes very large, as shown schematically in Figure 5. The plane stress model is representative of the behaviour of a macrozone which impinges on a free surface. This is interesting because locations of dwell fatigue facets have predominantly been found sub-surface, particularly so in aero-engine components such as compressor discs, so this analysis may provide an explanation for the experimental and component observations.

Figure 4 shows a polycrystal containing an embedded macrozone. (a) Geometry, where colour indicates crystal orientation; (b) macrozone embedded in the bulk polycrystalline material (multiple lengths of macrozone are considered as indicated); (c) crystallography of the macrozone; (d) dwell loading history (applied in the Y-direction).

Figure 5 polycrystal models for (a) plane strain and (b) the same orientation combination as the macrozone in Figure 4. For plane stress conditions, the front surface in (a) is free from constraint while other boundary conditions remain the same as those for plane strain.

Figure 6 Schematic of the quasi-plane-strain condition for a high aspect ratio macrozone.

Figure 7 shows the σ_{22} stresses (equivalent to the basal stresses for the hard grains) distributions after stress hold at the mid-section of the macrozone (Figure 7(a)) and for the quasi-2D plane strain and plane stress models. Two extreme cases of the macrozone aspect ratio $r = 1$ and $r = 12$ are compared together with those for the plane strain and plane stress conditions. In all cases at the end of the stress hold, the local σ_{22} (basal) stresses (Figure 7(b-e)) within the hard grain peak at the grain boundaries of the soft-hard pairs. The effect of macrozone aspect ratio r is demonstrated to be important and it is noted that for high aspect ratio, the stress distribution and magnitude are

as anticipated similar to those developed under plane strain conditions. With a macrozone aspect ratio of $r = 12$, the peak stress achieved is substantially higher than that for the low aspect ratio. The peak stress σ_{22} for aspect ratio $r = 1$ is lower, and its location is different from all the other cases, while still at the hard-soft grain boundary. The high stress generated in the macrozone with high aspect ratio (or similarly for the case of plane strain conditions) is driven by the more severe creep development in the neighboring soft grain as shown in Figure 7(c) and (g). Previous investigations in IMI-834 [37] make clear that dwell fatigue cycling leads to progressive creep ratcheting in the soft grain and corresponding increasing basal stress in the hard grain. A high aspect ratio macrozone is therefore far more damaging under cyclic loading than an equiaxed macrozone. The plane stress result shown in Figure 7 (b) shows significantly lower stress build up at the hard-soft grain boundary to the extent that it demonstrates that high aspect ratio macrozones are most damaging only when located significantly sub-surface. The stresses established by the macrozone (even if high aspect ratio) on a free surface are sufficiently low such that their damaging effect is marginal (see later) and hence the result provides a mechanistic explanation for the absence of observations of free-surface dwell facet nucleation. In contrast, the highly damaging effect of high aspect ratio macrozones which only generate the appropriate (approximately plane strain) stress states sub-surface provides persuasive explanation of the observation of sub-surface facets in aero-engine discs [38]. Recent multi-scale modelling methods by Ozturk et al [11] provide an additional explanation for the preference for facets to be nucleated sub-surface based on appropriate statistically representative polycrystals. However, their study did not examine macrozone morphology and high-aspect ratio effects which are considered here and both effects may therefore be important.

The stress σ_{22} distribution within the soft-hard-soft grain combination along path A-A' is shown in Figure 8 for differing macrozone aspect ratios before and after the stress hold. Just prior to the stress hold, the σ_{22} stress concentration level at the boundary of the soft-hard grain pair tends to decrease as the aspect ratio increases. During the load-up, the hard grain carries the stress and accommodates the corresponding elastic strain, whereas slip and plastic straining occur in the soft grain. During the stress hold, stress redistribution occurs from the soft grain to the hard grain. As the aspect ratio increases, the load transfer magnitude increases since the creep in the adjacent soft grain also increases during the load hold (see later in Figure 9 (b)). For the point in the loading history immediately after the stress hold, as the macrozone aspect ratio increases, so the σ_{22} stress concentration within the hard grain at the grain boundary increases as shown in Figure 8 (c).

Figure 7 shows (a-d) stress σ_{22} and (e-h) strain ϵ_{22} distributions within the soft-hard-soft grain combination for macrozone ratios $r = 1$ and $r = 12$, and for plane stress and plane strain conditions, all at the end of the applied stress dwell.

Figure 8 spatial distribution of stress σ_{22} along path A-A' (a) before and (b) after the stress hold.

Figure 9 (a) and (b) summarize the evolution of peak stress σ_{22} in the hard grain and effective plastic strain $\hat{\epsilon}^p$ at the adjacent location in the soft grain for differing macrozone aspect ratios during the stress hold (Figure 9(d)). Here effective plastic strain is defined as

$$\hat{\epsilon}^p = \int_0^t \sqrt{\frac{2}{3} \dot{\epsilon}^p : \dot{\epsilon}^p} dt. \quad (5)$$

The peak stress points and the neighboring strain points are marked in the stress and strain distributions respectively in Figure 7. Figure 9 (a) shows that the peak stress σ_{22} level increases rapidly with the remote applied loading and then progressively increases due to local stress redistribution during the remote stress hold, with corresponding creep accumulation in the adjacent soft grain shown in Figure 9 (b). In particular, the macrozone aspect ratio is shown to have a very strong effect with increasing aspect ratio leading to considerable increase in stress in the hard grain resulting from the higher creep strain evolution in the adjacent soft grain.

The maximum peak stresses σ_{22} achieved both at the end and the beginning of the stress hold for given macrozone aspect ratio r_n are shown in Figure 9 (c), together with the corresponding stresses determined from the plane stress and plane strain analyses. The result makes clear that as the macrozone aspect ratio increases, so the peak stress σ_{22} (at the mid-section of the hard macrozone)

after the stress dwell increases, progressively approaching a saturated value corresponding to the conditions given by plane strain. Conversely, the peak stress at the beginning of the stress dwell decreases with increasing aspect ratio. The peak stresses both before and after stress dwell are found to saturate with a macrozone aspect ratio of 10 or higher. The plane stress condition results in an intermediate stress σ_{22} lying between that for a macrozone with lowest and highest aspect ratio. Figure 9 (d) shows the stress redistribution during stress dwell onto the hard grain as a function of aspect ratio making clear that the effect of the latter occurs predominantly during the stress dwell period. In addition, the plane stress condition gives an intermediate load transfer, but still higher than that resulting from the equiaxed condition (i.e. macrozone aspect ratio of 1) indicating that sub-surface macrozones with high aspect ratio are the most damaging, followed by free-surface-impinging macrozones. Equiaxed conditions are least damaging.

Figure 9 shows the effect of macrozone aspect ratio on (a) hard grain stress, and (b) adjacent soft grain strain evolution during the stress dwell (see Figure 4(d)). (c) shows the peak hard grain stress prior to and just after the applied remote stress hold against macrozone aspect ratio and (d) the stress redistribution on to the hard grain with increasing macrozone aspect ratio. The results for quasi-2D plane strain and plane stress analyses are also shown in (c) and (d).

We note that other authors have investigated the role of macrozones (of various geometries) [18,29,30] on slip initiation in polycrystal alloys. Here, however, we focus on the interaction of macrozone geometry with the stress redistribution (from the intrinsic crystal rate sensitivity) occurring due to soft grain creep during load hold periods in dwell fatigue. Macrozones have long been associated with facet nucleation in dwell fatigue in aero-engine disc components but the mechanistic explanation has been elusive. The characteristic geometries of macrozones, often having very high aspect ratios, transpire to be crucial, and here we show that subsurface, high aspect ratio macrozones generate a local stress state at hard-soft grain pairs which approaches that of plane strain. Interestingly with these conditions, during remote stress hold, the creep of the soft grain leads to a non-intuitive increase in the stress redistribution on to adjacent hard grains thus pushing up the local basal stress making this condition the most damaging for facet nucleation. An aspect ratio of ~ 4 or greater was found to be necessary to drive the highest basal stresses due to stress redistribution. Hence there is a very clear reason why macrozones should be associated with preferential sub-surface facet formation. When the high-aspect ratio macrozone impinges on a free surface, giving rise to conditions of plane stress, the stress redistribution is less pronounced leading to lower hard grain basal stresses and less likelihood of facet nucleation. Hence dwell facets are predicted to be preferentially nucleated sub-surface as observed in disc spin tests [38], and at macrozones. Macrozone aspect ratio does therefore seem to be important in dwell fatigue, and hence a potential key measure with which to define a macrozone. However, the directional nature of the high aspect ratio is also important since the plane strain effect resulting from it only comes in to play when the applied loading is normal to the direction of the highest macrozone length. The next section addresses another attribute which is also important in a possible definition.

4. Macrozone Crystallographic Orientation with Respect to Remote Loading

Experimental characterization of macrozones indicates that sometimes, a clear region of uniform crystallographic orientation of high aspect ratio exists (see Figure 1 (d)) [8] but that other macrozone-like features are more ambiguous with regions which contain many grains with hard-grain orientation interspersed with those which are differently orientated (e.g. Figure 1 (a)) [18]. It is therefore useful to investigate what magnitude of misorientation is necessary before an adjacent grain ceases to be a part of the hard region. Because a key contributor to dwell fatigue is argued to be the high basal stresses established by a hard-soft grain combination, it is appropriate to determine the critical misorientation angle on the basis of the basal stress which results. That is, what misorientation is required above which the adjacent grain should no longer be considered 'hard'.

4.1 C-axis orientation for identifying macrozone size

During dwell fatigue loading, the basal stress developed on the hard grain is argued to be important and is generally highest when the grain's c-axis is near parallel with the remote loading. This, however, can depend crucially on the constraint effect provided by adjacent grains in turn determined by their crystallographic orientations. A consequence is that for a given grain with c-axis perfectly parallel with remote loading, the local primary principal stress direction acting on the hard grain may deviate by 10° or more from the c-axis direction. The macrozone configuration shown in Figure 4 is utilised to investigate the central hard grain orientation angle and its effect on the magnitude of the grain's basal stress. The c-axis orientations with respect to X- and Z-

directions are considered separately for the central hard macrozone and the orientations of surrounding macrozone grains are set the same as those in Figure 4. Rotations from 0 to 90° about the X- and Z-axis are defined separately as δ_1 and δ_2 , respectively.

Figure 10 shows (a) the high aspect ratio macrozone embedded in an equiaxed polycrystal and (b) the crystal orientation changes to the central hard grain of the macrozone region by rotating through δ_1 and δ_2 about X- and Z-directions, respectively.

The dependence of the peak basal stress after the remote stress hold on the central hard grain orientation is shown in Figure 11. Here the basal stress σ_{basal} is given by

$$\sigma_{\text{basal}} = (\sigma \mathbf{n}) \cdot \mathbf{n} \quad (6)$$

where $\mathbf{n}$ is the normal to the crystal basal plane. Peak basal stress is seen to decrease with increasing c-axis rotation away from the loading direction as anticipated. The basal stress approaches zero with a rotation about the Z-axis of 90° since the crystal basal plane becomes parallel to the remote loading direction (no shear) but a rotation of 90° about the X-axis leads to a significant reduction in basal stress to ~400 MPa but it remains non-zero because of the plane strain constraint (normal to the basal plane). A re-orientation of up to 15° (in either direction) is found to lead to a decrease in peak basal stress of less than 10%, but the latter increases to over 15% of the total stress level with ~25° rotation about either X or Z axes.

Figure 11 shows the basal stress after the stress hold at the same peak location as a function of crystal rotations of δ_1 and δ_2 about X- and Z-directions.

Determining a threshold stress for which a given ‘hard’ grain orientation is considered to have become ‘soft’ for given loading direction is arbitrary but on the basis that a decrease of 10% in basal stress arises from a c-axis orientation deviation of 15° away from the remote loading direction (or strictly, the local primary principal stress direction), we choose the latter as the threshold crystal orientation deviation at which the potential for macrozone damage is sufficiently reduced. Hence, a further attribute required for the definition of a macrozone is for the hard grains within the macrozone to have c-axis orientations within 15° of the local primary principal stress direction (strictly) but which we relax for simplicity here to the remote loading direction (pragmatically, since this is the only available data for a given component undergoing, e.g., ultrasound examination to identify the presence of macrozones).

Hence we conclude that two key requirements for the definition of a macrozone (or MTR) region are that (i) the hard grains comprising the macrozone (exclusively or partially) have c-axes within 15° of the applied maximum principal stress direction (note that most aero-engine discs carry multiaxial stress states); (ii) the macrozone identified on the basis of crystallographic orientation in (i) has an aspect ratio of four or higher where the high aspect ratio direction is normal to the principal loading direction.

4.2 Assessment of proposed macrozone criteria against experimental EBSD orientation data

EBSD data for a rotor grade Ti-6Al-4V alloy has been provided by [35]. The grain orientations are analysed and any grain with c-axis misorientation less than the threshold is considered to be part of a potential macrozone and its orientation changed to that of a hard grain. Grain crystallographic orientations are specified by three Euler Bunge angles $[\varphi_1, \Phi, \varphi_2]$. Since the third Euler relates only to orientation about the crystal c-axis, the direction of the latter is determined from Euler angles φ_1 and Φ and the corresponding rotation matrix $\mathbf{R}$ relating the crystal reference orientation to its current configuration within the polycrystal is

$$\mathbf{R} = \begin{bmatrix} \cos \varphi_1 & -\sin \varphi_1 \cos \Phi & \sin \varphi_1 \sin \Phi \\ \sin \varphi_1 & \cos \varphi_1 \cos \Phi & -\cos \varphi_1 \sin \Phi \\ 0 & \sin \Phi & \cos \Phi \end{bmatrix} \quad (7)$$

which is shown schematically in Figure 12 (a).

Here the loading direction is defined as $\mathbf{L} = [l_1, l_2, l_3]^T$ and the c-axis $\mathbf{C}$ is $[0,0,1]^T$ in the macroscopic coordinate system. Thus the rotated $\mathbf{C}'$ axis of each crystal is,

$$\mathbf{C}' = \mathbf{R} \cdot \mathbf{C} \quad (8)$$

Thus, the misorientation angle θ between c-axis of crystal and the loading direction is given by

$$\theta = \arccos \left(\frac{|\mathbf{C}' \cdot \mathbf{L}|}{|\mathbf{C}'||\mathbf{L}|} \right) \quad (9)$$

If the c-axis misorientation angle θ is less than the threshold, the grain is provisionally identified as being potentially damaging and its crystal orientation is changed to be the same as a hard grain orientation. Otherwise, the grain is not considered part of the macrozone and retains its original crystal orientation.

Figure 12 illustrates (a) the crystallographic configuration of misorientation between (macroscopic) c-axis and loading direction (y) and (b) the EBSD scan provided by [35] is an IPFZ map with three potential principal loading directions.

Surface EBSD crystal orientation data for a representative forged rotor grade Ti-6Al-4V alloy has been analysed against the macrozone criteria above. The EBSD scan shown in Figure 12(b) provides inverse pole figures for a surface so does not regrettably provide sufficient information from which to capture 3D macrozone geometry. This is important since the macrozone aspect ratio direction (i.e. high length direction) with respect to loading direction transpires (see above) to be crucial. Hence in this analysis based on a single surface EBSD scan, we contrast the differences obtained which result from considering three differing principal loading directions, shown in Figure 13. More generally, access to the full 3D geometry of potential macrozones is essential and

this information may be extracted from orthogonal EBSD scans or possibly in the future from tomographic ultrasonic methods.

Figure 13 shows identified macrozones with c-axes within 15° of the potential loading direction along (a) X direction, (b) Y direction and (c) Z direction. (d) shows those macrozones satisfying the morphological and crystallographic criteria (c-axes within 15° of principal loading direction; morphological orientation $< 15^\circ$; effective aspect ratio > 4).

Figure 13 shows the provisional macrozones which result from applying an angular misorientation threshold of 15° for principal loading directions in the X-, Z- and Y-directions respectively (shown

in red). For loading along the X-axis, only a few potential macrozones are identified in that they satisfy the misorientation criterion. However, they all have characteristic length similar to the average grain size and hence do not satisfy the conditions stated above to qualify as dangerous macrozones (for which an aspect ratio of 4 or greater is required with the high aspect ratio direction being normal to the principal loading). The dwell stresses generated in these grains would likely not exceed that required for facet nucleation. For loading along the Y-direction in Figure 13(b), multiple potential macrozones are revealed within the material. In these macrozones, the c-axis is near parallel (within 15°) to principal loading and the high aspect ratio direction is near perpendicular to the loading direction, which would create the approximate plane strain condition, leading to much higher stress development within each dwell period due to more severe load shedding, as shown in Section 3. For Z-direction loading, several potential macrozones are also identified as shown in Figure 13(c). They are somewhat more sparsely spaced than those for Y-direction loading. Some of their characteristic lengths are smaller than average grain size, such that dwell stress levels would not be anticipated to be critical for facet nucleation because the macrozone aspect ratio condition has not been met. We note in addition that this analysis is based solely on a 2D EBSD scan, for the purposes of establishing a methodology. But in practice, crucial 3D information on macrozone geometry would also be required.

Thus, the dwell debit, which is the ratio of conventional fatigue life to dwell fatigue life, $\eta = t_{\text{fatigue}}/t_{\text{dwell-fatigue}}$, of this 2D microstructure depends on the principal loading direction. In addition, it's clear from, for example, Figure 13(b) that not all of the potential macrozones have their high aspect ratio directions normal to the principal loading direction, but in fact are at some other morphological orientation which also needs to be established in order to define the effective aspect ratio with respect to the remote loading direction.

4.3 Effective length of orientated critical macrozones

The high aspect ratio direction of a macrozone (a region with c-axis aligned within 15° of principal loading) need not necessarily be normal to the loading direction, but what is the relationship between the macrozone morphological misorientation and its effective length which is that normal to the loading direction? (Here, we define the macrozone morphological misorientation as the angle between its high aspect ratio direction and the normal to the loading direction.) This is shown schematically in Figure 14 and arises because the macrozone damaging effect in dwell comes from a high aspect ratio of four or higher with respect to the remote loading direction. Hence, high aspect ratio macrozones with directions which are orientated away from the normal to loading become less damaging. We hence need to establish a threshold orientation below which the aspect ratio is greater than or equal to 4 (see above for this choice of critical aspect ratio).

Figure 14 (a) a high aspect ratio macrozone morphology with principal loading along Y; (b) the effective length L_{effect} of the macrozone with respect to loading direction; (c) the relationship between L_{effect} and orientation angle ω ; and (d) the effective aspect ratio r_{effect} changing with ω .

Figure 14 (c) shows various high aspect ratio macrozones orientated differently to the remote loading direction in which effective length L_{effect} and grain size a_{effect} are also defined. The effective aspect ratio r_{effect} is thus

$$r_{\text{effect}} = \frac{L_{\text{effect}}}{a_{\text{effect}}} \quad (10)$$

and this has been determined over macrozone misorientation angles between 0 and 90° shown in Figure 14 (d) where a misorientation of ~15° or below gives an effective aspect ratio of 4 or larger. Hence the critical aspect ratio criterion required for a potential macrozone to satisfy the criterion to be damaging is that its morphological misorientation is less than 15°. Finally then, returning to the microstructure loaded in the Y-direction indicated in Figure 13 (b), the macrozone aspect ratio criterion taking account of the morphological misorientation is applied which results in a final diagnosis of macrozones shown in Figure 13 (d) for this loading condition.

5. Conclusion

This work presents an assessment of the stresses that are developed in titanium alloy polycrystals containing macrozones (or MTRs) under dwell fatigue conditions and demonstrates particularly that macrozone morphology and crystallographic orientation are both key factors in the magnitudes of the stresses achieved at macrozones. In addition, we put forward some possible criteria which may be useful in defining a macrozone (or MTR). The major conclusions are:

- i) High aspect ratio (above about 4) macrozones are much more damaging than those which are equiaxed since the stress redistribution on to hard zones during dwell fatigue is considerably higher than that for low aspect ratio macrozones. This results from the approximately plane-strain stress states established by high aspect ratio macrozones.
- ii) As a consequence of the above, a high aspect ratio macrozone which is subsurface is much more damaging than one which impinges on a free surface since the former generates stress states of plane strain while the latter produces states of plane stress which result in considerably lower stresses.
- iii) Dwell fatigue facets are observed in experiments and component tests predominantly to be sub-surface and this follows from conclusion (ii).
- iv) The relationship between macrozones and dwell fatigue debit has, until now, remained anecdotal. The mechanistic link between the presence of macrozones and dwell fatigue damage has been established in this paper.
- v) Hard orientated macrozones of high aspect ratio generate high stresses which depend on both crystallographic orientation and aspect ratio ‘direction’ with respect to principal loading direction. As a consequence, essential criteria for defining a macrozone have been introduced. These are that (i) hard macrozone regions must be orientated with their c-axes within ~15° of the principal loading direction, (ii) macrozone morphology must have high aspect ratio of > ~4, and (iii) the high aspect ratio direction must be near normal (within ~15°) to the principal loading direction.

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