Plastic strain localization and fatigue micro-crack formation in Hastelloy X

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1. Introduction

Fatigue crack initiation is a complex phenomenon for which a comprehensive quantitative understanding is still in progress [1]. Part of the intricacies are associated with the fact that the local deformation response and the driving forces for fatigue crack initiation can vary depending on material composition, microstructure, loading conditions, etc. [2]. In the case of pristine materials, the formation of persistent slip bands (PSBs) and their interactions with grain boundaries (GBs) have been identified as a primary source of crack initiation [3–8]. In general, it is widely accepted that localized plastic deformation, which is a precursor to PSB formation, is essential for fatigue crack initiation [9]. However, it is less clear how the localization of plastic strains influences the length of the fatigue cracks which initiate later in the fatigue life after strain localization has occurred. In this work, during interrupted loading experiments, high resolution deformation measurements using digital image correlation are made on polycrystalline Hastelloy X subjected to fatigue loading. The sub-grain level strain measurements are made prior to the formation of micro-cracks. The correlation between the localization of plastic strains very early on during the loading (e.g., less than 1000 cycles) and the micro-cracks which are detected later in the life of the sample (e.g., around 10,000) is discussed in this paper. Particular focus is given to the difference in grain boundary response, either blocking or transmitting slip, and the associated fatigue micro-crack lengths generated in the vicinity of these boundaries. The results show a clear correlation between both the locations and lengths of fatigue micro-cracks, which form later in loading, and the localization of plastic strains very early in the loading process. For the same number of cycles, the transmission of slip across grain boundaries resulted in longer transgranular cracks compared to cracks near grains surrounded by blocking grain boundaries which were shorter cracks and confined within single grains.

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reaction and the strain magnitudes across transmitting GBs [26–32]. Another important aspect in slip–GB interaction, which pertains to cyclic loading conditions, is slip irreversibility across the GB resulting in the accumulation of heterogeneous plastic strains with continued loading [6,9,33–35]. In this work, we measure the local heterogeneity of deformation developing under fatigue loading and utilize the results to shed further light into the influence it has on fatigue crack formation. Particularly we focus on the deformation response in the vicinity of GBs which are known to influence fatigue crack formation.

The manifestation of the deformation heterogeneities introduced by GBs at the mesoscale can be in the form of strain localization [26]. An example, also a focus in the current paper, is the interaction of slip with a GB which may lead either to transmission across the boundary or to the creation of a pile-up and blockage of slip as illustrated schematically and with photographs of each case in Fig. 1. The analysis of these types of slip–GB reactions is complicated and may involve leaving residual dislocations in the GB plane (in the case of partial dislocation transmission) or the formation of GB steps (to relieve the high stresses associated with pile-ups) [27,36,37]. Nevertheless, one may generally expect high strains across the interface in the case of transmission and high strains on only the pile-up side in the case of blockage. Fatigue cracks initiating in the vicinity of transmitting and shielding GBs can potentially be different due to variation in the area, i.e., number of grains, with localized plasticity. For example, in the shielding case, slip may be confined in a single grain with a pile-up created at the slip–GB interface and in the case of transmission, slip dislocations continue their motion through transmitting GBs which results in a longer PSB length. Note that transmission of slip through multiple GBs leads to the formation of grain clusters which are important in fatigue failure as discussed by many authors [13,17,38]. The correlation between these two different deformation mechanisms (shielding and slip transmission) in the vicinity of GBs and fatigue crack initiation, particularly the length of fatigue cracks that form upon transformation of the slip band to a finite crack size, requires further investigation. Also, it is noted that no clear connection between slip transfer and crack formation exists. One viewpoint is that as slip is allowed to traverse the GB, and therefore relieve stresses, these transmitting GBs will not crack [39]. Another perspective is that the accumulation of residual dislocations in the case of partial transmission will create stress concentrations and nucleate fatigue cracks. These fundamental issues, and the correlation with fatigue crack lengths, will be addressed in the current paper. The results are important as they shed light into crack formation lengths based on the understanding of deformation mechanisms which localize plasticity in the vicinity of GBs prior to cracking.

From an experimental standpoint, much of the previous works in fatigue has been focused on macroscopic measurements such as nominal stress/strain evolution and fatigue life. Modeling approaches at the same length scale have utilized these works in developing total life models where distinction between initiation and crack propagation is not generally made. These approaches have enabled much progress but do not provide insight into the experimentally observed scatter in fatigue life under similar loading conditions. This scatter has been typically associated with the local microstructure and the influence it has on fatigue crack initiation [40,41]. Also, the microstructural features (e.g., GB types) susceptible for fatigue crack initiation cannot be assessed or predicted. In critical applications, such as in turbine engines, more accurate predictions of the number of cycles to initiate cracks are of great importance and require more refined and focused experimental and modeling work. On the modeling side, several approaches at different length scales have been put forward for local crack initiation predictions (crack initiation models) [41]. For example, researchers have proposed fatigue indicator parameters based on a critical accumulated slip
[42,43], indicators based on the Fatemi–Socie parameter for multi-
axial fatigue [44] which includes the plastic shear strain within slip
bands and the normal stress to the plane of maximum shear strain
[45,46], critical stress, or on energy considerations [47]. In general,
the local strain or stress measurements required for these crack
initiation parameters were obtained using finite element crystal
plasticity simulations, e.g., [13,41–43,47–49]. Other modeling
approaches rely on dislocation–GB interaction. The work of Lin
and Ito [50], Tanaka and Mura [51], and Mughrabi and coworkers
[52] on persistent slip band (PSB) mechanisms provided the basis
for these types of models. More recently, the use of improved
computational tools such as atomistic simulations [17,53] has
enabled much progress in this field. Another body of works has
formulated fracture initiation parameters based on the slip transfer
concept [14,54,55]. These parameters are geometric in nature
related to slip planes and slip directions across GBs, normal to
GB plane, and Schmid factors) and were used to predict the
susceptible GBs for crack nucleation. For the most part, supportive
experimental work with local measurements at the same length
scale as considered in computational studies has been lacking due
to the challenges associated with making such quantitative assess-
ments. Not only microscale strain measurements are required, but
the relation to microstructural features, in particular GBs, is crucial
for model verification, refinement, and to help remove some of the
controversy and ambiguity as to what critical conditions can be
used to predict fatigue crack initiation.

Microstructural analysis of fatigued samples using techniques
as TEM and SEM provided the basis for the fundamental under-
standing of the critical features (e.g., GB types) vulnerable to crack
initiation [2,8]. Nevertheless, it is evident that only a limited
number of cases can be practically investigated using TEM and
SEM techniques. Also, no direct correlation with strain accumula-
tion prior to crack initiation is possible, quantitatively. Full field
defformation measurements at a length scale of individual grains,
but yet over substantial regions spanning 1000s of grains, can
overcome some of the limitations associated with the much
higher resolution TEM and SEM techniques. By surveying large
areas one can focus on critical regions which may not be
observable with a single length scale technique or with focused
analysis on a limited region. Extension of full field measurement
techniques to high resolution assessment of deformation in
relation to the underlying microstructure (characterized using
techniques such as electron backscatter diffraction, EBSD) has
been well demonstrated in the literature for monotonic loading
[56–62] and fatigue crack growth [63]. In previous work by the
authors [26], digital image correlation (DIC), which is one of the
major techniques for full field and local deformation measure-
ments [64], was utilized to study deformation behavior in the
vicinity of GBs with a focus on determining the local slip system
activity, quantitatively, slip transmission across GBs, and the influ-
ence it has on local strain magnitudes in uniaxial tension. There
has been less work, however, considering fatigue crack
initiation in a structural alloy where local strain accumulation
and microstructural information are addressed simultaneously
[65,66]. Such a quantitative assessment of the local material
response and deformation heterogeneities at the microstructural
level can improve our understanding of the localization of plastic
strains leading to fatigue crack initiation. In the current work,
high resolution strain measurements with sub-grain level accu-
arcy are provided in conjunction with microstructural character-
ization in the same region under cyclic loading conditions.

In summary, this paper is focused on the experimental analysis of
fatigue crack formation in polycrystalline Hastelloy X. We utilize
deforation measurements with sub-grain level resolution (from
DIC) and microstructural characterization (from EBSD) to evaluate the
heterogeneous material response under cyclic loading conditions. The
localization of plastic strains is discussed in relation to the micro-
cracks (observed in the SEM) which develop later in the life of the
sample. The correlation between the length of fatigue cracks, which
includes initiation, and micro-crack propagation to lengths where it is
still dominated by the local microstructure (i.e., crack formation)
and the length of strain localization bands (i.e., bands of high strains
surrounded by relatively low strain regions) is established. We further
consider the difference in GB response in blocking and transmitting
slip and demonstrate how these two mechanisms influence strain
magnitudes across GBs and consequently the fatigue crack lengths.

2. Material and methods

2.1. Material and sample preparation

A nickel-based superalloy, Hastelloy X, was considered in this
study. This alloy is known for its oxidation resistance, fabricability,
and strength at elevated temperatures. Strengthening is achieved
through solid-solution heat treatment at 1177 °C (2150 °F). Fatigue
specimens were electro-discharge machined from a 3.2 mm thick
sheet in the as received condition. Hour glass specimen geometry
(i.e., relatively small gage section) was adopted to enable investiga-
tion of the entire gage area for fatigue cracks. The constant
(reduced) gage area was 2.0 mm × 1.0 mm and the thickness was
1.5 mm as shown in Fig. 2a. The selected gage area was the
maximum possible for practical EBSD/high resolution DIC measure-
ments on the entire region.

The surface of the specimen was mechanically polished using
SiC paper (up to P1200) followed by finer polishing using alumina
polishing powder (down to 0.3 μm) and vibro-polishing with
colloidal silica (0.05 μm). The final surface finish was adequate
for microstructural surface characterization using EBSD and was
also sufficient for high resolution deformation measurements
using DIC. Prior to deformation, the microstructure in the region
of interest (marked with Vickers indentation markers) was
characterized using a Scanning Electron Microscope (SEM)
equipped with an EBSD detector (a measurement spacing of
1.5 μm was used). Fig. 2b shows a grain orientation map of the
sample investigated in this study. The total number of grains in the
region of interest was 4492 grains with an average grain
diameter of ~24 μm (annealing twins are considered as indivi-
dual grains in our analysis). The percentage of annealing twin
boundaries (Σ3 type GBs using the coincident site lattice, CSL,
notation) was about 30% of the total number of GBs, which
corresponds to about 65% of the total CSL content.

2.2. High resolution DIC measurements

In DIC, a random speckle pattern is introduced on the sample's
surface (region of interest) before deformation. Optical images of
the undeformed (reference) and deformed surface are captured
and used to track the speckle pattern and therefore measure the
in-plane surface displacement and strain components [64]. Accu-
rate strain measurements with sub-grain level resolution can be
achieved by increasing the imaging magnification [67,68]. The
challenge associated with higher magnification imaging is that it
reduces the field of view and thus imposes limitations on the
area/number of grains that can be studied. The ex situ technique
used in this study, and described in detail in [67], addressed this
problem and enabled high resolution measurements over rela-
tively large areas by capturing enough high magnification images
to cover the required region of interest.

In the results reported in this work, a fine speckle pattern was
achieved by roughening the highly polished surfaces, after EBSD
measurements were completed, with silicon carbide powder
(1000 Grit). Arrays of reference and deformed images were captured using an optical microscope at 25x (0.174 μm/pixel) magnification. The method for creating the speckle pattern and the imaging magnification allowed for a subset size of ~4.7 μm (27 pixels). Arrays of 72 overlapping images, for reference and deformed states, were required to cover the selected region of interest for DIC measurements. In each case, the sample had to be removed from the load frame to acquire the images using the optical microscope. Therefore, the measured strain fields using ex situ DIC represent the residual strains (plasticity dominated) at a particular deformed state after unloading the sample.

DIC correlations were run for each combination of reference and deformed image (72 correlations) and the results across the entire region of interest were stitched together as described in [67]. Alignment with EBSD measurements was accomplished using the Vickers indents as fiducial markers (an example shown in the upper right of Fig. 2b). Establishing this alignment enabled quantitative analysis of the plastic strain fields in relation to the underlying microstructure of the polycrystalline specimen. We note that the speckle pattern quality, selected magnification, and the achieved DIC resolution in this work allows for sub-grain level deformation measurements (average number of DIC correlation points per grain = 600, subset size/average grain size ≈ 0.2) and can therefore resolve the local deformation heterogeneities introduced at the microstructural scale.

2.3. Fatigue loading

After characterizing the microstructure and capturing reference images for DIC, the sample was fatigued in load control at a rate of 0.4 Hz, loading ratio, \( R \), of -1, and stress range of 900 MPa (using a servohydraulic load frame). After 1000 cycles (point marked ‘A’ in Fig. 3), the test was stopped and the sample removed from the load frame to capture deformed images for ex situ DIC. The DIC strain measurements reported in this paper are for this deformed state for which, as will be shown later, no cracks were observed under an optical microscope. Loading was resumed with an additional 9000 cycles (a total of 10,000 cycles, point marked ‘B’ in Fig. 3). Optical images at this deformed state revealed numerous micro-cracks covering the entire gage area and therefore no additional loading cycles were applied except for a half tensile cycle to open the initiated micro-cracks for better visualization (point marked ‘C’ in Fig. 3).

3. Analysis and results

3.1. DIC strain measurements

Fig. 4a shows an example of a selected region imaged before loading (reference images for DIC). The subset size used in this work, also the smallest possible at the selected magnification and speckle pattern quality, is shown with a red box in Fig. 4a. The same region but at deformed state ‘A’ (i.e., after 1000 fatigue loading cycles) is shown in Fig. 4b. No visible cracks were observed at this state given the resolution of the optical system used and the length scale of interest in this work. The red arrows in Fig. 4b point to the regions for which cracks were observed at deformed state ‘B’ (i.e., after 10,000 fatigue loading cycles) as shown in the optical microscope images in Fig. 4c. For better visualization of the initiated micro-cracks, the sample was subjected to a half cycle (state ‘C’, tensile portion of a complete cycle only) to open the cracks, and images were taken in the SEM as shown in Fig. 4d. Through comparison of Fig. 4c and 4d, we note that the optical images (Fig. 4c) provide sufficient resolution to detect the micro-cracks that are clearly observed in the SEM (Fig. 4d). For additional clarity, the regions outlined in Fig. 4a–c are enlarged as shown in Fig. 5). Notice the similarity between the reference images shown in Fig. 5a and the deformed images.
shown in Fig. 5b and that no micro-cracks are visible. Cracking is clear at deformed state ‘B’ as shown in Fig. 5c.

All the DIC deformation measurements are based on correlations between images which contain no cracks as the examples shown in Fig. 4a and b (i.e., between the undeformed state and the deformed state ‘A’ with no micro-cracks observed). Figs. 6a–c show contour plots of the vertical residual strain field $\varepsilon_{yy}$ (along the loading direction), the horizontal strain field $\varepsilon_{xx}$ and the shear strain field $\varepsilon_{xy}$ over the entire gage area after 1000 cycles of loading. These three components of the strain tensor were measured using DIC through differentiation of the vertical and horizontal displacement fields. The measured strains were made ex situ with the sample unloaded and therefore represent residual strains that are plasticity dominated. Any elastic strains are expected to be small and insignificant, although they might still be present because of kinematically imposed constraints of neighboring grains. By assuming plastic incompressibility, the component in the residual plastic normal strain along the third direction, $\varepsilon_{zz}$, was also obtained using:

$$
\varepsilon_{zz} = - \left( \varepsilon_{xx} + \varepsilon_{yy} \right).
$$

Contour plot of normal residual strain field ($\varepsilon_{zz}$) is shown in Fig. 6d.

Microstructural information from EBSD analysis (i.e., crystal orientations and GB locations) was numerically overlaid on the
DIC strain fields. Eventually, for each of the 2,739,321 DIC measurement points in the gage area, four strain components were established ($e_{xx}$, $e_{yy}$, $e_{xy}$, and $e_{zz}$) and the underlying crystal orientation was determined (i.e., Euler angles [69]). By knowing the crystal orientation, the GB locations were established and overlaid on all the strain contour plots in Fig. 6a–d.

Another important advantage of the combined EBSD and high resolution DIC measurements is that the local slip system activity can be quantitatively and spatially estimated by solving the following equation for the crystallographic shear strains:

$$d e_{ij} = \frac{1}{2} \sum_{s=1}^{s} \left( n_s l_x^s + n_s l_y^s \right) d \gamma_{ij} = \sum_{s=1}^{s} \left( m_s^x \right) d \gamma_{ij}$$

where $s$ is the slip system number, $s$ is the number of slip systems (12 for fcc), $n^s$ is the vector defining the normal to slip plane for system $x$, $l^s$ is the vector defining the slip direction (notice that $n^s$ and $l^s$ are known for fcc crystal structure), and $d \gamma_{ij}$ is the shear strain increment for system $x$. Solving for the scalar quantities $d \gamma_{ij}$ at each spatial point (i.e., DIC measurement point) yields local information about slip system activity across the selected region (nonlinear system of equations). The information attained from this calculation are important and can help determine the possible slip–GB reactions as will be shown later in Section 3.3. Details of this calculation procedure along with specific examples and comparisons with slip trace analysis are given in [26].

As it will be advantageous to consider a single strain measure which combines all the measured strain components into one term, an estimate of the effective plastic strain, $\varepsilon_{eff}$, was calculated spatially using the following equation:

$$\varepsilon_{eff}^{xyz} = \sqrt{\frac{2}{3} \left( \varepsilon_{xy} \times \varepsilon_{yz} \right)}$$

Fig. 7 shows a contour plot of the effective plastic strain estimate ($\varepsilon_{eff}^{xyz}$) with GBs overlaid. Heterogeneities in the plastic strain field are clearly observed with many regions showing localized and high strains (up to ~20%). Mean field average = 0.58%. Some of the strain localizations are concentrated around GBs and

Fig. 6. (a–d) Contour plot of the horizontal ($e_{yy}$), shear ($e_{xy}$), vertical ($e_{xy}$), and normal ($e_{zz}$) residual strain fields with overlaid grain boundaries. The reference and deformed images for DIC are a composite of 72 images at 25x magnification. The deformed images were taken after 1000 cycles and showed no evidence of micro-cracks.
others extend through multiple GBs. In the next section, we study the correlation between the localization of plastic strains and crack formations which were observed considerably later in the fatigue life of the sample (deformed state ‘B’ with 10,000 loading cycles).

3.2. Fatigue crack formation and the correlation with prior strain localizations

As explained earlier (Fig. 3), all the DIC measurements were made using deformed images that showed no cracks in the optical

Fig. 7. Contour plot of the effective plastic strain field ($\varepsilon_{\text{eff}}$) across the entire gage area. Heterogeneities in the plastic strain field are clearly observed with many regions showing localized and high strains (up to ~2%). Mean field average = 0.58%. Some of the strain localizations are concentrated around GBs (examples are marked with blue and white arrows) and others extend through multiple GBs (examples are marked with black and white arrows). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 8. Stitched image of the 72 individual deformed images at state ‘C’ (10,000+1/2 Cycles). Micro-cracks of varying lengths are distributed across the entire gage area. The $\varepsilon_{\text{eff}}$ plastic strain field from Fig. 6 prior to crack formation was also overlaid on the optical images. A strong correlation between strain localization and the locations and lengths of the observed cracks is clear from the figure.
microscope (State ‘A’). Crack formation was observed at deformed state ‘B’ after 9000 additional loading cycles. At this stage it is unknown precisely when each micro-crack formed and how it evolved with cycles in the range between 1000 and 10,000 loading cycles. Determining such information would require removing the sample multiple times and would involve considerable amounts of ex situ microscopy. Therefore the exact determination of the number of cycles versus crack lengths is outside the scope of this work. We focus here on the crack formation lengths, which include initiation and micro-crack propagation, and how they are influenced by the strain localizations which were established at an earlier deformed state.

Fig. 8 shows a stitched image of all the high magnification optical images at deformed state ‘C’ (72 images). The \( e_{\text{eff}} \) plastic strain field from Fig. 7 prior to crack formation is also overlaid on the optical images. Visually, we observe many micro-cracks distributed across the entire gage area. The cracks vary in length and no single crack seems to dominate the field. The strains overlay reveals a strong correlation between not only the locations of the observed cracks, but also the crack formation lengths and the high strain regions. To further elucidate this correlation, a specific region is enlarged and shown in Fig. 9. The localized strains in Fig. 9a clearly show examples of accumulation of strain on one side of the GB and strain bands extending across some interfaces. The length of the localized slip bands varies (see for example \( L_{s1} \) and \( L_{s2} \) in Fig. 9a) and correlates very well with the observed cracks shown for the same region in the SEM image in Fig. 9b (compare for example \( L_{s1} \) and \( L_{s2} \) in Fig. 9a to \( L_{C1} \) and \( L_{C2} \) in Fig. 9b).

For a more quantitative assessment of the correlation between the fatigue crack formation lengths and the length of the localized slip bands (i.e., strain localization length), all the lengths of the strain localization regions and fatigue cracks were measured across the entire gage area. A histogram of the strain localization lengths (\( L_s \)) across the entire gage area is shown in Fig. 10a. The corresponding histogram of the crack lengths which were measured 9000 cycles after the strain measurements is shown in Fig. 10b (recall that these measurements were made 9000 cycles after the strain measurements). The similarity between both histograms confirms the strong correlation between the localization of plastic strains and the fatigue crack formation lengths. The crack formation lengths were easily measured from the SEM images. We note that every crack type was measured and not every crack in the region. For example, in the region shown in Fig. 9b, several parallel cracks similar to the marked crack \( L_{C1} \) exist. \( L_{C1} \) represents the length of the longest of these similar and parallel cracks. The strain localization lengths were based on the generally sharp gradients in strain magnitudes around the regions with strain localization (i.e., sharp drop/rise in strain magnitudes). Several examples displaying these sharp gradients through line scans are shown in Fig. 11. A clear cutoff strain magnitude to delineate the length of the localization region was not defined in this work. However, we note that the strain magnitudes in the localized regions, which were measured and shown in Fig. 10a, represent approximately the top 30% of strain magnitudes in the entire gage area as shown in the strain histogram in Fig. 12.

3.3. Influence of grain boundaries

In this section, the focus is on the difference in GB response in blocking (thus creating a pile-up) or transmitting slip, henceforward referred to as shielding and transmission respectively. The association
between shielding and crack initiation at the slip–GB interaction region (intergranular cracking) has been well documented and discussed in the literature. Transmission represents another possible outcome of slip–GB interaction, where full or partial slip transmission across the interface takes place. In the case of partial transmission, the cross boundary reaction creates a residual dislocation (residual Burgers vector \( b_r \)) in the GB plane. Many factors contribute to specifying the final GB response (blocking, full or partial transmission) including the geometric relation between the slip planes across the GB (see schematic in Fig. 13), resolved shear stress (or Schmid factors), and more importantly the magnitude of the residual Burgers vector [26–28]. Some of these factors are discussed below (through two specific examples) with focus on the correlation with fatigue crack formation lengths.

Fig. 11. The strain localization length measurements were based on the generally sharp gradients in strain magnitudes around the regions with strain localization. Several examples displaying these sharp gradients through line scans are shown in this figure. In all the contour plots (a), (c), and (e), a line scan across the region with localized strains is shown. The corresponding strain magnitudes are given in (b), (d), and (f). Notice a sharp increase in strain magnitudes while the region with localized strains is approached and a drop in strain magnitudes after crossing the region. These large gradients in strain magnitudes were visually used to measure the strain localization lengths (see also Fig. 12).

Fig. 12. Histogram of the effective plastic strain field (\( \varepsilon_{\text{eff}} \)) in the entire region of interest. The wide range of strain magnitudes is indicative of the level of deformation heterogeneity developing at the microstructural level. The strain localization length measurements are made for bands with high strain magnitudes (~top 30% of \( \varepsilon_{\text{eff}} \) strain magnitudes).
this case (Fig. 14b) showed that micro-cracks were confined within the grain which exhibited pronounced slip activity (Fig. 14a) and did not extend across the shielding GB (i.e., no transgranular cracking). The exact initiation site is not obvious although the slip–GB interaction region is the most likely location. By determining the local slip system activity (i.e., the calculation of \( d\gamma^s \) as described briefly above and in detail in [26]), we are able to shed light into possible slip–GB reactions for this specific case. Particularly, an estimate of the residual Burgers vector due to possible slip transmission can be established using the Burgers vector of the incident and transmitted slip systems across the GB:

\[
\bar{b}_r = \bar{b}_1 - \bar{b}_2.
\]  

(4)

The magnitude of \( b_r \) has a major influence and in the case where its magnitude is high, slip transmission will not occur or will seize due to the accumulation of residual dislocations in the GB plane. For the grain with pronounced slip system activity in Fig. 14a, one of the activated slip systems is \( b_1(111)[101] \), this system has the highest Schmid factor among the 12 possible slip systems (fcc crystal structure). Across the interface, the two slip systems with the highest Schmid factors (0.38 and 0.34 respectively) are the \( b_2(T11)[110] \) and \( b_3(111)[100] \). Using Eq. (4), the possible \( b_r \) associated with activation of any of these systems through transmission of the incident slip (i.e., \( b_1(111)[101] \)) through the GB was found to be 0.7a (where a is the lattice spacing) as shown in the table at the bottom of Fig. 14. This magnitude of \( b_r \) is rather high and can partially explain why transmission of slip has not occurred. Another contributing factor is the relatively low magnitudes of the Schmid factors for both of the slip systems considered in the grain across the GB. Also, and primarily for \( b_3(111)[100] \), the geometric relation between the incident and possible transmitted slip planes is unfavorable for slip transmission (visually observed through large misalignment between the incident, marked blue in Fig. 14b, and transmitted, marked red, slip planes). Nevertheless, and regardless of why shielding has occurred, the results shown in Fig. 14 show that this GB response (i.e., shielding) limits the strain accumulation and crack formation to only one side of the GB. In addition, the results serve to strengthen the observed correlation between strain localization and crack formation lengths.

Fig. 15 shows a different example where evidence of transmission was observed from the DIC strain measurements (notice high strains across multiple GBs in Fig. 15a). Crack formation for this case exhibited a relatively long crack through the transmitting
GBs as shown in Fig. 15b. Similar to the shielding case shown in Fig. 14, the exact initiation site is not visible from the results but the correlation with strain accumulation across the interfaces and the transgranular crack is clear. Analysis of the local slip system activity and the slip transmission reactions for the three grains involved in localizing strains and crack formation are shown in Fig. 16. Contour plots of the shear strains ($\gamma_{ij}$) for the incident and transmitted slips across the GBs are shown in Fig. 15a. Traces of the activated slip planes are shown on the EBSD grain orientation map in (b). Notice that the transmitted system through the first GB acts as incident slip for the other GB to the left of the figure. This sequence of slip transmission through multiple GBs leads to the formation of a grain cluster and a long band of strain localization.

**4. Discussion**

Although the correlation between strain localization and fatigue crack initiation is well known, a quantitative assessment of the locally heterogeneous material response prior to fatigue crack initiation and an association with fatigue crack formation lengths was lacking. The results presented in Figs. 8–10 provide clear evidence of the connection between regions with high magnitudes of plastic strains ($\varepsilon_{\text{eff}}$ strain magnitudes as shown in Fig. 12) early during loading, and each of the fatigue cracks which were observed later in the life of the sample. These results are important since they can help crack initiation models introduce a length scale (i.e., crack length) to their analysis that is neither arbitrary nor based on experimental observations, but is rather based on local plastic strain accumulation prior to crack nucleation. Also, the results can help remove some of the ambiguity regarding when to make the transition between models based on initiation to the well-developed fatigue crack growth models.
In the analysis presented in Section 3.3 of this manuscript, the role of GBs in blocking slip (shielding as shown in Fig. 14) and allowing slip transmission (transmission as shown in Fig. 15) along with the impact on fatigue crack formation was considered. On the one hand, the smaller crack lengths measured in the fatigued sample were confined in single grains surrounded by shielding GBs. On the other hand, transmitting GBs resulted in relatively longer cracks (see Fig. 15). These experimental observations lead to the conclusion that transmission can be more detrimental to the fatigue life due to the longer fatigue cracks that form transgranularly. Although shielding, which results in the creation of a pile-up and stress concentration, may lead to crack initiation before transmission, the associated cracks were found to be shorter in length. Another important implication of this observation is that the consideration of a single fatigue initiation parameter, as has been typically done in initiation models, can only point to a critical location where cracks may initiate first, but does not necessarily capture the most detrimental feature (e.g., grain cluster with GBs allowing slip transmission) for the fatigue life. For example, a shielding GB may result in the highest magnitude of plastic strains, and thus initiate cracks within a single grain, leading to its selection as the critical location controlling the fatigue life. Based on the observations made in this work, these cracks may be confined to a single grain and do not represent the most critical case. A group of grains with transmitting GBs and lower magnitudes of the strain can lead to the formation of a much longer crack. Therefore, a better assessment of the critical conditions for fatigue crack formation requires not only knowledge of the local strain magnitudes, but also an evaluation of the role of GBs in blocking or transmitting slip.

The importance of deformation mechanisms (i.e., shielding and transmission) in the vicinity of GBs in predicting damage nucleation has been also emphasized by other researchers [14,30,70]. However, similar and related concepts/interpretations to slip transmission and transmission also exist in the literature. Kim and Laird [71] showed through slip trace analysis that slip directed towards the GB over a long slip distance is necessary to form GB steps and induce cracks. We note that such an outcome (GB steps) can be observed in either the blocking or transmitting [36] GBs. Davidson et al. [38] explained crack initiation using the concepts of grain clusters (i.e., group of grains connected by low angle grain boundaries allowing slip transmission). In their interpretation, slip transmission mainly results in the group of grains acting as one larger grain (supergrain). The increase in the effective grain size explains the tendency for nucleating cracks based on experimental observations of fatigue cracks being found in larger grains. The results presented in this work supports the idea of the formation of grain clusters (considering slip transmission), but the correlation we make with fatigue cracks is through the accumulation of high magnitudes of plastic strains and not grain size. Zhang and Wang [72] have associated crack initiation sites with the misorientation of grains across GBs. In the case of high angle grain boundaries, cracks initiate at the GBs while in the case of low angle grain boundaries, which allow easy transmission of slip, cracks initiate along PSBs similar to fatigue cracks in single crystals. These observations strongly relate to the concepts of shielding and slip transmission as discussed in this paper. However, we emphasize that although the misorientation between grains influences the GB resistance to slip transmission, it does not represent by itself a sufficient condition describing whether transmission may or may not occur. Additional factors, primarily the residual Burgers vector and resolved shear stresses on slip planes, are required for a better description/prediction of the GB response. For example, a twin boundary, which is a high angle GB, can represent a strong barrier for dislocation motion (shielding) or it can allow easy transmission across the GB by cross-slip [26]. The difference in response depends on many factors (e.g., residual Burgers vector and Schmid factor) besides the misorientation angle. In conclusion, this work emphasizes that by capturing the correct GB response, the localization of plastic strains at the surface can be predicted. With an accurate assessment of strain localization prior to crack formation, the locations of potential fatigue cracks and their severity can be predicted.

It should be pointed out however that the prediction of fatigue crack lengths based on localized plasticity might be influenced by different loading conditions resulting in dissimilar magnitudes of local plastic strains (e.g., high cycle versus low cycle fatigue results in different magnitudes of localized strains). If relatively large magnitudes of plastic strains localize through multiple GBs, then fatigue cracks will follow with formation lengths comparable to the length of regions with high strains. This could be different in the case of high cycle fatigue where localized plastic strains may be confined to a fewer number of grains, or even a single grain. These localized strains will be associated with initiation of cracks but the growth of fatigue cracks to lengths equivalent to the measured cracks in this paper may be better described and predicted based on other considerations. Some works have addressed this issue using small crack propagation analysis at the microstructural level (e.g., [73,74]). This issue requires further investigation and additional experimental work to help focus on the difference between cases with lower strain magnitudes compared to what was done in this effort.

A limitation worth pointing out regarding the results presented here is that the exact initiation sites were not determined (i.e., nucleation at the atomic level). Our analysis focused on crack formation which, as explained earlier, includes initiation and micro-crack propagation. Nevertheless, potential candidate sites for initiation can be deduced through some of the analysis made in Section 3.3. For shielding, initiation sites from slip–GB interaction regions are well documented (e.g., [75]) and can be delineated in the experimental results presented in this manuscript. For transmission, shielding at the end of the slip band which has transmitted through multiple GBs can act as an initiation site. Another candidate is based on the magnitude of the residual Burgers vector following slip transmission. For example, in the transmitting GBs shown in Fig. 16, one of the reactions results in a higher magnitude of \( \mathbf{b} \) (0.5a compared to 0). The accumulation of residual dislocations in the GB plane can be envisioned as an initiation site. Experimental observations of fatigue cracks initiating in the vicinity of GBs following partial slip transmission and dislocation accumulation in the GB plane has also been reported by other researchers (see for example [76]).

Finally we note that although the results in this work unambiguously point out to where fatigue cracks form, they do not address the equally important question as to when (exact number of cycles) initiation takes place. In situ experimental work where deformation is monitored real time, as opposed to ex situ (after deformation), will be required to address this point. Work in this area is much more limited compared to ex situ studies due to numerous challenges associated with such endeavors (e.g., [56,65]). For example and particularly for DIC measurements, an in situ imaging setup allows capturing deformation images at a much lower magnification compared to an ex situ setup. The consequence is that in situ strain measurements are at a lower resolution and cannot in general be related to microstructural features (e.g., grain boundaries). Resolving the issues associated with in situ strain measurements to enable real time deformation measurements and fatigue cracks observations will provide a better and a comprehensive assessment of strain localization leading to fatigue crack initiation [77].
5. Conclusions

The experimental results and analysis in this paper support the following conclusions:

1. The localization of plastic strains at the microstructural level prior to fatigue crack formation determines the location and length of micro-cracks which form later in the fatigue life.

2. The deformation mechanisms (i.e., shielding and transmission) in the vicinity of GBs influence strain localization in the vicinity of GBs and thus affect fatigue crack formation.

3. A better assessment of the critical conditions for fatigue crack formation requires not only knowledge of the local strain magnitudes, but also an evaluation of the role of GBs in blocking or transmitting slip.

4. For the same number of cycles, the transmission of slip across grain boundaries resulted in longer transgranular cracks compared to cracks near grains surrounded by blocking grain boundaries which were shorter cracks and confined within single grains.

In summary, this work suggests that the locations of potential fatigue cracks and their severity can be predicted with an accurate assessment of strain localization prior to crack formation which should also take into account the deformation mechanisms in the vicinity of GBs.

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