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The physics of fatigue crack initiation

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ABSTRACT

The fatigue life of a component can be expressed as the sum of two segments of life: (a) the number of loading cycles required to initiate a crack and (b) the number of cycles it takes that crack to propagate to failure. In this review, the primary emphasis is relating the fatigue crack initiation to the microstructure of the material. Many studies have focused on this phenomenon over the years and the goal of this paper is to put this work in perspective and encourage future work of fatigue in polycrystals based on the material's microstructure. In order to address fatigue, it is necessary to understand the mechanisms that facilitate crack initiation. Slip irreversibilities exist in a material and accumulate during fatigue loading. At the defect level, irreversibilities are a result of dislocations: annihilating, cross-slipping, penetrating precipitates, transmitting through grain boundaries, and piling-up. These slip irreversibilities are the early signs of damage during cyclic loading. The dislocations subsequently form low-energy, stable structures as a means to accommodate the irreversible slip processes and increasing dislocation density during cyclic forward and reverse loading. The result is strain localizing in a small region within the materials, i.e. persistent slip bands and dislocation cells/bundles. Strain localization is a precursor to crack initiation. This review paper will focus on experimental observations of strain localization and the theory and numerical analysis of both slip irreversibilities and low energy configuration defect structures. This fundamental understanding is necessary to study persistent slip bands in FCC metals and alloys including the appropriate characterization, theory, and modeling. From this fundamental knowledge both micromechanical and crystal plasticity models can be used to predict crack initiation, which are also reviewed. Finally, this review ends with a discussion of the future of fatigue modeling and experiments.

1. Introduction

The importance of fatigue is evident; although exact numbers are not available, it is expected that at least half of all mechanical failures are due to fatigue [1]. The relative cost of these failures constitutes approximately 4% of the gross national product of the US [1]. For this reason, it is essential to understand the physics of fatigue, in order to create a cause and effect relationship in an effort to reduce the probability of such failures. For this reason, we present a critical view of fatigue crack initiation in modern engineering. We note that this article is not intended to be a comprehensive review of crack initiation; in this case, we present a pointed review of the seminal crack initiation mechanisms in FCC materials during low cycle fatigue.

The aim of this article is to elucidate the role of the microstructure in crack initiation mechanisms. From this perspective and the combination of experiments, modeling, simulations, and theory, it is possible to construct the structure to fatigue performance relationship. This link enables prediction of fatigue life in components, which consist of different heat lots of materials and further allows the ability to engineer materials with optimized microstructure for extended fatigue lives.

We start by reviewing classical fatigue experiments with respect to localization of strain as a precursor to crack initiation. Strain accumulates primarily through dislocation motion resulting in slip within the grains of the polycrystalline aggregate. Upon forward and reverse loading, slip moves in distinct paths within each cycle, in which the slip processes are *not* fully reversible. We present an overview of slip irreversibilities and the arrangements of dislocations in low energy configurations as these phenomena define the unique nature of fatigue and the existence of persistent slip bands (PSBs). Persistent slip bands represent a critical mechanism of crack initiation in ductile FCC materials. Due to their importance in the fatigue process, we present a thorough review of theoretical, experimental, and modeling efforts to rationalize the nature of PSBs and their role in crack initiation of PSBs in single crystals, polycrystals, and alloys. This information is key as we explore crack initiation in relation to microstructural features within the material. Finally, we close with a discussion on the future of research in the area of fatigue in materials.

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2. Fatigue experiments and strain localization

Fatigue is characterized by a series of forward and reverse loading. Specifically in low cycle fatigue, plasticity is induced in each cycle. Over the course of accumulated cycles, during the fatigue process, defects in the form of dislocations multiply and accumulate within the material. This behavior results in an increase in the dislocation density [2–4], which form unique structures in an attempt to minimize the total energy of the system [5]. As a consequence, in many materials strain is localized in the form of slip bands, as first pointed out during fatigue of polycrystalline (coarse-grain) Swedish iron by Ewing and Humphrey [6]. The slip lines appeared fine and sharp in several favorably oriented crystals within the specimen and as more cycles accumulated within the specimen, more crystals displayed signs of slip bands, the existing bands widened, and ultimately some of the slip bands developed into small cracks [6].

Seeger et al. [7] and Friedel [8] discussed the mechanism of work hardening in FCC crystals and the associated slip band formation. In this work, a combination of experiments displaying the stress–strain response indicating the role of the flow stress and theory of the underpinning dislocation mechanics creates a foundation for a discussion of slip band formation as depicted on the surface of the cyclically loaded specimens [7,8]. Hence, the results display that strain localization occurs in the form of slip bands, which are precursors to crack initiation. As shown in Fig. 1, slip bands form during cyclic loading resulting in crack initiation [5]. In the formation of slip bands, the dislocation mechanics play an important role in the fatigue response of the material. Specifically, the dislocation response is strongly dependent on the temperature, stacking fault energy, slip character, and applied strain amplitude (cycles to failure) [5,7–11]. As discussed in this article, the dislocation mechanics create the impetus for strain localization and ultimately crack initiation.

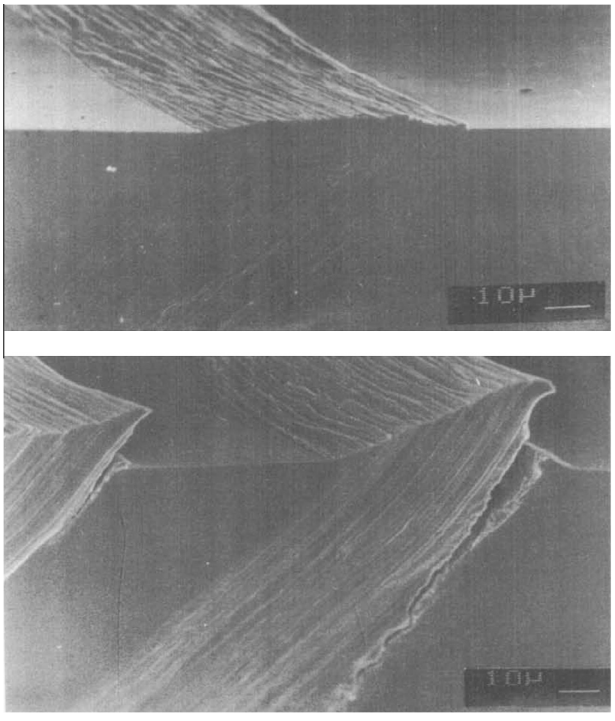

Fig. 1. (a) Slip bands form at the surface of a crystal as a result of fatigue (54.5 kilocycles). (b) Due to the accumulation of strain, a crack initiates at the interface between the slip band and the matrix (72 kilocycles) [5].

Through the use of powerful microscopy tools, several groups have superimposed the strain fields spatially across boundary traces pertaining to the microstructure, including Tschopp et al. [12], Clair et al. [13], Abuzaid et al. [14], and Daly [15]. Primarily, digital image correlation (DIC) is used to analyze strain fields and strain localization spatially on the surface of a specimen combined with electron back-scatter diffraction (EBSD) scans indicating the grain orientation and grain boundaries within the specimen, during in situ or ex-situ loading. The results illustrate the role of strain localization across the microstructure as a result of loading. For instance, we use the experimental work of Abuzaid and Sangid et al. to depict strain localization, as shown in Fig. 2 [14]. This specimen has been loaded to a uniaxial strain of 2.2% and unloaded while recording the microstructure from EBSD and the strain fields from DIC, ex-situ, before and after loading. After unloading, the residual strain is nominally 2% across the specimen, although as shown in Fig. 2, the material deforms heterogeneously and the strain varies spatially across the microstructure, especially in the presence of twin and grain boundaries. Many high stress regions are visible where the strain accumulation is greater than 5%. Additionally, other regions have nearly zero or compressive strains resulting from the loading cycle [14]. This, it can be seen that the microstructure plays an important role in strain localization, and, during cyclic loading, it is expected that a crack will nucleate in the vicinity of a region containing a large amount of strain accumulation.

3. Slip and irreversible slip processes

In order to understand crack initiation during low cycle fatigue in metals, it is necessary to understand the deformation mechanism within the material at the atomistic scale (dislocation level). In metals, the mechanism of plastic deformation is dislocation motion, which is accomplished via slip or twinning of the crystalline lattices. In most polycrystalline alloys during fatigue, we see slip as the primary mechanism. As slip accumulates during cyclic loading, plastic deformation manifests into eventual strain localization leading to crack initiation. This process is determined by the individual microstructure and strengthening mechanisms within the material.

In an attempt to describe the fatigue process at the dislocation level in a generic engineering alloy, slip follows a series of steps as follows: (i) dislocations are present from the processing of the materials or nucleate at the grain boundaries, (ii) upon reaching the critical resolve shear stress on a slip system in preferentially oriented grains, dislocations begin to glide on that slip system, (iii) slip continues until the dislocations reach an obstacle in the form of an elastic field originating from a solute particle, another dislocation, grain boundary, or precipitate, (iv) upon subsequent loading, the local stresses cause the nucleation of additional dislocations or the blocked dislocations to supersede their obstacle by either a climb, jog, kink, cross-slip, shearing, or looping process, (v) steps i–iv repeat during cycle loading along the same path as this path represents a low energy pathway to deformation, which can be planar (two-dimensional in materials with a low stacking fault energy) or wavy (three-dimensional in materials with a high stacking fault energy), (vi) due to the preference of dislocations to move on low energy pathways, slip continues on these pathways resulting in the formation of persistent slip bands (PSBs), (vii) due to plastic deformation resulting from forward and reverse loading, positive and negative dislocations are produced and configure themselves into preferred structures to minimize the energy of the dipole configuration (as discussed further in Section 4), (viii) if positive and negative dislocations are close enough, they annihilate via cross-slip (screw components) or climb (edge components), which produces vacancies, (ix) due to the increase in

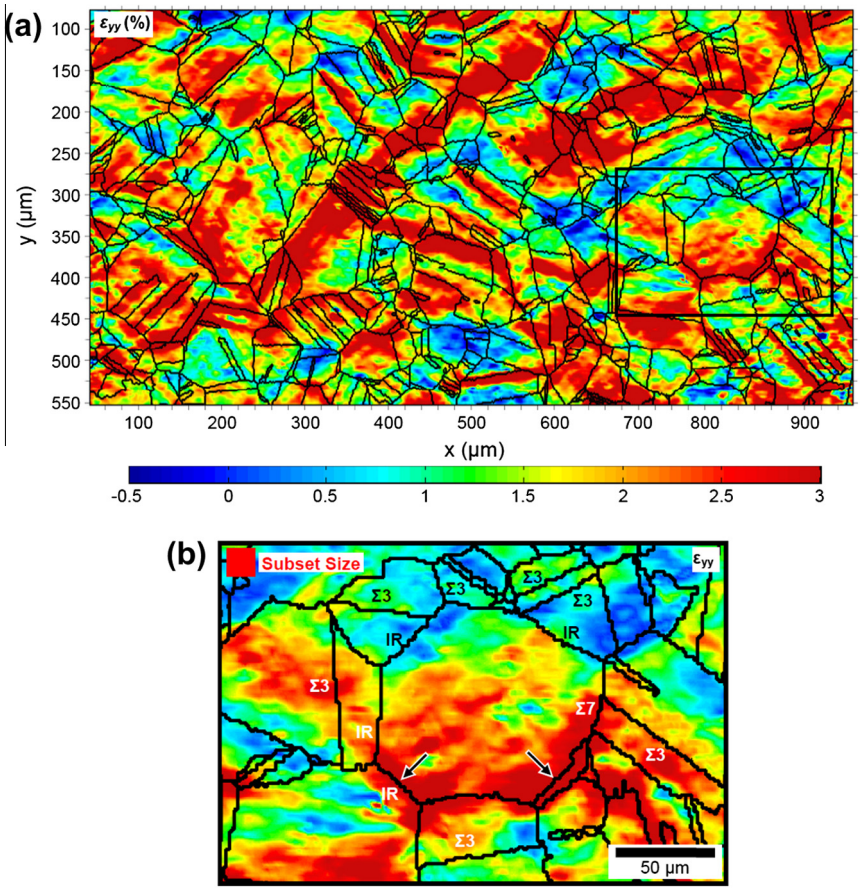

Fig. 2. (a) Strain fields measured from digital image correlation after loading/unloading a sample in tension to 2.2% strain overlaid with the material's microstructure from EBSD. (b) Enlarged view of the black box in (a), which illustrates the GB role in greater detail [14].

dislocation density within this slip band and the dislocation to dislocation interactions, the slip band exhibits work hardening resulting in the formation of either a ladder structure or a parallel slip band in the material, (x) vacancies diffuse within the material resulting in the formation of ledges, intrusions, and extrusions at the grain boundaries and free surfaces, (xi) the increase in defects which pile-up at the grain boundaries result in a stress concentration that activates slip in a neighboring grain, and (xii) as the accumulated plastic strain increases (within a grain or across several grains), the strain is localized into a small volume within PSBs in the material, the dislocation patterning forces the material to be very hard or soft, which results in crack initiation at the soft/hard interface, as shown in Fig. 1.

Thus, the physics of crack initiation are directly influenced by the interaction of defects and dislocations in the material, which can lead to complex dislocation arrangements. The result of this process is slip irreversibilities during fatigue loading. The slip introduced during forward loading is not recovered fully during reverse loading due to the following:

- Cyclic loading produces equal number of positive and negative edge dislocations, which arrange themselves in low energy dipole configurations.
- Cross slip and different paths for forward/reverse glide of screw dislocations during a complete fatigue cycle leads to irreversibility and possibly annihilation.
- Point defects are produced, due to the dynamic equilibrium between dislocation generation and annihilation. The flux of vacancies within the material produces extrusions and intrusions (surface roughness) at a free surface or grain boundary.
- Dislocation–dislocation interactions lead to the formation of nodes, jogs, or dislocation locks, which impede motion during a portion of a fatigue cycle.
- Differences in dislocation back stress due to slip on different glide planes during the tension and compression portions of fatigue results in irreversibility.
- Shearing of precipitates localizes slip into planar deformation.
- The discontinuous nature of slip and strain incompatibility at grain boundaries (GBs) leads to activation of different slip planes as dislocations interact with GB during forward and reverse loading.

Hence, fatigue damage is governed by irreversible plastic flow [16]. Mughrabi quantified the cyclic slip irreversibilities p, defined as the fraction of plastic shear strain that is microstructurally irreversible [17]. In this case, p varies from 0, as is the case in low loading amplitudes, to 1, for high loading amplitudes and near stress concentrators such as notches in components. As we see in this review, slip irreversibilities form the foundation to crack initiation, as the irreversible nature of slip is unique to cyclic loading.

4. Defect structures in low energy configurations

In order to gain a more thorough understanding of the effects of cyclic loading on the material, we must analyze fatigue dislocation arrangements. As previously mentioned, during cyclic loading, dislocations arrange themselves into preferred defect structures to minimize the total elastic strain energy of the system. In 1977, Kuhlmann-Wilsdorf discussed, in detail, the theory of low energy dislocation arrangements. She showed that dipolar walls and dislo-

cation cell structures form in order to minimize the stored energy per unit length of the dislocations, which results in extrusions and intrusions of the material's surface and work hardening [18,19]. Fatigued materials consist of numerous dislocations with opposite signs that nucleate from forward and reverse loading, which arrange themselves in dipole configurations. In 1986, through a simple force balance of the stresses exerted by an edge dislocation on a Taylor lattice, Neumann showed that several specific configurations result in stable structures, including ladder (series of walls, as seen within PSBs) and vein (diamond multipole) configurations, as shown in Fig. 3 [20–22]. This approach displayed an early form of modeling discrete dislocation dynamics, which computational efforts for this type of modeling have evolved over time. Using 3D dislocation dynamics, Depres et al. simulated the associated surface topography and roughness profile resulting from fatigue loading. The dislocations arranged themselves into slip bands to localize plastic shear strain. In order to relieve stress, intrusions and extrusions form on the material's surface, as shown in Fig. 4 [23–25], creating a rough surface topography. From these simulations, Depres et al. suggests that cross-slip is responsible for the formation of the dipole structure of the dislocations and the origin of irreversibility of the plastic strain.

There have been a few attempts to develop a closed-form solution to the stress field developed by the dislocation arrangement resulting from fatigue. Brown used the Airy's stress function to develop an expression for the stress field by the dislocations of a dipole arrangment, which he used to explain long-range stresses from the wall structures [26–28]. Van der Giessen and Needleman developed a dislocation dynamics model to verify that the stress field from a series of planar edge dislocations can be modeled as a series of hyperbolic terms [29]. Brinckmann extended this model to account for two opposing series of edge dislocations, which provided a good approximation for the dislocation arrangement in a slip band and the resulting stress field [30]. These models represent the stress field of dislocations in a PSB from 2D dislocation dynamics, which provides information that is crucial for modeling the unique dislocation arrangements resulting from cyclic loading.

5. Persistent slip bands in single crystals

5.1. Experimental observations of PSBs

Due to slip irreversibilities, vacancies are generated creating a flux within the PSB resulting in surface intrusions and extrusions. Meanwhile, dislocations agglomerate into the walls of a PSB, which act as strong barriers to slip, resulting in a hardening response of the material. Both the hardening behavior and dislocation density are seen to saturate as the fatigue cycling continues [31–33]. Thus, PSBs represent significant localization of plastic deformation, slip, and dislocations, therefore hardened (PSB) regions are adjacent to the relatively soft matrix material. The result produces a relatively well-defined 3D structure of a PSB in the material, as shown in Fig. 5. The interface between the PSB and matrix is a plane of discontinuity across which there are abrupt strain gradients, resulting in a preferred site for crack initiation [34–38]. As the PSB evolves during cyclic loading, dislocation multiplication leads to a strain (cyclic) hardening response in certain materials, while rearrangement of pre-strain-induced dislocation networks leads to a strain (cyclic) softening response in other materials.

Many of the physical insights into the mechanisms that form a persistent slip band were theorized by Mughrabi and Essmann et al. in the late 1970s and 1980s, specifically on the generation and annihilation of point and line defects within a PSB [39–41]. Cyclic loading produces positive and negative edge dislocations, which attract each other, forming dislocation dipoles agglomerating in the walls of the PSB resulting in a nearly zero net Burgers vector [42–45]. Only edge dislocations of opposite sign are likely to form such dipoles because positive and negative screw dislocations can easily cross slip and mutually annihilate [39,46,47]. Similarly, edge dislocations of opposite sign on different glide planes can annihilate via climb on glide planes resulting in formation of a vacancy.

Within the PSB, dislocation glide even at low temperatures and as aforementioned there is a flux of vacancies resulting in intrusions/extrusions at the surface. During the surface roughening process, the average dislocation distance in the fatigued matrix approaches the annihilation distance for dislocations, which Mughrabi calculated for edge and screw dislocations in copper. The annihilation distance provides an upper limit for dislocation density and vacancy concentration in the walls of the PSB, whose dislocation density values are much greater compared to the fatigued matrix domains [39,48,49].

5.2. Modeling PSBs in single crystals

Essmann and Mughrabi created a model for extrusions and intrusions resulting from a PSB, focusing on randomly distributed irreversible slip processes, as a product of a dynamic equilibrium between dislocation multiplication and annihilation in a PSB [39]. The result of the above model leads to elongation of the PSB, extrusions/intrusions at the surface of the single crystal, and an increase in surface roughness. In their model, they estimated the surface roughness, *Ra*, which displays a square root dependency on the number of loading cycles, *N*:

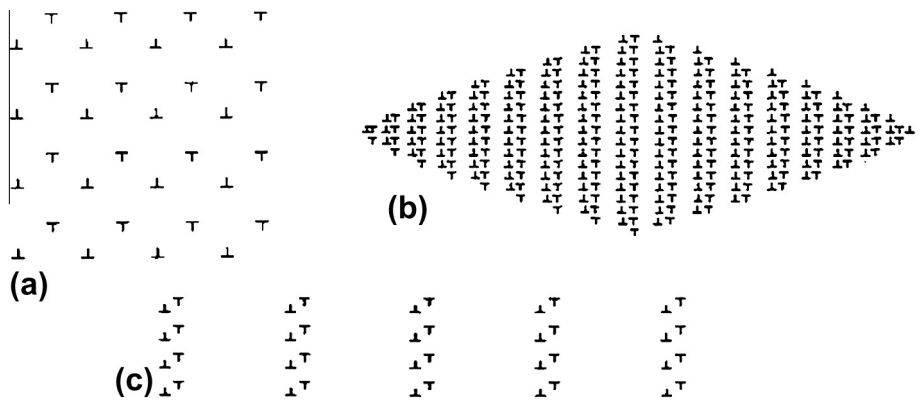

Fig. 3. From simulation under applied loading, stable arrangements of edge dislocations form on a (a) Taylor lattice, (b) in a vein structure, and (c) in a ladder configuration [21].

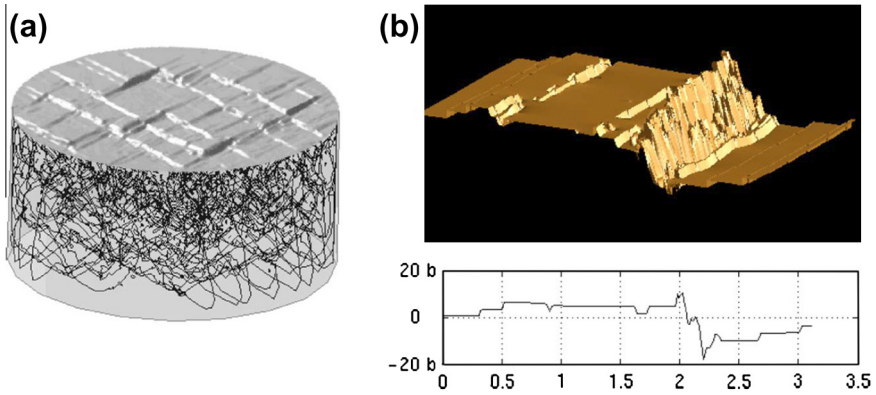

Fig. 4. Surface topography associated with dislocation arrangements and extrusions/intrusions during cyclic loading by discrete dislocation simulations [23].

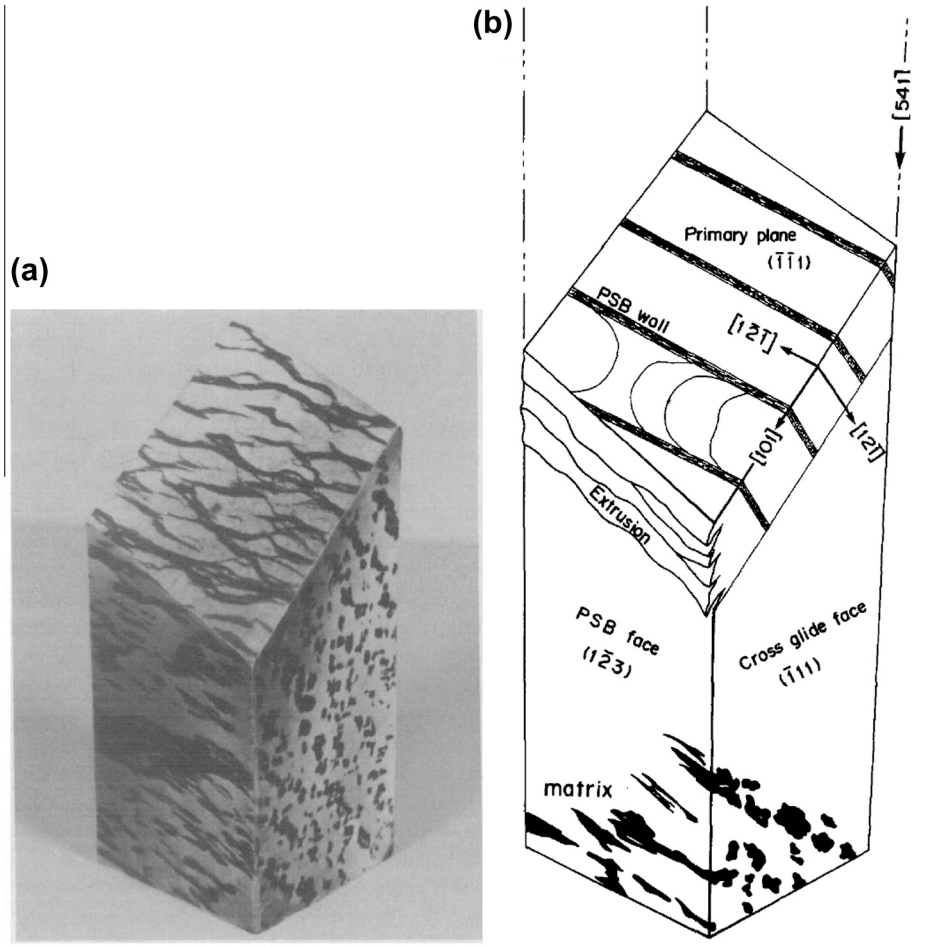

Fig. 5. (a) 3-D appearance of the dislocation structure of a fatigued crystal and (b) a schematic depicting the PSB configuration [5].

$$R_a = 2F\sqrt{Nb\gamma_{PSB}p_{PSB}h_p}, \quad (1)$$

where p_{PSB} is the ratio of irreversible strain to total strain, γ_{PSB} is the plastic strain amplitude in the PSB, h_p is the thickness of PSB, b is the Burgers vector, and F is a proportionality constant [40,41]. Many parameters are used that cannot be simulated or measured prior to failure. Hence, only logical quantitative estimates can be given for the model's variables. This model is physically-based and well thought-out and serves as an important foundation to researchers on modeling irreversibilities in fatigue.

Many PSB models build on the insights and techniques of Essmann and Mughrabi for single crystals [9,50–52], including Ortiz and Repetto who created a finite element model for the development of a PSB in an initially defect-free single crystal FCC material. The result leads to an outward flux of vacancies and the formation of surface roughness and stress concentration as a precursor to a sharp surface crack that may result in failure [52]. The Ortiz and Repetto model relies on fitting a constitutive model to the diffusion of vacancies in a single-crystal and delivers insightful results.

6. Persistent slip bands in engineering materials

6.1. PSBs in polycrystals

To this point, we have only discussed PSB formation in single crystals, although dislocation walls and PSBs can form in the most favorably oriented grains within a polycrystalline material [53–55]. The dislocation arrangements in polycrystals are similar to those in single crystals, except that the dislocations are impeded by the GB resulting in pile-up and additional stress concentration [49], as shown in Fig. 6a. Blochwitz et al. studied PSB interactions with GBs during fatigue of polycrystalline material; their results showed that PSBs affect the local stress at the GB, further the process is influenced by the misorientation between grains [56–59] or the presence of a twin [60]. The resulting stress is relieved by formation of a static extrusion at the GB (Fig. 6b); expressions are formulated for the resulting slip and static extrusion height at the GB [49]. Over an increasing number of cycles, the stress concentration and extrusion height increases assisting in crack nucleation at the PSB-GB interface.

GBs have been described as impenetrable obstacles to PSBs that cause stress concentration resulting in cracking or PSB formation in adjacent grains [56]. Since that time, the misorientation and Schmid factor of adjacent grains have been recognized as important parameters in determining PSB-GB interaction and crack initiation [59]. Based on experimental observation by Zhang et al., PSBs can transmit through low-angle GBs (LAGBs), hence cracking does not occur at these boundaries [61–67], as shown in Fig. 7a and c. LAGBs are defined as a misorientation between grains of less than 15°, also referred to, in literature, as a Σ1 GB according to the coincidental site lattice (CSL) [68,69] theory using the Brandon condition [70]. Interestingly, PSBs cannot transfer through general (random) high-angle GBs (HAGBs), resulting in impedance of dislocation motion, dislocation pile-ups, stress concentration, and possibly intergranular fracture [64], as shown in Fig. 7b and d. Further, the mechanism of HAGB cracking is independent of the angle between the applied stress axis and the GB plane [65]. From this analysis, the PSB-GB interaction can result in dislocations behaving by one of the following scenarios: passing through, piling-up, or partially passing through (resulting in a residual dislocation within the GB) [63,71]. In the case of partial transmission, the system orientation and GB character plays an important role [72]. The GB character can be quantified by the CSL notation, as an outcome special CSL boundaries do not experience intergranular cracking [73,74], especially the Σ3 boundaries also known as twins, which are discussed in Section 7.1.2. These experimental observations are important to the modeling community to predict fatigue crack initiation.

6.2. Modeling PSBs in polycrystals

Lin and Ito developed a model for plastic shear strain accumulation from a PSB in a polycrystal [75]; however their shear stress field was non-equilibrating. Building on their concepts, in 1981, Mura and Tanaka created a powerful micro-mechanical model for crack initiation at a PSB in a polycrystalline material [76–78]. Their approach created an energy balance of the dislocation structure along the PSB in the most favorably oriented grain. The PSB consists of two series of dislocations on opposing layers, which account for deformation as a result of forward and reverse loading, as shown in Fig. 8a. In order to incorporate slip irreversibility in the Mura and Tanaka model, it is postulated that the irreversibility of dislocation motion in the two adjoining layers arises from the different levels of back stress during slip in the forward direction on layer I and in the reversed direction of layer II.

The change in energy, ΔU, from forward to reverse loading is given by:

$$\Delta U = \frac{1}{2}\Delta\gamma(\Delta\tau - 2k), \tag{2}$$

where $\Delta\tau$ is the alternating applied stress and k is the frictional stress of the matrix, which must be exceeded for dislocation motion (in this model it is assumed that $\Delta\tau > 2k$). The plastic strain, γ, is given by integrating the distribution of continuous dislocation within the PSB, D, where $D(x)$ is the dislocation density of a layer within the PSB, given as an unbounded function near the GBs, $D_1(x) = 2x(\tau_1 - k)(1-\nu)/(\mu b\sqrt{(a^2 - x^2)})$.

$$\gamma = \int_L \vec{b}D(x)xdx \tag{3}$$

By taking the difference in layers I and II during cyclic loading, the alternating plastic strain, $\Delta\gamma$, can be given as follows:

$$\Delta\gamma = \frac{(\Delta\tau - 2k)a^2\pi(1-\upsilon)}{\mu}, \tag{4}$$

where $2a$ is the grain size, υ is the Poisson ratio, μ is the shear modulus, and $\boldsymbol{b}$ is the Burgers vector of the material. The total energy of the PSB, U, is the sum of the energy on the two layers of opposing

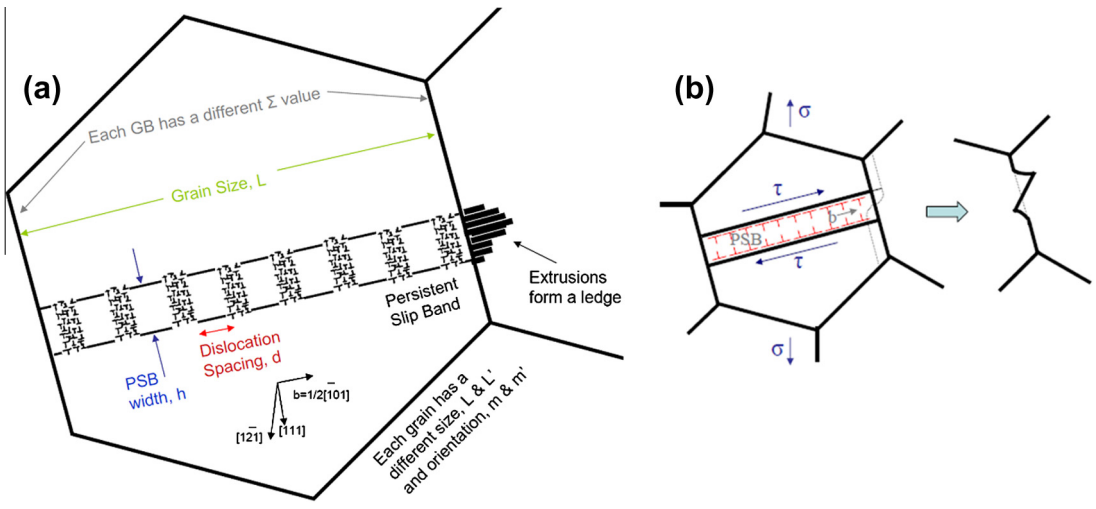

Fig. 6. (a) Schematic of the PSB geometry in the polycrystal [125]. (b) PSB interactions with GBs leads to static extrusions across the GB in the form of ledges and steps [125] redrawn from Ref. [49].

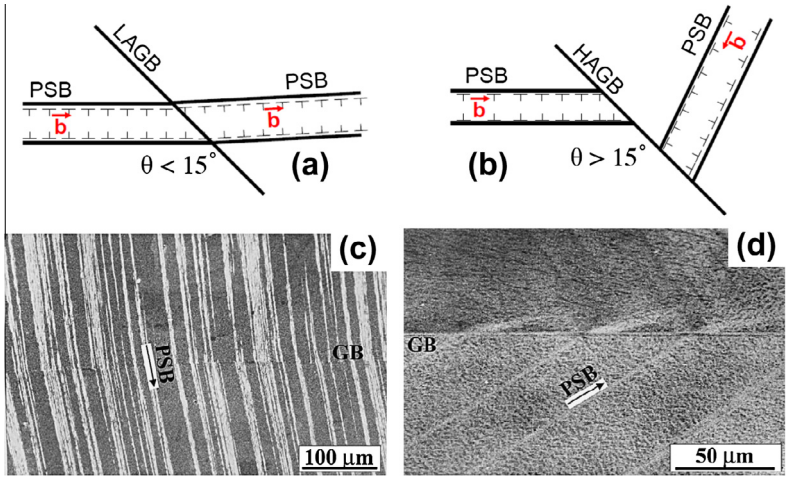

Fig. 7. (a) Transmission of a PSB through a LAGB (misorientation, $\theta < 15°$), (b) PSBs cannot penetrate through HAGBs ($\theta > 15°$). (c) PSB penetrate a LAGB [66], (d) PSB impeded by a HAGB resulting in dislocation pile-up and stress concentration [66].

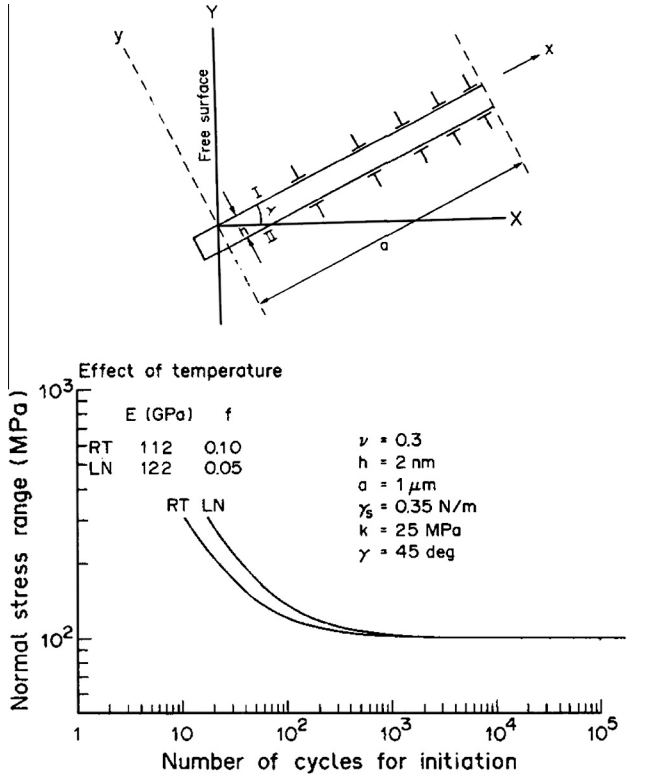

Fig. 8. (a) Schematic depicting a slip band as two parallel layers of dislocation dipoles impinging upon a free surface at an angle. (b) The results of the model in the form of a stress-life prediction for crack initiation at liquid nitrogen (LN) and room temperature (RT) [80].

dislocations, which can be equated to the alternating energy, ΔU, during reverse loading by the number of cycles, n. Failure is reached when the total energy of the PSB reaches the specific fracture energy of the material, W_s.

$$U = U_I + U_{II} = 2n_c\Delta U = 4aW_s \tag{5}$$

By rearranging this, the number of cycles to failure, n_c, can be written as:

$$n_c = \frac{4\pi(1-\upsilon)W_s a^3}{\mu\Delta\gamma^2} \tag{6}$$

Substituting Eq. (4) into Eq. (6) and rearranging, we can express this failure criterion into a Coffin–Manson type expression

$$\Delta\tau = 2k + 2\sqrt{\frac{\mu W_s}{\pi(1-\upsilon)n_c a}}. \tag{7}$$

Notice that the stress has an inverse square relationship with the grain size, a, hence this model is still reminiscent of the Hall–Petch model of grain size dependence on fatigue strength. This model was extended to account for notches, as dislocations pile-up in the presence of a notch, which acts as a stress concentrator.

Mura's and Tanaka's model was revisited in the 1990s, as the Gibbs free-energy evolution was calculated with increasing number of loading cycles. The change in the Gibbs free-energy, ΔG, is seen to increase, hit a maximum value, and sharply decrease during fatigue loading [79,80]. The change in the Gibbs free energy was used as their criterion for instability of dislocations within a PSB during fatigue and ultimately crack initiation. The free-energy considerations correctly predicted easier crack initiation in air as opposed to a vacuum, at higher temperatures, and closer to the material's surface, as shown by the stress-life prediction curve for liquid nitrogen and room temperature in Fig. 8b. This model works well and is comparable to experiments by adding an additional variable for degree of irreversibility, f [81].

There are some concerns and limitations with this model. For instance, this model consists of a simple energy balance and does not take into account the complicated geometry and dislocation structure of a PSB. Nor does it account for the normal stress, which is critical in fatigue. One layer of dislocations does not effect the other during reverse loading, which is an over simplification. Also, there is an energy discrepancy, as their model takes into account only the portion of the hysteresis loop above yielding; i.e. the energy does not account for the total area within the hysteresis loop, since the frictional stress parameter, k, must be overcame for the dislocations to move and is not incorporated in the energy.

6.3. Slip bands in alloys

Historically, the majority of the studies on PSBs have been on pure FCC materials, although PSBs have been observed in alloys [82,83] and superalloys [84–87]. Typically, superalloys are strengthened by an ordered γ' precipitate. Petrenec et al. studied the dislocation arrangements in Ni-based superalloys (IN713 and IN792) at room and elevated temperatures [88–90]. They concluded that persistent slip bands were evident and contained a

high density of dislocations. PSBs form as dislocations cut through the matrix and γ' precipitate in a planar slip manner at both temperatures and were the main source of crack initiation [88–90]. Therefore, the PSB structure in precipitate-hardened superalloys (i.e. multiple parallel thin bands and a planar concentration of plastic strain from shearing the precipitates) is noticeably different compared to the ladder-like structures observed in single-phase materials.

As previously mentioned, PSB formation manifests in surface roughness by means of intrusions and extrusions. This phenomenon is also seen across the grain boundaries in the bulk of a polycrystalline material [49]. Recently, inclusions and extrusions have been measured and quantified using atomic force microscopy (AFM) [58,91–93], which can be related to the irreversibility of slip/displacements in the material [94,95]. Risbet et al. measured the evolution of extrusions on the surface of cyclically loaded Waspaloy, a Ni-based superalloy [96–98]. The height of a PSB is seen to be nearly zero until a threshold number of cycles is reached, increase rapidly, and nearly saturate. As expected, this behavior is highly dependent on the applied strain range. In an extremely intensive experimental study, Huang et al. [99] used in situ neutron diffraction to measure the dislocation density in monotonic and cyclically loaded Hastelloy C-22HS, a Ni-based superalloy. The results show the dislocation density increases during cyclic loading and saturates, as a consequence the space between dislocation walls decreases as PSBs are formed, as shown in Fig. 9. The aforementioned work represents an extensive effort in capturing the slip behavior, dislocation density, wall spacing, PSB height, and extrusion length evolution with number of cycles during fatigue of Ni-based superalloys.

7. Crack initiation relative to microstructure

7.1. Experiments

7.1.1. Large grains and GB character

From experimental results, finer grain material generally experiences a longer fatigue life [100–106], since PSBs are prone to form in larger grains [55,58,107]; although these studies were performed on materials with uniform grain size and cannot address the response of materials with a wide distribution of grain sizes. Similarly, there have been a number of studies that examine the GB character, defined as the density of coincidental atoms between two lattices at the GB, where the density's reciprocal is denoted as the coincidental site lattice (CSL) Σ value. Experimental studies have shown that CSL boundaries of high CSL density/low Σ value do not crack during fatigue of Ni [73], stress corrosion of a Ni-based superalloy [108], and cavitation of Cu [109]. Hence, it is important to account for the GB character as this contributes to the formation and stability of a PSB. Moreover, there can be a combining effect between grain size and grain boundary character. Crack initiation is found to occur across adjacent grains with similar orientations. That is, the grain clusters are connected by low-angle GBs, thus allowing for slip transmission across the GBs. As a result, the grain cluster is coined as a *super-grain* and represents a preferred site for crack initiation [110].

7.1.2. Twin boundaries

Experimentally, twin boundaries (TBs) have been observed as another preferred sites for crack initiation [111–113], although there is still debate on the TB's fatigue response in FCC material. In other words, do TBs harden the material or degrade the fatigue life by acting as crack nucleation sites? Initially, Bottner, McEvily, Liu observed the formation of fatigue cracks at TBs [114]. In many cases, the PSBs form parallel to the TB's normal, resulting in PSB–TB interaction. They note coherent TBs as low energy interfaces within the material, but as PSBs intersect the TBs, non-coherent ledges, steps, or static extrusions form on the TBs. The resulting steps are non-coherent, facilitators of secondary slip, dislocation sources, stress concentrators, and preferred crack initiation sites. The same phenomenon was observed by Thompson [115]. He concluded larger grains and lower stacking fault energies (SFE) result in greater dislocation pile-ups and more secondary slip, respectively; as a consequence both factors result in more stress concentration and are more prone to cracking. In other words, TBs are inherently stronger against intergranular cracking in materials with high SFE, while in low SFE materials, TBs accommodate much of the plastic deformation leading to stress concentration and crack nucleation at the TB [116]. Interestingly, in nanocrystalline material, thinner twins (<1 μm) play an important role in strengthening the fatigue response of the material by affecting the type of PSB–TB interaction [117].

Many models are available to explain TBs as preferred sites for crack nucleation [59]. Kim and Laird argued that plastic incompatibilities caused by surface steps at the TB lead to irreversibilities and cracking [118]. Lim and Raj presented a dislocation model, in which they measured the residual or sessile dislocations at the boundary and from this quantity coined a continuity factor dependent on the slip transfer [119]. Neumann created a traction model to calculate the local stress concentration at TBs promoting crack initiation at low plastic strain amplitudes [120]. Peralta et al. modeled the elastic incompatibilities near a TB; from this analysis, they calculated the stress concentration, which is a maximum value when the tensile axis is a ⟨111⟩ direction, i.e. the loading axis is parallel to the TB [121]. In this model, the TBs promote early primary slip and secondary slip. Peralta's elastic incompatibility

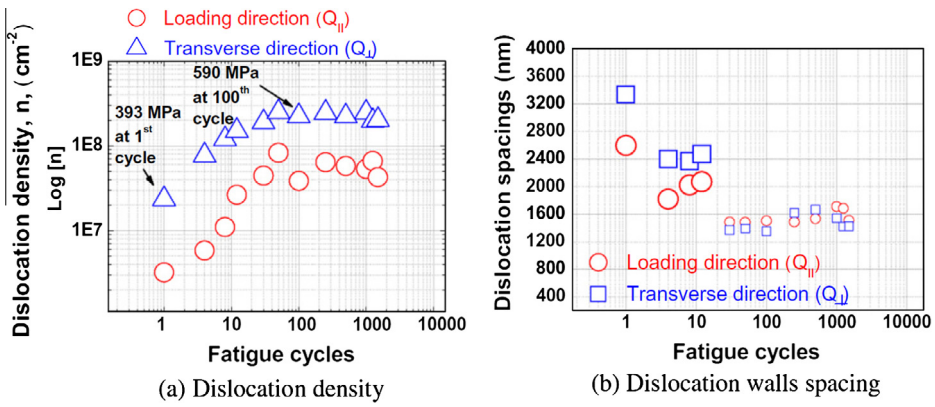

Fig. 9. (a) Dislocation density and (b) dislocation wall spacing as a function of number of cycles in 1% strain fatigue loading of Hastelloy C-22HS [99].

results were reconstructed using the finite element method [122,123]; the results are in agreement and show that coherent TBs have the highest elastic stress concentrations. Building on these concepts, Neumann's model was modified by Blochwitz and Tirschler to account for medium plastic strain amplitudes, thus representing an elasto-plastic solution [60,124]. Each of the aforementioned models demonstrates the role of TBs as preferred sites for fatigue crack initiation in polycrystalline material. These experimental results and analytical models provide a solid foundation, which overwhelmingly illustrate that cracks preferentially nucleate near TBs as a consequence of dislocation pile-up and stress concentration.

7.2. Microstructure models of crack initiation

7.2.1. Micromechanical models

Through a series of papers, a model is developed to predict micro-structurally driven fatigue failure from a specific failure mechanism in a Ni-based superalloy, i.e. PSBs [125–127]. The initial microstructure information is input in the form of an EBSD scan providing characterization of the grain size, grain orientation, and neighboring grains. From this measurement, the individual GB characters are calculated [128] and linked to atomistic simulations of bicrystals with similar types of GBs, which provides the energy barrier to plastic deformation for various types of boundaries [129,130]. Thus, a quantifiable characterization of the material's microstructure and local strength is used to monitor the energy of a PSB in a single grain or a grain cluster (group of grains connected by low-angle GBs) within the polycrystalline aggregate. The overall energy of the PSB is comprised of the following:

i. The formation of the PSB occurs as dislocations shear through the γ matrix and the γ' precipitate within the Ni-based superalloy, resulting in an associated stacking fault energy, γ_{SF}, and anti-phase boundary energy, γ_{APB}, respectively.
ii. After formation of the PSB, dislocations glide within the slip band, thus overcoming the existing local stress fields produced by the elastic strain energy of the sessile dislocations, work hardening within the PSB, and the external applied stress field, $\Delta\sigma^A$.
iii. The dislocation density, ρ, within the PSB increases with applied loading until saturation is reached. Additionally, the PSB interacts with the GB resulting in dislocation pile-up and transmission through the GB to form extrusions/intrusions at the boundary. The energy barriers associated with the dislocation nucleation process, $E^{\gamma\text{-nuc-}GB}$, and GB resistance to slip transmission, $E^{\gamma\text{-slip-}GB}$, are dependent on the specific character of the GB and determined through atomistic simulations.

Therefore, the total energy of a PSB is expressed as follows:

$$E = \left(f\int_o^L \gamma_{APB}dL + (1-f)\int_o^L \gamma_{SF}dL\right)n^{layers\text{-}eff}\partial X + \sum_i\left(\frac{\mu\vec{b}h\pi}{d^2(1-\upsilon)\left(\cosh\left(\frac{2\pi h}{d}\right)-1\right)} - \alpha\mu b\sqrt{\rho} - \tau_o - m\Delta\sigma^A\right)\vec{b}Ln^{layers}\partial X_i + \sum_i \partial X_i\cdot\left\{\sum_j E_j^{\gamma\text{-nuc-}GB}L_j^2\right\}(\rho-\rho_o)\vec{b}h + \sum_i \partial X_i\cdot E^{\gamma\text{-slip-}GB}n^{pen\text{-}dis}\vec{b}h \quad (8)$$

The total energy evolves as the number of loading cycles increases. The failure criterion in this model is defined as the PSB reaching a stable energy configuration, i.e., the energy of the PSB reaching a minimum value with respect to motion of the glissile dislocations, X_i.

$$\frac{\partial E}{\partial X_i} = 0 \quad (9)$$

Hence, the failure criterion is an energy balance with respect to plastic deformation, which is in accordance to other well-known energy balances for describing material behavior, such as Griffith's fracture criterion [131] or Rice and Thomson's brittle versus ductile behavior [132]. To physically describe failure, the dislocations within the PSB have reached an equilibrium position; hence the overall PSB has a minimum in energy. The dislocations do not want to be displaced from their equilibrium and would rather allow a crack to nucleate along the PSB at the GB. This failure criterion aligns with an in situ neutron diffraction study, which states that dislocation self-organization arises possibly during the formation of a microcrack [133]; that is analogous to self-organization in this model due to the dislocations reaching a stable position. Since, potential PSBs within each grain and grain cluster are monitored, failure is determined when the first PSB reaches a stable configuration, Eq. (9), resulting in crack nucleation. Thus, each feature in the microstructure is analyzed locally and used to identify the weakest link, which is most likely to nucleate a crack. For an EBSD scan, the most likely location of failure is predicted, as shown in Fig. 10a.

Using a Monte Carlo algorithm to create simulated specimens of different realizations of the material, this model can be used to calculate the influence of microstructure variability on the fatigue life. The results are shown in Fig. 10b, as the predicted fatigue life of 1000 simulated specimens are compared with 84 experimental fatigue specimens, therefore representing a similar volume of material. At each strain range, the averages, maximum, and minimum fatigue lives are in agreement between the model and experiments, thus providing an excellent prediction of fatigue scatter. In these simulations, failure is caused by mostly single large, preferentially-oriented grains, but also cluster of several grains connected by low-angle GBs acting in concert to promote failure. Furthermore, cracks initiate due to PSB-GB interaction, in which the $\Sigma3$ (twin) GB is the most preferential site for failure. From the atomistic simulations, the inherently stable structure of the twin boundary provides the highest energy barrier for slip transmission. Therefore, dislocations are likely to pile-up at twins resulting in strain localization and crack initiation [126,127].

7.2.2. Crystal plasticity models

Due to recent advances in computational power, finite element-crystal plasticity (FE-CP) models have become more elaborate and are used to predict microstructural phenomena in fatigue. Wong and Dawson used an FE-CP model to analyze the response of FCC metals subjected to cyclic loading. Their results showed the hysteresis response and complex stress state of individual crystals in the aggregate strongly depend on lattice orientation, elastic anisotropy as a result of neighboring grains [134]. Thus, the results show that the stress and strain distributions at the grain level are strongly dependent on the microstructure factors, such as crystal orientation, elastic–plastic response, and grain neighbors, which determines the heterogeneous macroscopic response of the material. Dunne et al. created a FE-CP model of C263, a nickel-based superalloy, which incorporates a back stress term to account for cyclic loading [135]. By taking the curl of the deformation gradient tensor, Dunne accounts for geometrically necessary dislocations and microstructural size effects through the material.

$$\Delta\rho_G^\kappa = \frac{\Delta\gamma^\kappa}{b}curl[n^\kappa F^P] \quad (10)$$

Hence, the evolution of geometrically necessary dislocations, ρ_G, influences the plastic velocity gradient, L^P, on the individual slip systems.

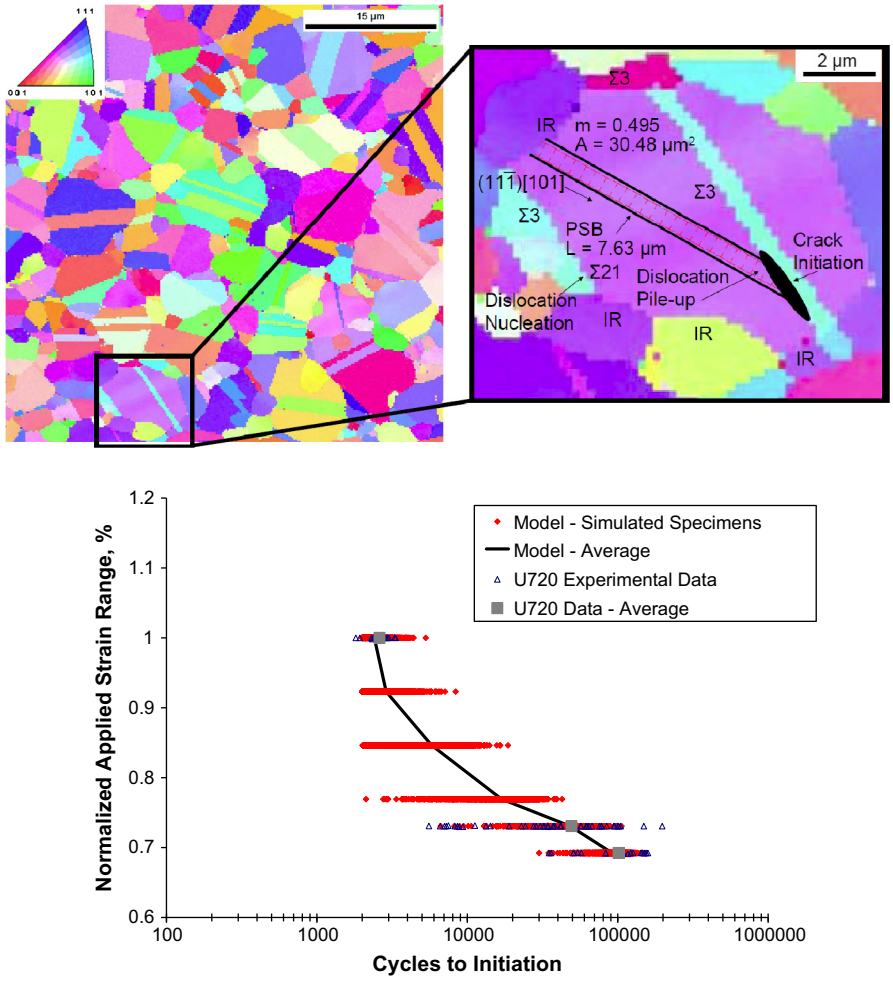

Fig. 10. (a) EBSD scans displaying orientation maps for U720. The inset displays the model's prediction for failure location from this specimen's EBSD scan. The crack initiates from a PSB of length 7.63 μm at a twin boundary. (b) Predicted fatigue results for 1000 simulated specimens at each strain range compared to specimen from 84 fatigue experiments [127].

$$L^P = \sum_{\kappa} \rho b^2 v exp\left(-\frac{\Delta F}{\kappa T}\right) \sin h\left(\frac{(\tau^\kappa - \tau_c)b^2}{\kappa T\sqrt{\rho G}}\right) S^\kappa \otimes n^\kappa \tag{11}$$

As shown in Fig. 11, the model predicts the overall macro-scale stress–strain response and gives information pertaining to the accumulated slip distribution at the micro-scale at each point in the loading history. Crack initiation occurs once a critical accumulated amount of slip (via the shear strains) is achieved based on individual slip systems reaching the critical resolved shear stress. Dunne's model predicts that PSBs are preferentially formed at triple points and the resulting crack initiation follows the Coffin–Manson relationship [135]. This model was extended to study cold dwell fatigue in titanium [136]. In this paper, rogue grain combinations are identified as having a combination of orientations leading to highest stresses normal to the primary basal plane (in hexagonal closed-packed material) of a central grain resulting in accumulated slip in adjacent grains. Each of these models represents a significant advancement in the field, in an effort to use crystal plasticity simulations to predict fatigue crack initiation.

Ghosh et al. studied the effects of creep-induced load shedding leading to stress concentration in titanium, which included a Hall–Petch parameter to include the effects of grain size, D [137].

$$g_o^\alpha = \bar{\bar{g}}_o^\alpha + \frac{K^\alpha}{\sqrt{D^\alpha}} \tag{12}$$

The result is captured in a power law relationship to model the strain rate, $\dot{\gamma}^\alpha$, on each slip system, which evolves with the back-stress, χ.

$$\dot{\gamma}^\alpha = \left[\dot{\gamma}_o\left(\frac{|\tau^\alpha - \chi^\alpha|}{|g^\alpha|}\right)^{1/m}\right] sgn(\tau^\alpha - \chi^\alpha) \tag{13}$$

The back-stress, χ, follows an Armstrong–Frederick nonlinear kinematic hardening rule and evolves according to the direct hardening, c, and dynamic recovery, d.

$$\dot{\chi}^\alpha = c\dot{\gamma}^\alpha - d\chi^\alpha|\dot{\gamma}^\alpha| \tag{14}$$

This model was extended to include a critical mixed-mode stress to nucleate a fatigue crack [138] and a novel wavelet decomposed dual-time scale to reduce the computational cost of cyclic loading in a FE-CP framework [139]. The decomposition of the nodal displacement with the rate dependent plastic variables results in a decoupled behavior between the monotonic coarse cycle-scale and an oscillatory fine time scale [140]. And as result it is possible to achieve crystal plasticity simulations with 100,000 applied loading cycles to mimic the crack initiation behavior in materials subjected to LCF conditions.

McDowell et al. modeled the fatigue behavior of Inconel 100 at elevated temperature through FE-CP [141,142]. This model accounts for microstructural features such as grain size and second-

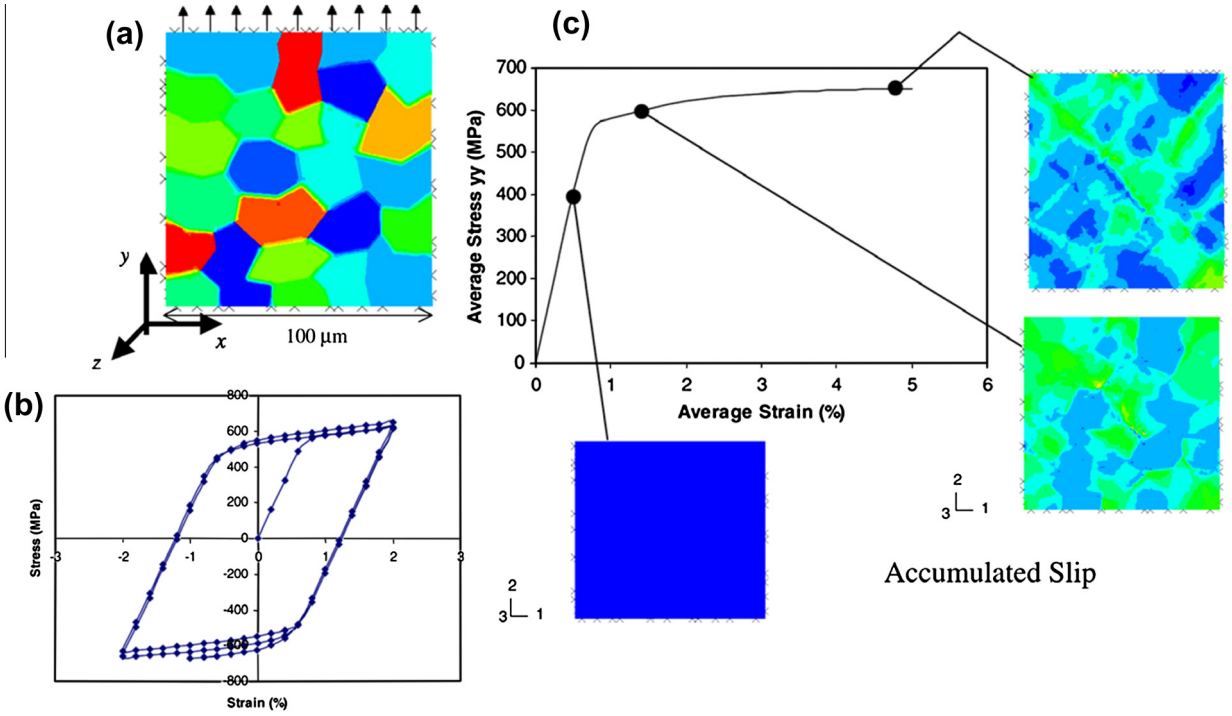

Fig. 11. (a) Crystal plasticity simulations of (a) a textured polycrystal displaying its (b) cyclic macro-scale stress–strain response. (c) For monotonic loading, the accumulated slip is shown at three distinct strains [136].

ary/tertiary γ' size and volume fraction by using a flow rule with a two-term potential.

$$\dot{\gamma}^{\alpha} = \left[\dot{\gamma}_0\left(\frac{|\tau^{\alpha}-\chi^{\alpha}|-\kappa^{\alpha}}{D^{\alpha}}\right)^{n_1} + \dot{\gamma}_1\left(\frac{|\tau^{\alpha}-\chi^{\alpha}|}{D^{\alpha}}\right)^{n_2}\right] sgn(\tau^{\alpha}-\chi^{\alpha}) \qquad (15)$$

In this flow rule, κ^{α}, is the threshold stress on the individual (octahedral or cube) slip system, which is a function of the local microstructure (grain size, γ' precipitate size distribution, and γ' precipitate volume fraction) through physically based micromechanical models. Thus, the microstructure plays a role in determining the mean free path of dislocations and the associated critical resolved shear stress on each slip system. Two internal variables are used to determine the evolution on each slip system, α, which are the dislocation density, ρ, and the back-stress, χ. Each parameter is calibrated based on the cyclic stress–strain response for extreme variations of microstructure by an optimization routine within a neural network [141,142]. From this analysis, the fatigue sensitivity in terms of the initial hysteresis loops (cyclic hardening behavior) are estimated based on the microstructure parameters, namely the average grain size and precipitates size distribution and volume fraction [142]. This framework has been extended to notch root analysis [143], and fatigue indicator parameters are used to determine the effect of varying microstructure in predicting crack initiation life [141,144]. This set of FE-CP modeling of Ni-based superalloys embodies a tremendous effort including the sensitivity of key microstructure parameters into the fatigue response of the material.

Another set of FE-CP models from McDowell et al. focused on slip band evolution within a Ti-64 alloy [145]. This work focused on the softening response of slip in a region within the microstructure while subjected to a cyclic load. The simulation of cumulative plastic strain distribution within the microstructure displayed good agreement with the qualitative images of surface slip trace micrographs measured from an in situ SEM experiment, as shown in Fig. 12 [145]. Additionally, a large prognosis effort developed a FE-CP framework to determine the tensile stress in particles within 7075 aluminum based on the strain level surrounding the particle, parent grain orientation, and particle aspect ratio [146]. A microcrack develops in the particle, if the stress in the particle exceeds its strength, which is determined mechanistically through experimentally measured probability distributions. This framework is extended to study fatigue crack initiation [147]. The model depicts a fatigue crack nucleating from a cracked Al_7Cu_2 particle once localization and cyclic accumulation of slip is present as well as a local driving stress, which is once again strongly based on the local microstructure [148]. In general, the FE-CP models presented in this section represent significant progress in balancing the microstructure level understanding of material behavior with the associated computational costs. We see that these approaches offer tremendous benefits in predicting the response of the material and eventually fatigue crack initiation, especially given the multi spatial scales and time scales simulations achieved in these studies.

8. Discussion on future of fatigue: experiments and modeling

Rather than try to summarize and conclude on the physics of crack initiation, we close with brief comments on the future of fatigue experiments and modeling. Fatigue is a topic that has attracted research interest for a long time; there have been significant phenomenological advances in the 1960s through the early 1980s that shape our modern understanding of microstructural influences in fatigue today. The historical understanding of fatigue is critical to allow the current generation of scientists and researchers to build on this fundamental knowledge given the vast improvements in material characterization and computational power. Hence, we are now in a position, to make major strides in addressing and solving the microstructural influence and prediction of fatigue crack initiation in metals, which remains a pressing issue to the materials science and engineering community.

Simulation-based predictions of material performance including fatigue crack initiation have been recognized as a means of

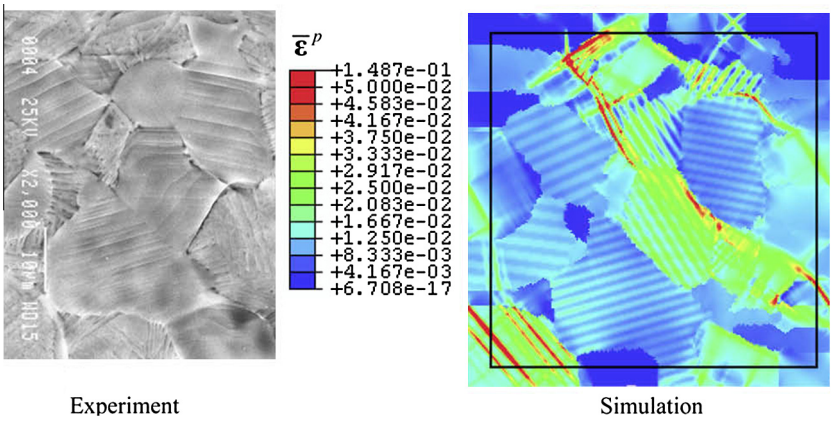

Fig. 12. Crystal plasticity simulation of cumulative plastic strain distribution compared with experimentally measured slip traces for Ti-6-4 at 2% applied strain [145].

accelerating the insertion of new materials by reducing the associated cost and time for materials development [149]. Given the recent enhancements in all facets of high-performance computing, predictive simulations and models will continue to enhance our analysis of reliable fatigue components. A long-standing goal of the engineering and materials science community is the ability to build connections between the complex microstructure of advanced engineering alloys and the performance of the material. Researchers and scientists appear to be approaching this goal by determining physics-based cause and affect relationships. The models presented in Section 7.2 represent advancement in cyclic slip behavior of polycrystalline microstructures, which simulate the slip irreversibilities and unique defect arrangements that are critical to fatigue. These multi-scale (spatial and temporal) methods serve as an integrated foundation to predict damage evolution, fatigue crack initiation, and the minimal reliable safe life, in order to prevent failure of critical components. Many current approaches are built on the fundamentals of uncertainty quantification to predict variability in the micro- and meso-structure that result from processing advanced materials to elucidate propagation of variability within the models and supply the associated risk assessment. Moreover, these modeling results allow microstructure-based failure prediction tools to be linked to existing process modeling software to reverse engineer components that are resistant to failure. As discussed in other review papers certain fundamental challenges in modeling still exist [150], and as more robust fatigue models are created, additional complexities will surmount building generalized models with competing failure mechanisms and combinatorial effects of fatigue variables (temperature, hold times, multi-axial loading, notches, etc.).

As previously stated, the development of emerging materials and their incorporation into component design can be accelerated while simultaneously improving the material performance by establishing computational materials models, which connect microstructure and fatigue properties/performance. The aforementioned efforts need detailed material characterization activities combined with validation and verification of their test readiness in order to implement the models into a design methodology. Previous model validation efforts were completed based on large-scale testing programs, which may look at an ensemble of test data at the specimen or component scale. These traditional testing strategies jeopardize the implementation of new advanced materials or design methodologies due to large time and financial investments. Today, we see the most advanced characterization and interrogation methods at each scale are used to verify and validate predictions of the simulations, including 4-D mapping of 'defect' features, strain fields, and complex stress states within the material.

Initial 3-D microstructure characterization is valuable as a starting point for building computational fatigue models for structural materials. In order to fulfill this need, software is available to reconstruct the microstructure from EBSD images via destructive serial sectioning of the material [151], which can be used as an input to modeling efforts. Higher fidelity 4-D microstructure characterization is obtained through use of advanced synchrotron sources [152]. Using near field high-energy X-ray diffraction (HEXRD), complete non-destructive 4-D microstructure information can be obtained including the grain size, orientation, topology, and position [153]. Additionally, far field HEXRD techniques have been used to measure the in situ averaged elastic stress tensor evolution within each grain during loading [154]. This offers tremendous insight into the microstructure. Moreover, using diffraction and phase contrast tomography, the evolution of small cracks can be seen relative to the microstructure as captured in an ex situ experiment by Ludwig et al. [155]. These techniques offer profound microstructurally-sensitive implications by experimentally capturing and detecting in situ fatigue crack initiation, as these efforts are currently underway by Suter et al. [156].

As a research community, we employ both experiments and computational modeling efforts to explore the physics of fatigue crack initiation in materials, although at times, these efforts are disjoint. Over the last decade, with an increase in computational power, we have been able to simulate the 3-D response of the microstructure due to external stimuli during processing or loading. Previously, this behavior could not be experimentally interrogated at the microstructural level within the material's bulk. With the combined grain orientation mapping and stress tensor measurements efforts based on synchrotron techniques, tremendous amounts of information are accessible at the microstructural level. Now we are in a unique position to directly compare the results of experiments and modeling on the same scale. This represents an exciting time for fatigue research.

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