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1	On the mechanism of fatigue and dwell-fatigue crack initiation in
2	Ti-6Al-4V
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8	
9	Abstract
10 11 12 13 14 15 16	In the present study, the mechanism of fatigue and dwell-fatigue crack initiation was investigated in Ti-6Al-4V with a bi-modal microstructure. While substantial dwell-fatigue life debit was evidenced, microstructural configurations associated with crack nucleation are similar and suggest a unique mechanism for fatigue and dwell-fatigue loadings. Pairs of α grains well oriented for basal slip and separated by a (0001) twist grain boundary were found to be critical configurations for crack initiation. Intense slip is localized at the boundary and precedes crack formation along this boundary. These findings offer a new understanding and improved crack initiation prediction insights.
17	Keywords
19	Titanium alloys; fatigue; slip; grain boundary; dwell-fatigue

20

21 Main body

Titanium alloys are widely employed for aerospace applications including gas turbine components owing to a combination of superior mechanical properties with a relative low density [1]. In-service conditions imply complex cyclic loadings that include a hold time at high stress. This hold period leads to a reduction in number of cycles to failure [2,3]. This phenomenon, which is referred to as "dwell effect", is a major industrial concern and has been an active research field for more than 40 years. The life debit resulting from the introduction of a load hold is accompanied by a transition from surface to subsurface crack initiation of the crack leading to failure [2–6].

29 Early characterizations of the crystallographic orientation of subsurface initiation facets formed 30 during dwell-fatigue tests revealed that the c-axis of the α titanium lattice is nearly parallel to the loading 31 direction [2,3]. Using electron back-scattered diffraction (EBSD) and electron channeling techniques, it 32 was also evidenced that the facet plane is close to the basal plane [4-6]. As a consequence, the 33 misorientation between the c-axis of initiation α grains and the loading direction (denoted as declination 34 angle in the following) is lower than 15° [6]. Evans and Bache introduced a modified version of the Stroh 35 model in order to include a preliminary slip activity [7]. In this model, basal slip in the initiation grain, 36 which is poorly oriented for $\langle a \rangle$ slip, is triggered by the stress concentration due to a dislocation pile up 37 in an adjacent soft grain. Crystal plasticity simulations were used to update this model [8] to account for 38 load shedding from the soft grain on to the hard grain [9-11] which assists crack nucleation [12-14].

39 Further analyses revealed declination angles up to 45° in α grains where dwell-fatigue facet 40 nucleation occurred [15–18]. Basal slip activity being reported to occur in the 15 ° - 45° range [19–22], it is 41 not clear whether cracks nucleate in hard or soft grains. Interestingly, this orientation domain is the same 42 as reported for surface crack initiation that occurs in the primary α phase during low cycle fatigue tests 43 [23,19,24–26]. In particular, several authors have shown that low cycle fatigue crack nucleation proceeds 44 along basal slip bands in a grains well-oriented for basal slip [19,26-30]. While dwell-fatigue and fatigue 45 crack initiation mechanisms are often addressed as different topics, literature data suggests that it might be 46 rightful to consider a common crack initiation mechanism. This is the main motivation for the 47 investigation of the crack initiation mechanism in Ti-6Al-4V submitted to fatigue and dwell-fatigue 48 loadings reported in the present article.

49 Ti-6Al-4V with a bi-modal microstructure was studied. The microstructure is composed of 50 equiaxed α (α_p) grains and secondary α (α_s) lamellas embedded in a β phase matrix. The surface fraction of 51 the equiaxed α phase is 36% and the mean diameter is about 13 µm. Load controlled fatigue and dwell-52 fatigue tests were carried out using an INSTRON 1362 testing machine with a 100 kN loadcell. The strain 53 was continuously acquired using an extensioneter. Prior to testing, the surface of specimens was polished 54 finishing with a mixture of colloidal silica with a particle size of 0.04 μ m with 10% of H₂O₂. Loading and 55 unloading segments were performed in 1s. The load ratio was equal to 0.1. The peak stress was set to 90% 56 of the 0.2% proof stress, which was determined using a tensile test with a strain rate equivalent to the 1 s 57 loading ramp. The minimum load was held for 1 s and the maximum load was held for 1 s or 120 s in 58 order to obtain fatigue or dwell-fatigue loading conditions. Three fatigue tests and three dwell-fatigue tests 59 were carried out up to failure in order to assess the fatigue and dwell-fatigue lives as they usually exhibit a 60 substantial scatter [31]. Cylindrical fatigue specimens with a diameter of 4.3 mm and a gauge length of 13 61 mm were used for that purpose. This specimen geometry is referred to as T1 in the following.

Additional tests on differing sample types were stopped before failure in order to study crack initiation sites. The features of surface crack initiation sites were investigated using a modified specimen geometry including flat surfaces such as required for EBSD analysis. Three 2.5 mm wide and 8 mm long flat areas were machined on the gauge length of cylindrical fatigue specimens with a 6 mm diameter and a 8 mm gauge length. The flats were regularly distributed around the specimen circumference. Further 67 details about the geometry can be found in [19]. This geometry is referred to as T2 in the following. In 68 order to characterize subsurface dwell-fatigue cracks, a third geometry was introduced to facilitate 69 mechanical sectioning parallel to the surface. This geometry is referred to as T3 in the following. Flat dog 70 bone specimens with a gage length of 10 mm, a gage width of 2 mm and a thickness of 1 mm were used 71 for that purpose.

A JEOL 6100 scanning electron microscope (SEM) was employed to detect initiated cracks and to observe fracture surfaces. The local crystallographic orientations nearby the cracks were characterized using the same microscope which is equipped with an EBSD detector provided by EDAX. A step below 1.5 μm was chosen to accurately describe the local crystallographic orientations. EBSD data were processed using the OIM analysis software. Cross-section views were obtained via focused ion beam milling using a FEI Helios Nanolab G3 CX.

The cumulated plastic strain versus the number of cycles for fatigue and dwell-fatigue tests is shown in figure 1a. The mean cumulated plastic strain at failure is 9% and the average number of cycles to failure is about 3700 for dwell-fatigue tests carried out up to complete fracture (i.e. T1 specimens). For the fatigue tests, the mean plastic strain at failure is 3.6% and the average number of cycles to failure is about 10800. Thus, failure of dwell-fatigue tested specimens occurred at a higher cumulated plastic strain and a lower number of cycles, indicating a substantial dwell debit with the present testing conditions. The number of cycles to failure is reduced by a factor 2.9 with the increased load hold duration.

85

Figure 1 a. Cumulated plastic strain as a function of the number of cycles. Black and grey curves show a higher cumulated plastic stain and a lower number of cycles to failure for the dwell-fatigue tests. For T2 and T3 specimens, only plastic strain accumulation before test interruption is reported. b. Fracture surfaces of specimens tested up to failure showing surface crack initiation for fatigue loadings and subsurface crack initiation for dwell-fatigue loadings

91 SEM micrographs showing typical fracture surfaces are presented in figure 1b for fatigue and 92 dwell-fatigue tested specimens. For the fatigue tests, the crack leading to the failure was initiated at the 93 surface. No such surface crack initiation site was found for the dwell-fatigue tested specimens. However, 94 numerous facets, which occasionally form clusters, are found in the center of these specimen. This 95 observation reveals the initiation of multiple subsurface cracks for the dwell-fatigue test condition.

96 In order to study surface crack initiation on the fatigue tested T2 specimen, the test was 97 interrupted after reaching a cumulated plastic strain of 1%. It corresponds to 2447 cycles. One crack 98 among the 46 observed is presented in figure 2a. No surface crack was found on the dwell-fatigue tested 99 T2 specimen after reaching a similar cumulated plastic strain level, which was achieved after 105 cycles. 100 The dwell-fatigue test was then continued up to a cumulated plastic strain of 2.5%, which corresponds to 101 1333 cycles. 53 surface cracks were found at this stage. An example of a crack found at 2.5% plastic strain 102 is shown in figure 2b alongside with a micrograph showing the same region after 1% plastic strain. A 103 dwell-fatigue test on a T3 specimen was interrupted at a cumulated plastic strain of 4% and 941 cycles to 104 investigate subsurface crack initiation. The high cumulated plastic strain was chosen to increase the 105 probability of meeting internal cracks with mechanical sectioning. A 300 µm thick layer was removed and 106 20 subsurface cracks were found. A typical example is shown in figure 2a. Due to the similar features 107 exhibited by microstructural regions surrounding the initiated cracks for all loading conditions and 108 specimens, they are discussed altogether in the following.

109 As shown in figure 2, all cracks are located within α_p grain clusters and arrested nearby the 110 boundary with transformed β regions for any loading condition. As a limited growth of surface and 111 subsurface cracks occurred, the identification of crack initiation sites was straightforward. Except for sub-112 surface dwell-fatigue cracks where slip markings have been removed by the mechanical sectioning process, 113 slip traces indicate slip activity in α_p grains on both sides of the cracks. The slip traces are parallel to the 114 crack. The crystallographic orientation maps suggest that crack initiation may occur at the boundary 115 between two α_p grains. Examination of the microstructural region shown in figure 2b where dwell-fatigue 116 surface crack initiation occurred was carried out before and after crack nucleation. It reveals that intense 117 slip activity is localized at the interface between two α_p grains and precedes crack formation. Thinner basal 118 slip traces are noticed in the surrounding α_p grains. The crack plane was investigated in 3D using a cross

- 119 sectional view realized by FIB milling. The sharp crack extends until a grain boundary. Its path matches
- 120 the basal planes on both sides of the crack in 3D. As no boundary is visible on the cross-sectional view,
- 121 cracking is likely to occur along a (0001) twist boundary, which would then be aligned with the basal plane.
- 122 These features are analyzed with a statistical significance in the following.
- 123

Figure 2 a. SEM micrographs and inverse pole figure maps along the loading direction showing initiated cracks and the surrounding microstructure on the surface of the fatigue tested T2 specimen, on the surface of the dwell-fatigue tested T2 specimen and in the bulk of the T3 dwell-fatigue tested specimen at different cumulated plastic strain levels and b. Micrographs of a microstructural region where crack nucleation occurred on surface of the T2 dwell-fatigue tested specimen alongside with the inverse pole figure map along the loading direction and a cross-sectional view of the crack realized using FIB milling.

The inverse pole figure shown in figure 3a reveals that the initiation α_p grains exhibit similar 130 131 orientations for any loading condition and for surface or subsurface initiation. In particular, most grains 132 exhibit declination angles between 10° and 60°. The angle between the basal plane trace and the crack 133 path, which is denoted as \varkappa in the following, has been measured on both sides of all cracks. This angle is 134 schematically represented in figure 3b along with the corresponding distribution frequencies. A maximum 135 frequency is observed for values lower than 5°. The basal plane trace is thus aligned with the crack path 136 for any loading condition and both surface and subsurface cracks. As this statement holds for subsurface 137 crack initiation, where the observation plane is randomly set during mechanical sectioning, the crack 138 seemingly matches the basal plane in 3D.

139 The crystallographic misorientation across all cracks has been characterized as well and its 140 distribution is plotted in figure 3c. While most values are lower than 30°, the maximum frequencies are 141 obtained in the 10°-20° range. These values are too high to result only from crack opening. This is 142 supported by the SEM micrograph of figure 3b that shows a crack opening about 1°. Therefore, a 143 boundary seems present at crack initiation sites. As this holds for subsurface crack initiation, where the 144 observation plane is randomly set during mechanical sectioning, the crack seemingly matches the 145 boundary plane in 3D. Only 10 - 15 % of cracks is found in the $[0^{\circ}-5^{\circ}]$ interval, where no boundary might 146 be present. The misorientation between the c-axis of α_p grains on both sides of the crack, which is 147 denoted as χ in the following, was also measured. The associated distribution frequencies are shown in 148 figure 3d. Most χ values are lower than 5°. The interface between α grains is thus a (0001) twist grain 149 boundary. This feature is consistent with the similar basal plane traces on both sides of the cracks.

150

Figure 3: a. Crystallographic orientation along the loading direction of the initiation α_p grains for fatigue
 and dwell-fatigue loadings, Distribution frequencies of b. x, c. Misorientation and d. χ for all test
 conditions demonstrating the presence of a (0001) twist boundary with a misorientation lower than 30° and
 that cracks are aligned with the basal and the twist boundary planes.

155 Several comments can be made about the previously identified features. Interestingly, no crack 156 was detected in grains with a declination angle lower than 10° while it could be expected according to the 157 dwell-fatigue crack initiation model initially proposed by Evans and Bache. In contrast, the analysis of the 158 crystallographic orientation of initiation α_p grains is consistent with the works of Uta et al. [17] and Pilchak 159 et al. [18]. Such orientations are associated with basal slip and lead to a combination of high normal and

160 resolved shear stress acting onto the basal plane [19,20,22,32]. Our observations are also consistent with

161 prior studies showing that the orientation of the crack matches the basal plane trace [19,23,24,27,28].

162 However, the specific role of (0001) twist boundaries had not been reported yet.

163 For instance, Bridier et al., who investigated fatigue crack initiation in Ti-6Al-4V with a similar 164 microstructure, have not reported the presence of such boundary at crack initiation sites [19]. The data 165 are presently revisited in order to clarify the potential role of (0001) twist boundaries. In that study, strain controlled fatigue tests were carried out with a frequency of 1 Hz, a strain ratio of 0 and a total strain 166 167 amplitude of 0.4 %. A micrograph of a secondary crack alongside with the associated crystallographic 168 orientation map are presented in figure 4a and 4b. The misorientation profile across the crack at the 169 nucleation site is also shown. The 14° rotation around the c-axis confirms the presence of a (0001) twist boundary. Such boundary is thus critical for fatigue and dwell-fatigue crack nucleation under a wide range 170 171 of loading conditions. Although the tests carried out in the present work involve a restricted volume and a 172 high stress in comparison with aero-engine components, they show that fatigue and dwell-fatigue crack 173 initiation are not necessarily related to different mechanisms. Tympel et al. and Wang et al. have reported 174 the presence of low angle (0001) twist boundaries accommodated by dislocation networks close to crack 175 initiation sites [33,34]. However, the underlying mechanism is still unclear. Stress concentration is unlikely 176 as i. no difference in elastic behavior is expected on both sides of such an interface due to the transversely 177 isotropic behavior of a titanium and ii. an effect of plastic anisotropy is also unlikely as boundaries with 178 twist angles as low as a few degrees were noticed. Interestingly, detailed transmission electron microscopy 179 characterization by Liu et al. suggested a presence of nanometric body centered cubic β-Ti layers on such 180 interfaces [34], which may allow the intense and localized slip that eventually leads to crack nucleation. 181 Further investigations are on-going.

182

183Figure 4: a. Secondary crack initiated in Ti-6Al-4V under strain controlled fatigue testing, b. The184corresponding crystallographic orientation map along the loadings direction taken from [19] and c.185Misorientation profile with respect to the origin along the I path of figure 4a showing the presence of a186(0001) twist boundary at the crack initiation site

187 In summary, crack initiation was investigated in Ti-6Al-4V with a bi-modal microstructure 188 submitted to fatigue and dwell fatigue loadings. The material was found dwell sensitive with a substantial 189 life debit for the applied test conditions. Surface and sub-surface crack nucleation sites exhibit similar 190 features for both fatigue and dwell-fatigue loadings. This finding suggests a common crack nucleation 191 mechanism with the following characteristics:

- The critical microstructural configuration for fatigue and dwell fatigue crack initiation is a α_p grain
 pair separated by a (0001) twist boundary. The associated misorientation is most frequently in the
 10° 20° range and the boundary plane corresponds to the basal planes.
- Both α grains exhibit a declination angle in the 10°-60° range, which favors basal slip activity and
 a high normal stress.
- Intense and localized plasticity occurs at the (0001) twist boundary before crack nucleation.
- The crack formation proceeds along the basal plane / the twist boundary.

199

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3 µm

FIB milling artifact Grain

boundary















b.







Fatigue and dwell-fatigue crack formation at (0001) twist boundaries

