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

17
18 **Keywords**

19 Titanium alloys; fatigue; slip; grain boundary; dwell-fatigue

20

21 Main body

22 Titanium alloys are widely employed for aerospace applications including gas turbine components
23 owing to a combination of superior mechanical properties with a relative low density [1]. In-service
24 conditions imply complex cyclic loadings that include a hold time at high stress. This hold period leads to
25 a reduction in number of cycles to failure [2,3]. This phenomenon, which is referred to as “dwell effect”, is
26 a major industrial concern and has been an active research field for more than 40 years. The life debit
27 resulting from the introduction of a load hold is accompanied by a transition from surface to subsurface
28 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 $15^\circ - 45^\circ$ 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 α 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 $13 \mu\text{m}$. 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 extensometer. Prior to testing, the surface of specimens was polished
54 finishing with a mixture of colloidal silica with a particle size of $0.04 \mu\text{m}$ with 10% of H_2O_2 . 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.

62 Additional tests on differing sample types were stopped before failure in order to study crack
63 initiation sites. The features of surface crack initiation sites were investigated using a modified specimen
64 geometry including flat surfaces such as required for EBSD analysis. Three 2.5 mm wide and 8 mm long
65 flat areas were machined on the gauge length of cylindrical fatigue specimens with a 6 mm diameter and a
66 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.

72 A JEOL 6100 scanning electron microscope (SEM) was employed to detect initiated cracks and to
73 observe fracture surfaces. The local crystallographic orientations nearby the cracks were characterized
74 using the same microscope which is equipped with an EBSD detector provided by EDAX. A step below
75 1.5 μm was chosen to accurately describe the local crystallographic orientations. EBSD data were
76 processed using the OIM analysis software. Cross-section views were obtained via focused ion beam
77 milling using a FEI Helios Nanolab G3 CX.

78 The cumulated plastic strain versus the number of cycles for fatigue and dwell-fatigue tests is
79 shown in figure 1a. The mean cumulated plastic strain at failure is 9% and the average number of cycles to
80 failure is about 3700 for dwell-fatigue tests carried out up to complete fracture (i.e. T1 specimens). For the
81 fatigue tests, the mean plastic strain at failure is 3.6% and the average number of cycles to failure is about
82 10800. Thus, failure of dwell-fatigue tested specimens occurred at a higher cumulated plastic strain and a
83 lower number of cycles, indicating a substantial dwell debit with the present testing conditions. The
84 number of cycles to failure is reduced by a factor 2.9 with the increased load hold duration.

85

86 **Figure 1 a. Cumulated plastic strain as a function of the number of cycles. Black and grey curves show a**
87 **higher cumulated plastic stain and a lower number of cycles to failure for the dwell-fatigue tests. For T2**
88 **and T3 specimens, only plastic strain accumulation before test interruption is reported. b. Fracture surfaces**
89 **of specimens tested up to failure showing surface crack initiation for fatigue loadings and subsurface crack**
90 **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

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

130 The inverse pole figure shown in figure 3a reveals that the initiation α_p grains exhibit similar
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 κ 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

151 **Figure 3: a. Crystallographic orientation along the loading direction of the initiation α_p grains for fatigue**
152 **and dwell-fatigue loadings, Distribution frequencies of b. κ , c. Misorientation and d. χ for all test**
153 **conditions demonstrating the presence of a (0001) twist boundary with a misorientation lower than 30° and**
154 **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
166 controlled fatigue tests were carried out with a frequency of 1 Hz, a strain ratio of 0 and a total strain
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
170 boundary. Such boundary is thus critical for fatigue and dwell-fatigue crack nucleation under a wide range
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 α 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

183 **Figure 4: a. Secondary crack initiated in Ti-6Al-4V under strain controlled fatigue testing, b. The**
184 **corresponding crystallographic orientation map along the loadings direction taken from [19] and c.**
185 **Misorientation profile with respect to the origin along the I path of figure 4a showing the presence of a**
186 **(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:

- 192 • The critical microstructural configuration for fatigue and dwell fatigue crack initiation is a α_p grain
193 pair separated by a (0001) twist boundary. The associated misorientation is most frequently in the
194 10° - 20° range and the boundary plane corresponds to the basal planes.
- 195 • Both α grains exhibit a declination angle in the 10°-60° range, which favors basal slip activity and
196 a high normal stress.
- 197 • Intense and localized plasticity occurs at the (0001) twist boundary before crack nucleation.
- 198 • The crack formation proceeds along the basal plane / the twist boundary.

199

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203 11-LABX-0017-01)

204

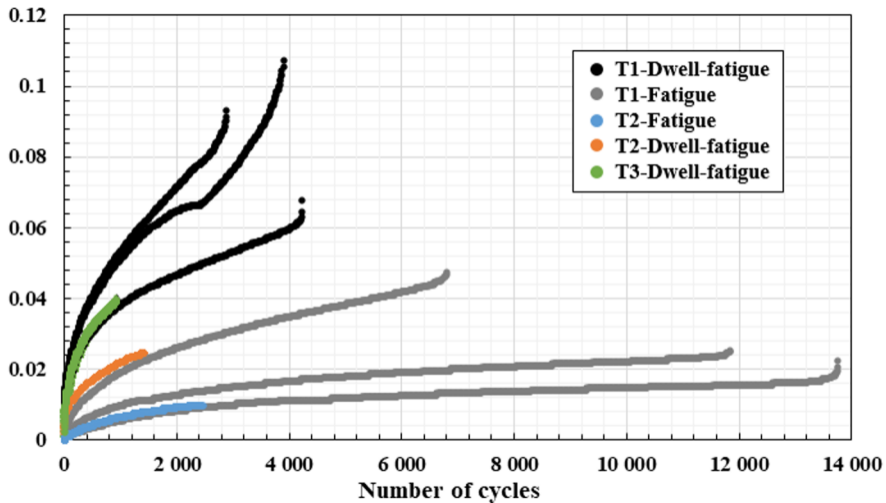
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a.

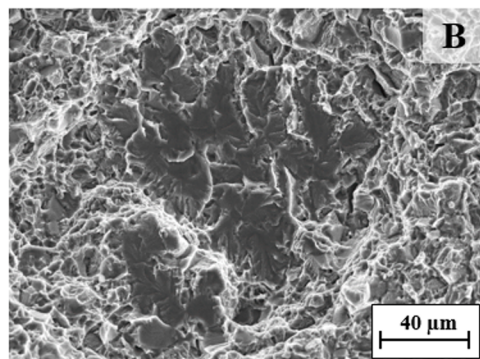
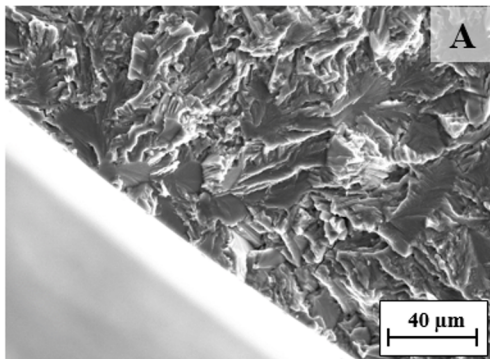
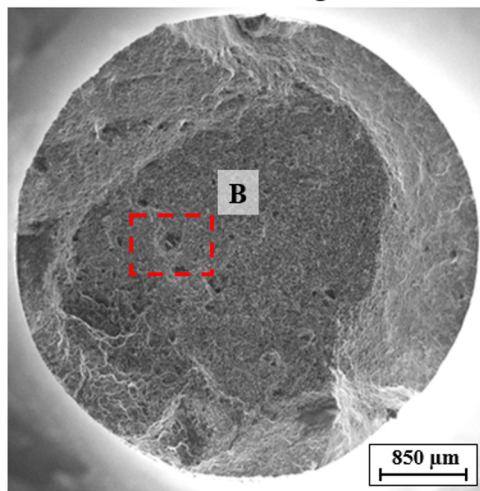
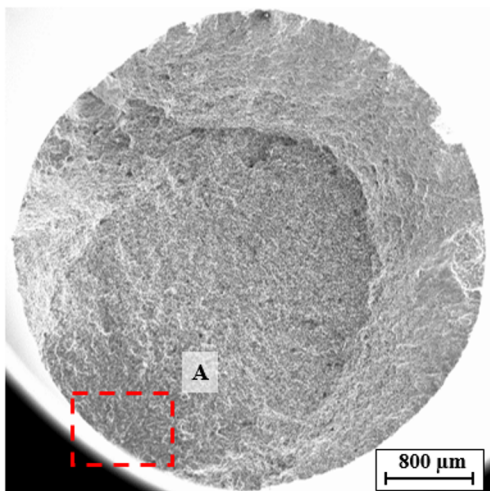
Cumulated plastic strain



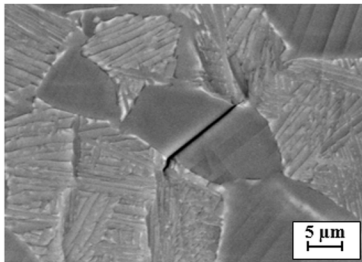
b.

T1- Fatigue

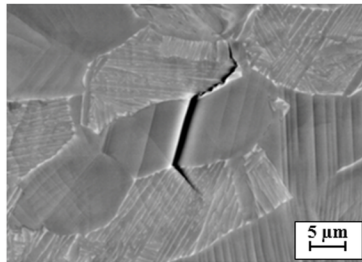
T1- Dwell-fatigue



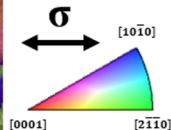
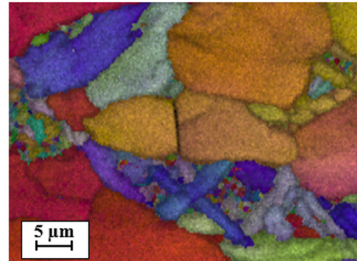
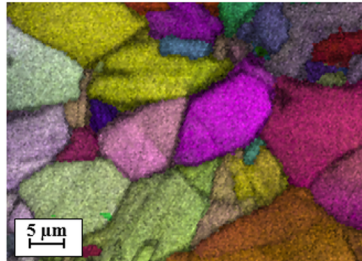
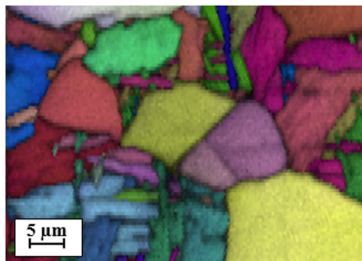
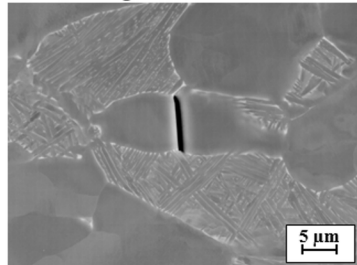
a. Fatigue – surface – T2



Dwell-fatigue – surface – T2

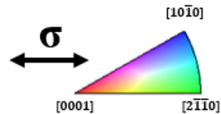
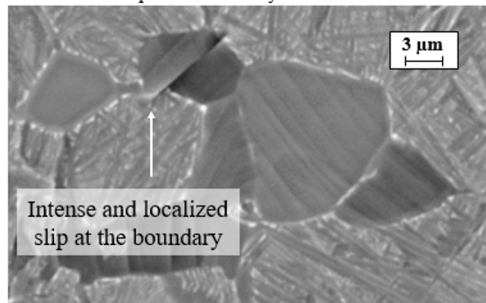
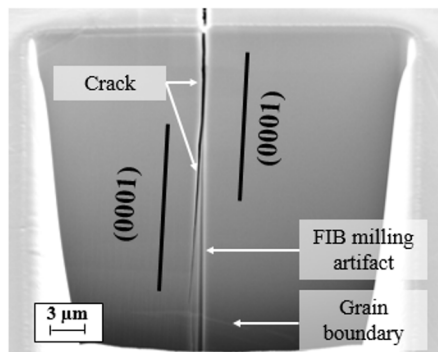
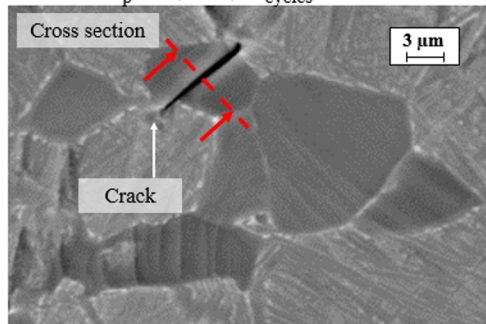


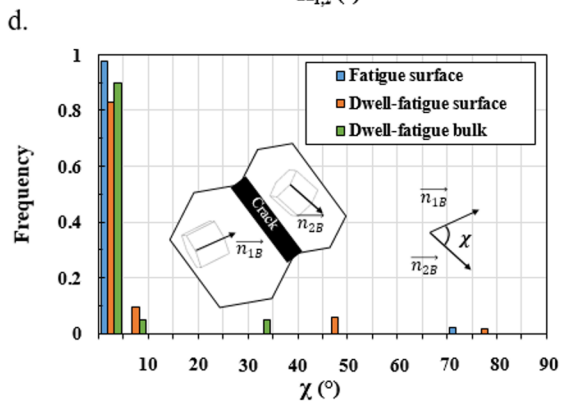
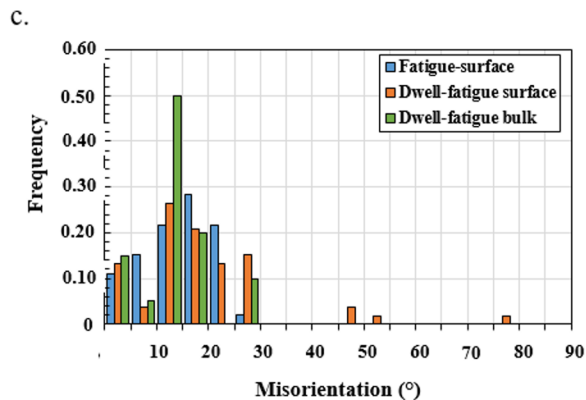
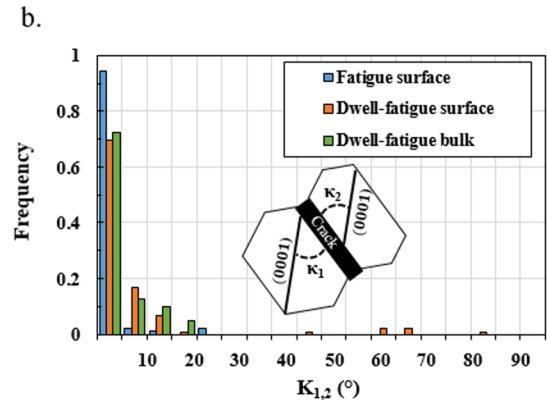
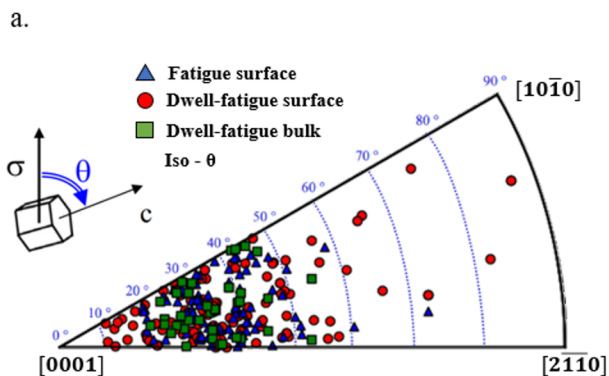
Dwell-fatigue – subsurface – T3



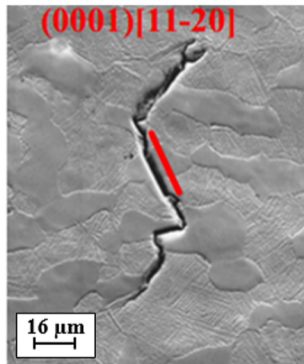
b.

Dwell-fatigue – surface – T2

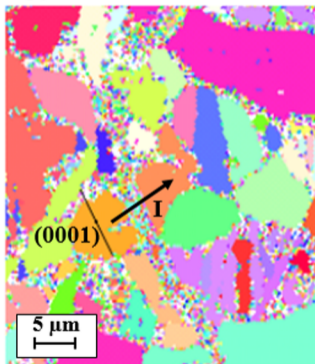
 $\varepsilon_p = 1\% ; N_{\text{cycles}} = 105$  $\varepsilon_p = 2,5\% ; N_{\text{cycles}} = 1438$ 



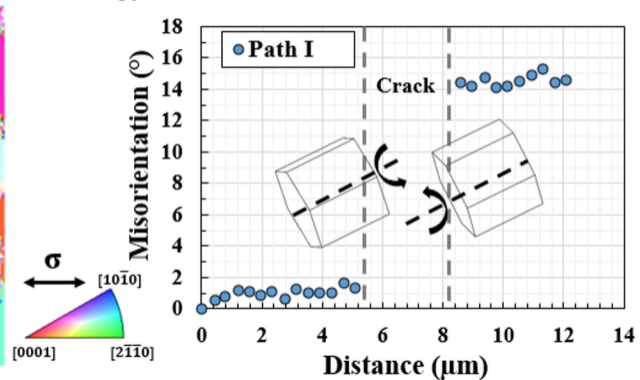
a.



b.

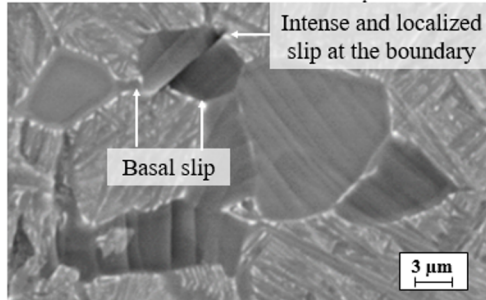


c.



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

After 105 dwell-fatigue cycles and $\epsilon_p = 1\%$:



After 1438 dwell-fatigue cycles and $\epsilon_p = 2,5\%$:

