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Microstructure-sensitive computational modeling of fatigue crack formation

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ABSTRACT

Recent trends towards simulation of the cyclic slip behavior of polycrystalline and polyphase microstructures of advanced engineering alloys subjected to cyclic loading are facilitating understanding of the relative roles of intrinsic and extrinsic attributes of microstructure in fatigue crack formation, comprised of nucleation and growth of cracks at the scale of individual grains or phases. Modeling of processes of early stages of fatigue crack nucleation and growth at these microstructure scales is an important emerging frontier in several respects. First, it facilitates analysis of the influence of local microstructure attributes on the distribution of driving forces for fatigue crack formation as a function of the applied stress state. This can support microstructure-sensitive estimates of minimum life, as well as characterization of competing failure modes. Second, it can inform modification of process route and its manifestations (e.g., residual stress, texture) to alter microstructure in ways that promote enhanced resistance to formation of fatigue cracks. Third, microstructure-sensitive modeling, even conducted at the mesocopic scale of individual grains/phases, can facilitate parametric design exploration in searching for microstructure morphologies and/or compositions that modify fatigue resistance. Fourth, such technologies offer promise for integration with advanced nondestructive evaluation methods for prognosis and structural health monitoring. Finally, as a longer term prospect in view of uncertainties in modeling mechanisms of cyclic slip, crack nucleation and growth, such modeling can serve to support more quantitative predictions of fatigue lifetime as a function of microstructure. We first discuss computationally based microstructure-sensitive fatigue modeling in the context of recent initiatives in accelerated insertion of materials and integration of computational mechanics, materials science, and systems engineering in design of materials and structures. We then highlight recent application of such strategies to Ni-base superalloys, gear steels, and α–β Ti alloys, with focus on the individual grain scale as the minimum length scale of heterogeneity. Finally, we close by outlining opportunities to advance microstructure-sensitive fatigue modeling in the next decade.

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1. Introduction

The past decade has witnessed a confluence of high performance computing, advanced experimental methods for in situ and ex situ measurement of evolving microstructure at various length scales under cyclic loading, and substantial advances in understanding deformation mechanisms, material degradation, and relevant modeling concepts in fatigue. Together, these various elements have introduced new possibilities to consider the role of microstructure in the formation and growth of small cracks in fatigue. This article focuses on microstructure-sensitive methods that involve explicit modeling of elastic–plastic behavior of individual grains in polycrystalline metals and alloys under cyclic loading conditions, with emphasis on advanced engineering alloys for loading amplitudes below the macroscopic yield point. The term "microstructure-sensitive" as used in this overview implies both an explicit treatment of the polycrystalline grain structure as well as constitutive models that reflect the role of crystallography in slip in addition to related microstructure size/scale effects. Such models are continuously evolving. As another point of clarification, we refer to the collective processes of grain scale fatigue crack nucleation and early growth as "crack formation" rather than the more common term "crack initiation," as the latter typically invokes an arbitrary length scale that varies widely through the literature. Use of the term "fatigue crack initiation" stems more from experimental convenience in reporting the number of cycles required to produce a crack of a predefined length to be measured experimentally, typically using somewhat coarse scale definitions relative to microstructure.

It is important to convey a realistic summary of the current state-of-the-art. In spite of the perception of maturity, the aforementioned coupling of computing and high resolution, experiments with sufficient field of view is of relatively recent origin;

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hence, in many respects we are in the infancy of grain/phase scale understanding of early stages of fatigue crack formation and design of fatigue-resistant microstructures. There are many outstanding issues that challenge our capability to bridge the scales of length and time necessary to address metal fatigue problems. In spite of substantial advances in first principles and atomistic modeling of the inelastic behavior of metallic materials, there is a substantial gulf between the length and time scales of first principles and atomistic modeling and those scales necessary to quantify the role of microstructure in formation of fatigue cracks. Fatigue is among the more daunting of the grand challenge problems in this regard, since the loading is non-monotonic and the number of cycles required of applications is often in excess of millions. Fig. 1 provides a gap analysis [1], with four orders of magnitude in length scale spanning the problem of linking the scale of nucleation of a fatigue crack in conventional polycrystalline metallic alloys to atomic level phenomena that give rise to the evolving state of irreversibility in fatigue. The gap has long been filled by experimental observations of cyclic deformation and fatigue crack formation as a function of microstructure, which of course limits the scope of exploration to studies of existing alloys under narrow sets of loading histories and environments. This is true not only of fatigue, but more generally of metal plasticity at either small or large strains.

Primarily building on computational simulations, progress is being made in addressing the gaps in modeling dislocation plasticity between atomic scales and scales of dominant microstructure attributes such as grains or phases [1]. Approaches such as microscopic phase field models and discrete dislocation dynamics that can accept information from experiments and atomistic modeling are advancing to the point where deformation mechanisms are beginning to be understood from a many body defect simulation standpoint. This can supplement and extend understanding gained over the past 20–30 years using SEM and TEM observations [2–12]. Modeling and simulation specific to dislocation structures in fatigue such as cells [9,10] or persistent slip bands [6–8,10–18] in single crystals has provided progress in addressing cyclic deformation aspects. Still, quantitative connection of such dislocation structures to crack nucleation is still in its very early stages.

There are multiple streams of related fatigue research. One body of research has addressed the issue of measuring and modeling dislocation substructure under cyclic loading [3,4,6–12,14–17] and experimental observations of slip offsets and progressive crack formation [6,15,18–23]. Another distinct body of work has been aimed at engineering applications requiring prediction of fatigue life of components under various loading conditions based smooth specimen testing. The latter approaches have largely settled upon the construct of "crack initiation" to circumvent the issue of bridging the scales in Fig. 1 up to the order of several hundred microns by introducing semi-empirical relations for the number of cycles to form a crack of predetermined size which is relatively large compared to dislocation substructure or grain size. One goal of this paper is to use simulations to bridge these two parallel branches of study to some extent, and to explore what applications might benefit from so doing. We may characterize this branch of study as microstructure-sensitive modeling of fatigue processes, with focus on the mesocopic description of the response of collections of microstructure attributes. The origins of these kinds of mesoscopic simulations of heterogeneous materials to understand the role of microstructure and related stochastic/probabilistic aspects with applications to failure modes can be traced back to the early to mid-1980s with the advent of computational micromechanics. For example, Asaro and colleagues developed early polycrystalline finite element models for shear localization in polycrystalline microstructures with ductility and strength in mind [24–28]. Needleman and colleagues [29–32] used finite element methods to consider the interactions of fibers with matrix material and processes of nucleation and growth of voids at grain boundaries in polycyrstals. They also extended these approaches to address interfacial failure in finite element models of idealized or actual microstructure representations using cohesive zone methods [33]. By the early 1990s, considerable efforts were underway in computational mesoscopic modeling of microstructure-property relations directed towards various classes of heterogeneous materials. Extending earlier works of Asaro, Needleman and colleagues, Zikry et al. [34–37] considered the effects of crystallite orientation distribution and grain boundary network on failure modes in large scale computational crystal plasticity using finite element methods.

The integration of modeling fatigue response of polycrystalline alloys with probabilistic failure descriptions was a natural outcome of the rapid development of the field of computational micromechanics modeling in the 1980s. Haddad [38] considered the effect of microstructure on distribution of slip in polycrystals. The work of Chamis and colleagues [39–41] integrated the notions of computational micromechanics simulation of heterogeneous materials

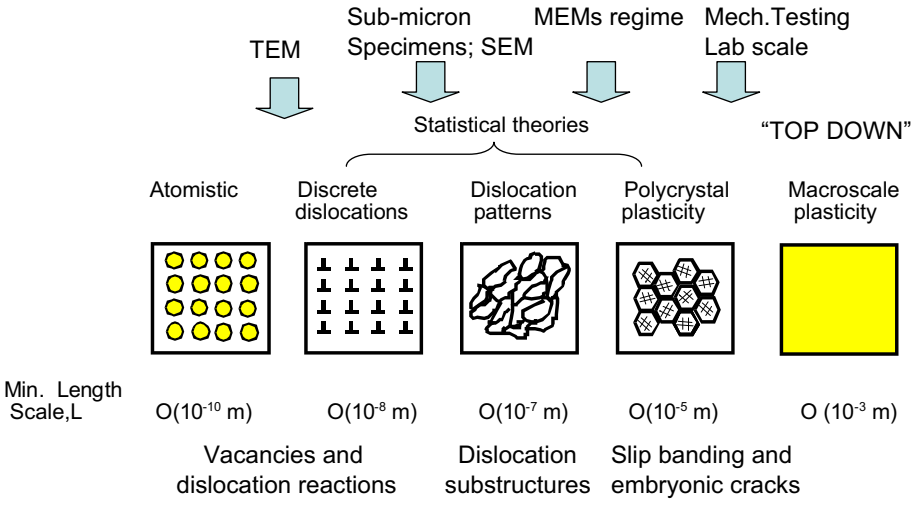

Fig. 1. Hierarchy of length scales in metal plasticity ranging from atomic (dislocation cores) to patterns of dislocations to multiple grains to macroscopic scale. The primary gap in modeling and simulation in multiscale modeling exists between the scales of atomistic simulations and dislocation pattern modeling, with discrete dislocation simulation playing an increasing role but phenomenological statistical theories presently dominant.

(composites) with probabilistic analyses to advocate low probability of failure design methods for different failure modes. Duva et al. [42] and Ruggieri and Dodds [43] employed computational simulations of heterogeneous materials and cracked to support probabilistic computational micromechanics characterization of damage evolution.

Appealing to earlier work on stochastic deformation and failure of random heterogeneous materials [44], and in recognition of the expense of finite element methods, lattice-spring methods were used by Ostoja-Starzewski et al. [45] to characterize probability distributions of damage evolution in random heterogeneous materials. Zhou and Zhai [46,47] built on the earlier work of Needleman to model dynamic fracture of realistic microstructures by placing cohesive zone elements throughout the microstructure in explicit finite element simulations, including effects of distribution of interface cohesive strength and energy. Variability of response (e.g., crack growth history) with microstructure is a natural outcome of such simulations.

Some of the earliest mesoscopic approaches to characterizing distributions of driving to support probabilistic fatigue crack formation for metallic polycrystals can be traced to early works such as those of Provan [48,49] and Sakai et al. [50]. The interaction of small cracks with microstructure and related mesoscopic models for crack growth in random microstructures had been understood and modeled in the 1980s [51]. McDowell [52] reviewed the status of microstructure sensitivity to formation and growth of small cracks in high cycle fatigue (HCF). Gall et al. [53] used finite element simulations to study the effects of crystallographic orientation on variability of microstructurally small crack growth rate in crystals using ΔCTOD concepts.

Mesoscopic modeling of distributed crack formation within grains of a polycrystalline ensemble by Hoshide and Socie [54] employed slip band cracking models and crack growth relations. This was an important precedent in motivating later work in the field, as all essential elements of crack nucleation in slip bands in grains and early growth were treated for metallic polycrystals with the approximation of the Sachs (isostress) assumption for intergranular interactions. McDowell [55] discussed the importance of such mesoscopic simulations to quantify the role of microstructure from the perspective of a frequency distribution of driving forces. This latter work also clarified that the notion of a statistically homogeneous representative volume element (RVE) for fatigue is problematic; for many practical cases, a RVE is simply too large to be relevant to actual specimens or structures, particularly in the HCF regime, given typical gradients of macroscopic field quantities. This had been stressed earlier in the work of Lacy et al. [56], which showed that the RVE size for elastic stiffness of a field of microcracks in a brittle material (e.g., polycrystalline ceramics) is much too small to be considered as a RVE for the evolution of damage. Of course, in this case one might argue that including higher order terms in the Taylor series expansion of the deformation gradient in the homogenization process would be necessary (e.g., second or higher gradient theory), but even this is insufficient to fully capture localization problems in damage evolution at the scale of the simulation window. Accordingly, it is necessary to build up statistics based on multiple computational realizations [57] of statistical volume elements (SVEs) to arrive at a complete statistical distribution of responses. In other words, it is not appropriate to select a size for a computational volume of a heterogeneous material by considering convergence of the average stress–strain behavior or elastic stiffness if fatigue crack formation and growth are the relevant responses of interest. The notion of a RVE for fatigue implies that even the higher order moments of the statistical distribution of fatigue driving forces are fully captured, not just the lowest order moments, a point made earlier by Lacy et al. [56] in general for microstructure evolution and by McDowell [55] in reference to fatigue.

Bennett [58] and derived papers by Bennett and McDowell [59,60] used finite element models with crystal plasticity to compute distributions of slip and to estimate distributions of fatigue cracks in polycrystals based on multiple realizations of a nominal microstructure. In addition, they computed the cyclic crack tip displacement range (both opening and sliding components) as a function of crack length relative to grain size from surfaces in polycrystals [61]. In the DoE USCAR program from 1995 to 2000 [62–64], finite element modeling of microstructure was employed to model formation and early growth of interdendritic cracks in A356–T6 casting alloys, culminating in the formulation of a probabilistic framework for fatigue response based on various distributions of microstructure attributes at five different length scales [65]. In the same timeframe, Tryon and Cruse [66–68] also related mesoscopic finite element modeling of microstructure to distributions of fatigue responses of polycrystalline microstructures, albeit within the context of a RVE.

A large body of microstructure-sensitive fatigue modeling work has evolved since the late 1990s, much of which is covered later in this manuscript. We focus here on microstructure-sensitive modeling of fatigue crack formation, i.e., the nucleation and growth of fatigue cracks up to a size at which the microstructure plays a less pronounced role in affecting variability of subsequent crack growth. Typically, this implies a crack length of less than three grains/phase domains in a polycrystalline and/or polyphase alloy system [69]. Some of the potentially important microstructure attributes that influence fatigue crack formation include microstructure unit size, morphology, and crystallographic orientation [69–72]; at smaller length scales, the development of lattice curvature, dislocation substructures, and effects of local grain boundary structure have profound effects on cyclic deformation and fatigue.

Concurrent with development of models to bridge the scales shown in Fig. 1 are associated experimental tools (top row in Fig. 1) for characterization and/or measurement of evolving structure at different levels of hierarchy to guide understanding of dominant mechanisms, spatial variation of microstructure evolution, and related size effects. They can also provide information that is key to quantifying realistic microstructure to support modeling and simulation, and to calibrate/validate models framed at various levels of the hierarchy. Once such modeling techniques are developed for a given class of materials, computational assessment/projection of microstructure sensitivity of various responses is enabled; this contrasts with costly experimental exploration that may not be able to effectively resolve the relative role of mechanisms occurring at various scales of hierarchy in Fig. 1. Attention can be increasingly devoted to design of experiments for model calibration and validation. Effective usage of microstructure-sensitive models requires the development of protocols for the extraction of relevant microstructure statistics. Only then may simulations be carried out to provide useful information regarding rare event slip localization processes that relate to minimum expected fatigue lifetimes, for example. An important topic of research in this area, therefore, is identifying and characterizing relevant statistical representations of microstructure attributes. As an example, both textures and micro-textures that result from different primary deformation processing routes should be characterized as key microstructure attributes of such models [73,74]. In addition, the development of micromechanical testing combined with a range of advanced microscopy techniques is essential for the development of mechanistic understanding and its embodiment within modeling techniques.

Microstructure-sensitive computational models, coupled with experiments for (i) calibrating specimen level and relevant grain scale cyclic deformation and cracking phenomena and (ii) validating algorithms and methodologies for interpreting simulations, can

offer value in understanding failure mechanisms and quantifying sources and magnitude of uncertainty. As such, the confidence limits of fatigue life prediction algorithms can be improved by such modeling. In such simulations, there can be tradeoffs between model accuracy and robustness for comparing responses among microstructures, depending on whether preliminary or detail design is under consideration. Given the complexity of phenomena shown in Fig. 1, absolute predictions of fatigue life is a grand challenge, not yet really practical, due to incomplete and/or uncertain models for deformation and damage mechanisms. Application domains that can be served by microstructure-sensitive modeling include the following:

- Supporting fatigue life prediction schemes, with emphasis on the role of microstructure in minimum life.
- Supporting selection/design of microstructure for application-specific scenarios.
- Enhancing depth of understanding in analyses of field service fatigue failures.
- Providing guidance for modification of process route to enhance fatigue resistance.

Different industry sectors conventionally design components for fatigue resistance with a focus either on crack initiation or crack propagation. In industry, two distinct approaches are commonly pursued: (a) fail-safe design based on fatigue crack initiation estimates or (b) damage tolerant design based on periodic inspection and use of fracture mechanics principles for fatigue crack growth. Both approaches are relevant to modeling total fatigue lifetime of components. Combined initiation-propagation approaches are also employed in certain industry sectors. Microstructure-sensitive models can provide a basis for predictive parametric exploration of the relation of microstructure to fatigue response across a range of microstructures, including *virtual* microstructures that have not yet been processed; they are perhaps of greatest value in applications that rely on fatigue crack initiation estimates. As resolution of crack detection schemes improves with advances in prognosis and structural health monitoring technologies (including signal processing), the need for microstructure-sensitive models will become even more pronounced.

There is considerable demand for microstructure-sensitive models to support emerging joint government–industry initiatives launched within the last decade in the USA. For example, the DARPA Accelerated Insertion of Materials (AIM) program [75,76] from 2000 to 2005 offered insight into how computational materials science and engineering can be harnessed in the future to assist in developing and certifying materials in a shorter timeframe to more closely match the system or product design cycle timeframe. AIM was a bold initiative that involved materials developers, original equipment manufacturers (OEMs), and government and academic researchers in a collaborative effort to build designer knowledge bases comprised of the various elements of systems design. These elements include databases, digital realizations of microstructure, modeling and simulation tools that address various levels of materials hierarchy, experiments, materials characterization, process and cost models, statistical approaches to uncertainty, metamodeling, and information protocols for managing workflow and communications. At the core of the AIM methodology are microstructure-sensitive models that facilitate the linkage of process path to properties and end-use applications. More recently, the *Integrated Computational Materials Engineering* (ICME) initiative has been defined by a NAE National Materials Advisory Board study group [77]. ICME is an approach to concurrent design of products and their materials to enhance product functionality, efficiency and sustainability. This is achieved by linking materials models at multiple length and time scales to address problems relevant to specific products and applications. A broad perspective regarding these initiatives is offered in Ref. [78].

2. Regimes of fatigue and cyclic microplasticity

Microstructure-sensitive simulations suggest definitions of the high cycle fatigue (HCF) and low cycle fatigue (LCF) regimes based on heterogeneity of cyclic plastic deformation at the scale of microstructure [65]. The HCF regime corresponds to stress amplitudes below macroscopic yielding for which cyclic plastic strain occurs within isolated regions of microstructure concentration (inclusions, favorably oriented grains, etc.). This is the regime of *constrained* cyclic microplasticity, in that surrounding regions are dominantly elastic [52,65]. Transition to LCF conditions occurs at higher applied stress amplitudes for which the cyclic plasticity becomes widespread and more homogeneously distributed. From a mechanics perspective, LCF can be regarded as an homogenization problem involving multisite cracking and coalescence. Variability of behavior in LCF is less pronounced for a given microstructure and arises chiefly in relation to crack growth phenomena.

In the HCF regime, crack formation and microstructurally small crack growth processes encompassing a scale of perhaps up to 10 grains often dominate the fatigue lifetime. Under HCF conditions, the cyclic plastic deformation is highly heterogeneous within the microstructure; accordingly, this is the regime in which variability and size effects are most pronounced. Variability in HCF is controlled by fatigue crack formation processes, with a significant role of microstructurally small crack growth behavior for many microstructures. Small crack growth behavior is quite sensitive to microstructure and accounts for much of variability of lifetime in practical alloy systems. Moreover, the issue of arrest of small cracks that form at isolated sites of cyclic plastic strain intensification is pertinent to estimation of an associated fatigue limit.

Table 1 outlines relevant mechanisms of crack formation and propagation in the HCF and LCF regimes. Microstructure-sensitive fatigue analysis is particularly useful as a means of gaining insight into fatigue responses in the HCF regime since experimental results are often limited or inconclusive in this regime – one complication is the low probability of finding critical formation sites – the rare event or "needle in haystack" problem. From a mechanics standpoint, HCF is a localization problem of extreme value type; strategy for computational HCF modeling of components that must last millions of cycles, such as shafts, bearings, and gears, for example, should focus on extreme value statistics of potential sites for microplastic strain localization and fracture that drive crack formation and early growth.

Stochasticity or randomness arises in fatigue behavior due to interactions of slip and crack path interactions with microstructure [52]. Operationally, there are at least three approaches for treating such stochasticity:

(i) Introduce stochastic models at all scales, including sub-grain scales associated with crack nucleation.
(ii) Embed microstructure-driven stochasticity into variability of parameters of mesoscopic or macroscopic fatigue crack initiation and growth models.
(iii) Adopt a deterministic methodology at some prescribe scale (e.g., crack nucleation and growth models at grain scale), capturing stochasticity at higher scales (e.g., polycrystal) via micromechanical simulations, and extracting statistics or informing Bayesian probabilistic models.

Approach (i) requires a robust multiscale modeling strategy with explicit treatment of microstructure degrees of freedom at scales ranging from tens of nanometers to tens or hundreds of

Table 1
Relative emphasis on fatigue micromechanisms in the LCF and HCF regimes.

Mechanisms	LCF – percolated, microplasticity	HCF – isolated, heterogeneous, microplasticity
Crack formation	Propagation-dominated: largest grains or inclusions establish initial crack length in propagation analysis	Initiation-dominated: largest grains or inclusions control number of cycles to form a crack or to escape arrest
Microstructurally crack growth	Cracks grow in elastic–plastic field with less microstructure influence	First few microstructure barriers control fatigue limit and scatter of lifetime
Physically small and long crack growth	Elastic–plastic growth persists well into crack growth history; coalescence of multisite cracks can occur	Transition to LEFM-dominated homogeneous crack growth; single dominant crack is common

microns, or understanding of appropriate scaling relations for phenomena at various length and time scales. It may represent an ultimate long term goal of stochastic modeling, but is presently infeasible. Approach (ii) has been commonly applied in crack growth models, and to some extent in fatigue crack formation. It requires physical intuition and an experimental database with which to compare. Approach (iii) is the one taken in several examples in this article, and consists of asserting applicability of physically based models at a certain scale (e.g., individual grain or sub-grain) and then developing statistics based on ensembles of polycrystal simulations. For this reason, we employ the term "microstructure-sensitive" to reflect the underlying physical basis, in contrast to approaches that indirectly prescribe dependence on microstructure based on random fields of parameters in mesoscopic or macroscopic models. In all cases, one key attribute of fatigue, particularly HCF, is that simulations are typically conducted over length scales (windows of microstructure) too small to target the response of a so-called representative volume element (RVE), defined on the basis of statistical homogeneity of response; in this case, the response is the probability density of slip-based driving forces for forming and growing cracks in the material, which is known to have strong size effects in HCF due to the very long correlation lengths of fatigue critical hot spots with highest probability of crack formation. This nuance renders microstructure-sensitive simulation of cyclic plastic deformation and fatigue processes completely different in nature from homogenization of heterogeneous material responses such as elastic stiffness or large offset-defined yield strength. Rather than focusing on RVE simulations, the focus in fatigue is more on statistical volume elements (SVEs) [1,55,57] which are computationally tractable and can serve to populate the statistics of the response function. A large number of such SVE responses are necessary to characterize the shape (including tail) of the probability density functions of cyclic slip that relate to fatigue crack formation and early growth. This is often overlooked in the literature which focuses more on homogenization than on higher order statistical moments.

Beyond addressing effects of microstructure randomness for a given material, we may further categorize microstructure-sensitive fatigue models according to the level of detail at which microstructure is represented, as follows:

(1) Those that introduce granularity/heterogeneity for purposes of injecting stochasticity (e.g., lattice models or damage mechanics models), but are concerned more with global response than local responses at the scale of microstructure. See McDowell [55] for a critical evaluation of such approaches for fatigue applications.
(2) Those that consider local details of microstructure in micromechanical modeling and are concerned with both local and global responses. Examples of microstructure attributes include inclusion/grain size, shape, and orientation distributions. In addition, models for each grain should employ realistic slip laws, track lattice rotation, etc. This body of work is much more limited in the literature (cf. [1,50,54,56–72]).

This discussion of emerging frontiers is more concerned with the latter category which offers potential for more utility in capturing local conditions for fatigue crack formation and linkage to experimental verification. Microstructure-sensitive modeling approaches of this type were employed as early as 1988 [54] and more recently within the context of polcrystal plasticity [1,59,60,69–72,79–92]. They have been applied to the formation and growth of microstructurally small fatigue cracks [93–99], including development of plasticity-induced crack closure [100]. Linear Elastic Fracture Mechanics (LEFM) theory is of limited utility in relating heterogeneous, localized slip to formation and growth of small fatigue cracks interacting with microstructure unless provision is made to explicitly incorporate the details of dislocation distribution and the discrete character of both dislocations and microstructure [101–106]; such discrete dislocation modeling is still in a very early stage. The extension of discrete dislocation modeling to consider realistic microstructure in fatigue is highly complex and has not really been addressed to date. The coupling of mechanical and chemical driving forces for crack formation and early growth in fatigue is an area of great importance, also still in its infancy; it is not addressed here. Finally, at present many factors (primarily computational time requirements) limit the ability to consider effects of many cycles necessary to address long term transients or complex, variable amplitude load histories; some progress is being made on this front [84]; as a result, most of the work considered here assumes that results from models executed over even limited numbers of cycles (say 3–30) can suffice to provide certain kinds of information useful to perform relative ranking of microstructures based on minimum expected fatigue life or other metrics. This state of affairs will be improved in due course with advances in computational methods for multiple time- and length-scaling, but this is not a problem that can be effectively solved in the foreseeable future by simply increasing computing power at projected rates. It demands advances in the mechanics treatment.

2.1. Hierarchical stages of fatigue crack formation and growth

It behooves us to carefully distinguish regimes of crack nucleation and early growth from those of growth in later stages. An operational decomposition of the total fatigue life among stages is given by [65,107,108]

$$N_T = N_{inc} + N_{MSC} + N_{PSC} + N_{LC} = N_{inc} + N_{MSC/PSC} + N_{LC} \quad (1)$$

where $N_{inc} = N_{nucl} + N^*_{MSC}$ is the number of cycles required to *incubate* or form a crack (comprised of nucleation plus small crack growth through the domain of influence of a large grain, cluster of inclusions, etc. that promoted nucleation) at a favorable site with initial length, a_i, on the order of the scale of certain microstructure attribute(s). In physical terms we may consider N_{nucl} to associate with a phase or order transition from uncracked to cracked lattice, an evolutionary process that depends strongly on underlying dislocation substructure. While N_{nucl} may comprise on the order of 5–20% of the total lifetime in the HCF regime [109], it serves as

a "trigger" for the process of forming and growing cracks; its linkage to microstructure hot spots is quite relevant. Moreover, the fraction of total lifetime consumed in nucleating cracks can increase substantially in the very high cycle fatigue (VHCF) regime. The term N^*_{MSC} represents the number of cycles required to propagate the crack beyond the influence of either the high slip concentration configuration of the nucleation site or beyond the first few strong microstructure barriers that resist crack advance and have a strong influence on apparent fatigue limit and overload effects; N^*_{MSC} can be a significant fraction of N_{MSC} under HCF conditions. Hence, the notion of "incubation" conveyed in Eq. (1) pertains more to local environments of microstructure attributes (e.g., extrinsic micronotch such as a pore or inclusion or a set of intrinsic attributes such as a large grain and its nearest neighbors, proximity of distinct phases, etc.); such environments are typically less than 100 μm in physical extent.

N_{MSC}, N_{PSC} and N_{LC} represent the number of cycles to propagate a crack in the regimes of microstructurally small (approximately 3–10 times the grain or second phase size/spacing that affects retardation of the crack driving force), physically small, and long crack growth, respectively. Physically small crack growth (N_{PSC}) is distinguished as a regime in which the crack is long compared to microstructure scale, but is subject to breakdown of similitude due to a cyclic plastic zone size that is on the order of grain size or other key microstructure correlation lengths that affect crack growth variability. At some point, cracks in the PSC regime have characteristics of fully developed, mechanically long cracks in that the crack front has reached a condition of self-similar crack growth. There are two aspects with regard to the notion of similitude or self-similar growth of cracks that are affected in the transition through the MSC and PSC regimes. First, the size and shape of the crack tip cyclic plastic zone relative to the crack length and microstructural unit size or barrier spacing changes substantially as the crack transitions from modes II to III dominated crystallographic Stage I shear growth [110] in the MSC regime to the Stage II, mode I-dominated regime. The cyclic plastic zone in the former case may be constituted by shear bands extending ahead of the crack tip, with dominance of single slip conditions within the first few grains. As a crack extends, the crack front has higher probability of sampling multi-slip conditions to accommodate extension and maximize the growth rate; given that the crack typically forms in a favorably oriented large grain, for example, the neighboring grains will affect this sampling process as the crack front meanders and percolates through the microstructure until multi-slip conditions are more uniform along the crack front. The lack of self-similarity due to this meandering process is an important three-dimensional manifestation that influences the transition from Stage I to Stage II crack growth, and effectively controls the limits of the MSC propagation phase. Beyond this point, lack of self-similarity of crack extension can still exist in the PSC growth regime if the cyclic plastic zone size is comparable to microstructure barrier spacing.

Finally, long crack behavior is typically realized for cracks with length and cyclic plastic zone size and damage process zone size suitably large compared to microstructure barrier correlation lengths, such that similitude requirements are met in terms of small scale yielding and damage. Crack lengths of several hundred microns and above are typically necessary to meet these conditions in conventional microcrystalline structural alloys, depending on amplitude and R-ratio of applied remote stress.

Emerging capabilities in microstructure-sensitive modeling and high resolution experimental characterization demand the more detailed decomposition in Eq. (1). High strength components for which the elastic strain amplitude dominates the plastic strain amplitude are subject to heterogeneous cyclic plasticity and cracks may form but frequently arrest; this is an important practical type of fatigue limit that can be eradicated by overloads. This is why the decomposition of incubation and subsequent growth is made. Second, advances in high resolution characterization via electron backscatter diffraction (EBSD), micro X-ray diffraction and chemical composition analysis, focused ion beam (FIB) serial sectioning, and computed tomography have enabled unprecedented levels of detail in rendering crack path and shape during the early stages of fatigue for which the incubation and microstructurally small crack regimes are applicable. It is also possible to machine artificial crack-like notches (crack starters) in a precise way in large, favorably oriented grains along slip planes having highest Schmid factor that replicate quite closely the behavior of naturally occurring cracks [111], something not possible with more coarse EDM-machined notches. Conventional cellulose acetate replicate techniques cannot render such detail. Also, high fidelity numerical simulations with reasonably realistic crystallographic models for dislocation glide offer the capability to interrogate the expected mechanical response of the individual grains and even sub-grain regions of polycystals, including reversed and cumulative slip. Accordingly, in spite of the experimental difficulty of imaging the crack tip displacements for such small cracks with present technology, means now exist to provide quantitative modeling of anisotropic elastic–plastic behavior of slip.

The more detailed decomposition in Eq. (1) is also important for the following reasons:

- In designing material microstructure for fatigue resistance, we must clarify what regime of crack length and characteristic life fraction is targeted. It is well known that design for "initiation" versus "propagation" of fatigue cracks often leads to conflicting material requirements in terms of ducility and strength.
- In modifying process path to enhance fatigue resistance, it is also necessary to understand which regime of crack formation and growth is to be targeted. Strategies for enhancing long crack propagation resistance by increasing grain size, for example, can severely degrade resistance to early stages of crack formation and growth. This depends on scale of notches and applied load history. Similarly, strategies for enhancing resistance to crack incubation at inclusions such as shot peening can compromise propagation life of longer cracks.
- In repairing in-service components, the credit on lifetime to be realized by the repair depends heavily on which stages of formation and growth that can be restored and those that will be bypassed by virtue of the length scales and processes involved.

The decomposition in Eq. (1) has been termed as a multistage formulation [65] since it corresponds largely to different physical aspects and mathematical modeling treatments in each successive regime. These stages are not to be confused with the aforementioned Stages I and II of crack growth as defined by Forsyth, although they are somewhat related. In a sense, they represent a perhaps more precise, specific decomposition, since the Stage I to Stage II transition depends not only on microstructure, but also on strain state and stacking fault energy. Early transition from Stage I to II growth behavior, termed by Socie [112] as conforming to "normal stress-dominated" response, is a manifestation of multi-slip conditions, refined microstructure relative to crack length, or some combination.

The Paris growth law based on Linear Elastic Fracture Mechanics (LEFM) should be applied unconditionally only in the N_{LC} regime. In view of the physical distinctions of the various stages of fatigue crack formation and growth, the apparent stress intensity factor, ΔK, based on applied loading and cracked geometry is not strictly applicable as a crack driving force for fatigue within the MSC regime and early portions of the PSC regime due to the roles of slip localization and microstructure; in such cases, the actual

value of ΔK is modified by shielding of the crack tip due to short and long range fields of dislocations [101–105]. Arguments of similitude that enable use of continuum plasticity models for shielding effects do not apply in this case. The cyclic crack tip displacement range ΔCTD (or other measures of geometry change near the crack tip) is a continuum concept that appears to provide common ground among virtually all stages beyond nucleation and can be computed [58,61,101–103]. The ΔCTD, defined as the magnitude of a vector of relative crack tip displacement range at some specified distance behind the physical crack tip, is readily computed using various computational methods listed above for MSC and PSC regimes, and has been shown in various investigations to collapse crack growth rate data for small/short cracks in the MSC and PSC regimes [52]. It reflects crack tip inelastic deformation which closely relates to the modes of crack extension, including irreversibility, crack opening and sliding. Micromechanical studies are necessary to capture ΔCTD interactions with microstructure [58,59,61]. Moreover, for long cracks under LEFM conditions there is a direct relation between ΔCTD and ΔK; the same is true for the ΔJ-integral in the Elastic–Plastic Fracture Mechanics (EPFM) case [113,114]. The latter often finds application in the PSC regime for which sensitivity of crack advance to microstructure has diminished and yet the cyclic plastic crack tip field does not yet meet requirements of small scale yielding. Much experimental work conducted in Japan in the 1980s and 1990s on physically small crack growth in polycrystalline steels, Ni-base superalloys, etc. clearly demonstrated the efficacy of separating the dependence of the fatigue crack growth rate on crack length and applied stress range [52]. In particular, in the MSC and early PSC regimes, the dependence of da/dN on $\Delta\sigma$ and a does not follow a power law scaling corresponding to the apparent applied ΔK. This is expected under EPFM conditions and is further complicated by a modification of crack length dependence associated with periodically encountering microstructure barriers in the MSC regime [51,52,64].

Plasticity and roughness-induced crack closure are also realized to varying degree depending on the stage of crack growth. In the MSC regime, by virtue of the limited crack length relative to microstructure and limited effects of free surfaces, plasticity-induced crack closure is thought to play a reduced role relative to long cracks [51,115]. Roughness-induced closure due to tangential shifts of the fracture surfaces in shear can play a more prominent role as MSC cracks propagate through a field of grains on a tortuous crystallographic path. Crack growth into the PSC regime is typically necessary to realize steady state levels of closure due to plastic wake effects. However, there are limited experimental studies in this regard, and realistic mesoscopic modeling and simulation of such effects for 3D cracks growing in the MSC regime in polycrystals are also limited.

Finally, it is worth mentioning that Miller [116,117] postulated the existence of two thresholds for fatigue, depending on the stage of crack growth. We can extend Miller's initial conception to a cascade of thresholds:

- absence of microplasticity (elastic shakedown)
- crack nucleation threshold (lack of irreversible slip, related to plastic shakedown limit)
- nonpropagating MSC cracks interacting with the initial set of strong microstructure barriers
- nonpropagating MSC or PSC crack that loses driving force in a gradient field at a micronotch with size typically below 100 μm
- LEFM threshold ΔK_{th}.

Only the LEFM threshold requires conditions of similitude and small scale yielding to be met; it has often been used (perhaps indiscriminantly) as a means of quantifying nonpropagating crack relations for MSC and PSC cracks based on an apparent ΔK. Traditional fatigue limits for alloys are of nonpropagating crack type in the MSC regime. The first two types of thresholds are typically too low in terms of applied stress level to have practical significance in design for applications. Clearly, the LEFM threshold is just part of the overall picture and its limits of applicability should be respected. It is quite likely that its historical application to very small cracks has been necessitated by a lack of explicit microstructure-sensitive models. Indeed, one promising emerging frontier in fatigue is more complete understanding and characterization of fatigue arrest limits beyond traditional LEFM concepts.

2.2. Nature of plastic strain accumulation

Comprehensive exploration of microstructure-sensitive fatigue phenomena demands consideration of the nature of plastic strain accumulation. Cyclic plastic strain behavior falls into three regimes: elastic shakedown, reversed cyclic plasticity, and plastic ratcheting [118]. Elastic shakedown is defined as the stress or strain level below which there is a cessation of cyclic plasticity. Reversed cyclic plasticity is the condition in which the material experiences reversed plastic straining during cycling with no net directional accumulation of plastic deformation; reversed cyclic plasticity is sometimes referred as plastic shakedown. Plastic ratcheting describes the condition in which the material accumulates a net directional plastic strain during each cycle. The ratcheting (directional) plastic strain increment per cycle is defined as

$$\left(\Delta\varepsilon_{ij}^{p}\right)_{\text{ratch}} = \left(\varepsilon_{ij}^{p}\right)\Big|_{\text{End of the cycle}} - \left(\varepsilon_{ij}^{p}\right)\Big|_{\text{Beginning of the cycle}} \tag{2}$$

The reversed cyclic plastic strain range is given by

$$\left(\Delta\varepsilon_{ij}^{p}\right)_{\text{cyc}} = \left(\Delta\varepsilon_{ij}^{p}\right)_{\max}\Big|_{\text{Over the cycle}} - \left(\Delta\varepsilon_{ij}^{p}\right)_{\text{ratch}} \tag{3}$$

The significance of this distinction is that multiple physical mechanisms of fatigue crack nucleation and early growth can operate, depending on the degree of reversed versus directional plastic strain. It has been noted that several mechanisms contribute to crack nucleation and early growth in ductile crystals that are related to reversed cyclic plastic strain range: (i) buildup of vacancies/free volume at the interface of the matrix with localized domains of slip (e.g., slip bands) that degrade material cohesion on slip planes [119–121], (ii) progressive formation of a spatial distribution of intrusions and extrusions associated with the intersection of slip bands (interaction of dislocation dipole structures) with external or internal free surfaces [13], or some combination. Similarly, with regard to directional plastic strain accumulation, impingement of dislocation pileups within slip bands can lead to high stresses at the leading edge that can drive microfracture of grain or phase boundaries. This mechanism is particularly pronounced under conditions that promote ratcheting, such as the imposition of mean stress.

2.3. Driving force parameters and microstructure-scale fatigue indicator parameters

To facilitate parametric studies of the effects of microstructure on fatigue, it is useful to introduce certain mesoscopic fatigue indicator parameters (FIPs) that reflect driving forces for fatigue crack formation (nucleation and limited microstructurally small crack growth). These FIPs invariably appeal to the notion of slip irreversibility in linking to fatigue damage. It is not necessary to establish specific functional relationships between these FIPs and components of life corresponding to nucleation and/or incubation in order to utilize them for comparing responses of a range of microstructures in parametric studies. In some cases, power law

relations are used to relate FIPs to number of cycles necessary to form a crack of a given microstructure scale, e.g., grain size [122–126].

Some authors [127,128] have argued that crack nucleation, MSC growth and limited PSC growth should depend upon local energy dissipation. However, in a material with low to moderate rate of work hardening, the differences resulting from consideration of energy dissipation compared to slip accumulation as a FIP are unlikely to be significant. Wilkinson et al. [129] and Ahmed and Wilkinson [130] have employed electron channeling contrast imaging (ECCI) to provide detailed information about the formation of persistent slip bands in fatigued single crystal samples of OFHC Cu. The experimental observations demonstrate that at the single crystal level, the establishment of persistent slip bands is a precursor to fatigue crack nucleation; the nucleated crack lies in the plane of the slip band. The accumulated plastic strain can be considered as a FIP for crack formation at this scale [125,126,131], i.e.,

$$p = \int_0^t \sqrt{\dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ij}^p}\, d\tau. \tag{4}$$

The cumulative plastic strain p does not distinguish between ratcheting and reversed plasticity outlined in Eqs. (2) and (3) per se, but is most closely related to the reversed cyclic plastic strain range in Eq. (3) for many cases involving dominance of reversed plasticity (e.g., $R = -1$) at the grain level (i.e., $\left(\Delta\varepsilon_{ij}^p\right)_{\text{cyc}} \gg (\Delta\varepsilon_{ij}^p)_{\text{ratch}}$). As a practical matter, microstructure-sensitive simulations are intensive and therefore are unable to pursue a large number of cycles; accordingly, the information contained in a measure of cumulative plastic strain based on $(\Delta\varepsilon_{ij}^p)_{\text{cyc}}$ differs little from that contained in p for limited numbers of simulated cycles [107,108]. For high R ratios [132] of $R = 0.7$ and above, ratcheting dominates $\left(\Delta\varepsilon_{ij}^p\right)_{\text{ratch}} \gg \left(\Delta\varepsilon_{ij}^p\right)_{\text{cyc}}$ and p may be more closely related to the cumulative directional plastic strain. For conditions under which slip impingement due to ratcheting might dominate crack formation processes, the same FIP might be used but with a different critical value, or a FIP based on $\left(\Delta\varepsilon_{ij}^p\right)_{\text{ratch}}$ might be used.

McDowell [108] introduced the notion of a set of FIPs that reflect in more explicit manner the relative roles of reversed and cumulative directional slip. For example, the Fatemi-Socie [112,133,134] shear-based parameter has been shown to correlate multiaxial fatigue crack initiation data very well in both LCF and HCF regimes at the grain scale and above [112]. It is defined by

$$P_{\text{FS}} = \frac{\Delta\gamma_{\max}^{p*}}{2}\left(1 + K'\frac{\sigma_{\max}^{n*}}{\sigma_y}\right) \tag{5}$$

where $\Delta\gamma_{\max}^{p*}/2$ is the nonlocal maximum cyclic plastic shear strain averaged over a finite volume of material, $\sigma_{\max}^{n*}$ and σ_y are the maximum stress normal to the plane of $\Delta\gamma_{\max}^{p*}/2$ and cyclic yield strength, respectively, and constant K' mediates the influence of normal stress. The spatial volume for nonlocal averaging of the driving force may be defined according to the nature of the simulation, and is desirable both for purposes of numerical regularization

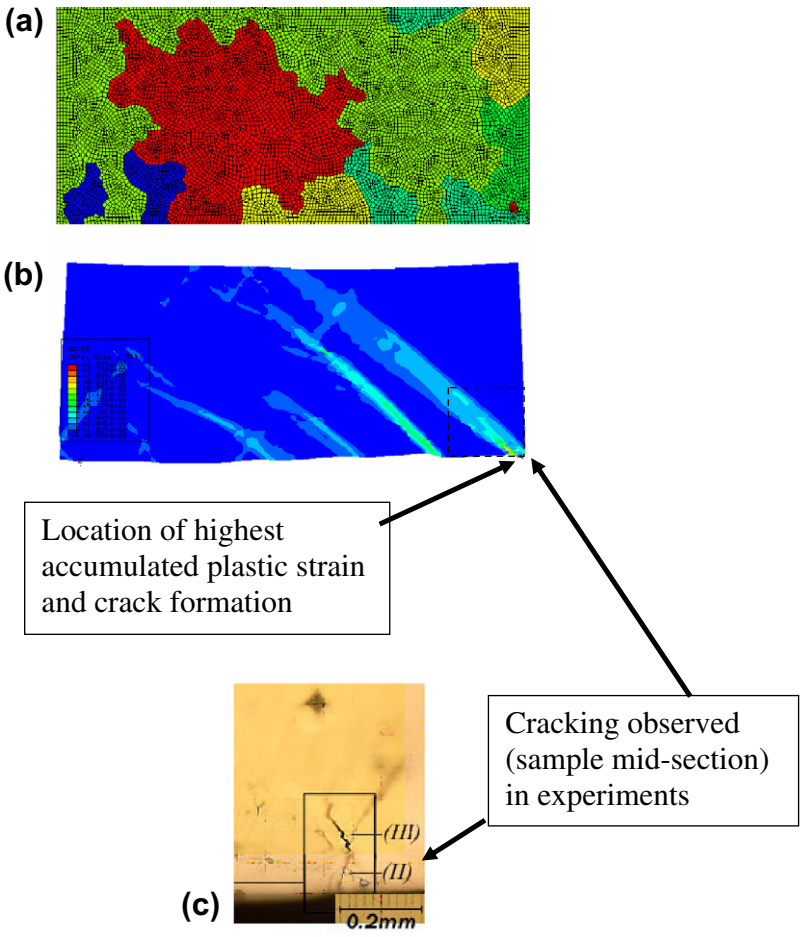

Fig. 2. (a) Mapped region showing the grain boundaries, (b) predicted effective accumulated plastic strain developing in the heterogeneous microstructure after two cycles, and (c) experimentally observed fatigue crack formation at the sample mid-section (approximate conditions of plane strain).

(mesh insensitivity) and targeting length scales associated with crack embryos (e.g., slip band width/spacing, inclusion size, etc.). A similar but distinct parameter has been introduced by McDowell [135] to address correlations of directional plastic strain accumulation with crack formation due to grain or phase boundary impingement, i.e.,

$$P_{ZP} = \gamma_{net}^{p*}\left(1 + K_z' \frac{\sigma_{GB}^{n*}}{\sigma_y}\right) \tag{6}$$

where $\gamma_{net}^{p*} = \max(n_i \varepsilon_{ij}^p m_j)$ among all planes with unit tangent and normal vectors **m** and **n**, respectively, is the maximum net plastic shear strain averaged over a finite volume of material, σ_{GB}^{n*} is the average peak stress normal to a boundary segment impinged by this slip, and K_z' is a constant that mediates the effect of this normal stress.

In fact, a range or approaches and parameters for multiaxial loading have been proposed and employed (cf. [54,136,137]) have been applied at the grain scale, some with more intimate potential link to fine scale driving forces for crack nucleation and early propagation. Building on mixed mode propagation arguments by Hoshide and Socie [138], McDowell and Berard [137] showed that the FS parameter in Eq. (5) is closely related to the Elastic–Plastic Fracture Mechanics (EPFM) ΔJ-integral and the cyclic crack tip displacement range (ΔCTD), as well as strain-based critical plane concepts [139]. Moreover, numerous experiments and modeling efforts in the literature point to the efficacy of ΔCTD (opening and sliding) to correlate crack advance [101,102,140–144].

However, the assessment of driving forces for fatigue crack nucleation at scales well below the size of individual grains remains an open issue. Crack nucleation can be regarded as a phase transition. As such, further research is necessary to elucidate material-specific driving forces for nucleation that may differ from the class of continuum FIPs listed in Eqs. (4)–(6). Current understanding is that the maximum plastic shear strain range $\Delta\gamma_{max}^{p*}/2$ or the cumulative plastic strain measure in Eq. (4) may provide most reasonable correlation with the site of nucleation of cracks less than the grain size in surface grains, as will be discussed later in connection to experimental data in Figs. 2–4. While continuum-based approaches for fatigue crack nucleation life have been introduced at the mesoscale [119,120], they do not typically deal directly with dislocation substructures or the discrete nature of defects within persistent slip bands that affect this process.

In the next section, we present a review of integrated computational and experimental strategies in fatigue modeling with an emphasis on crack formation at the scale of grains. We then present a range of recent applications of such methodologies to

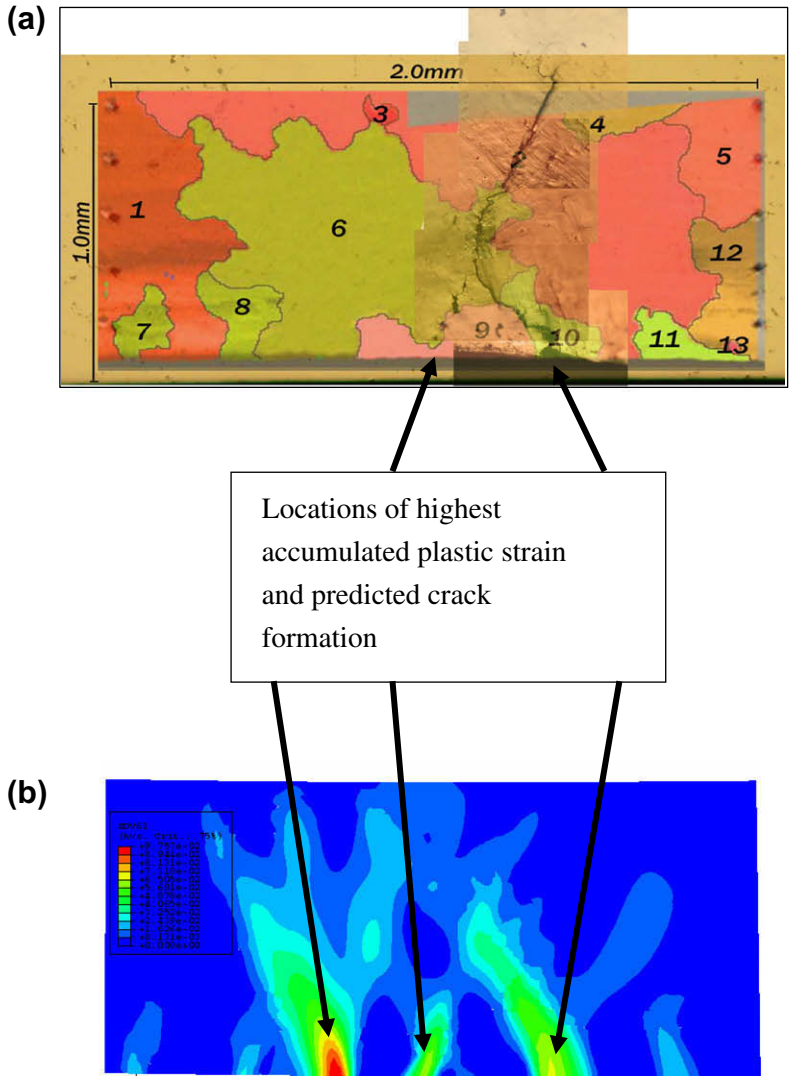

Fig. 3. (a) Experimentally observed crack formation and early and growth under plane stress conditions and (b) the predicted site of fatigue crack formation and orientation based on the accumulated plastic strain.

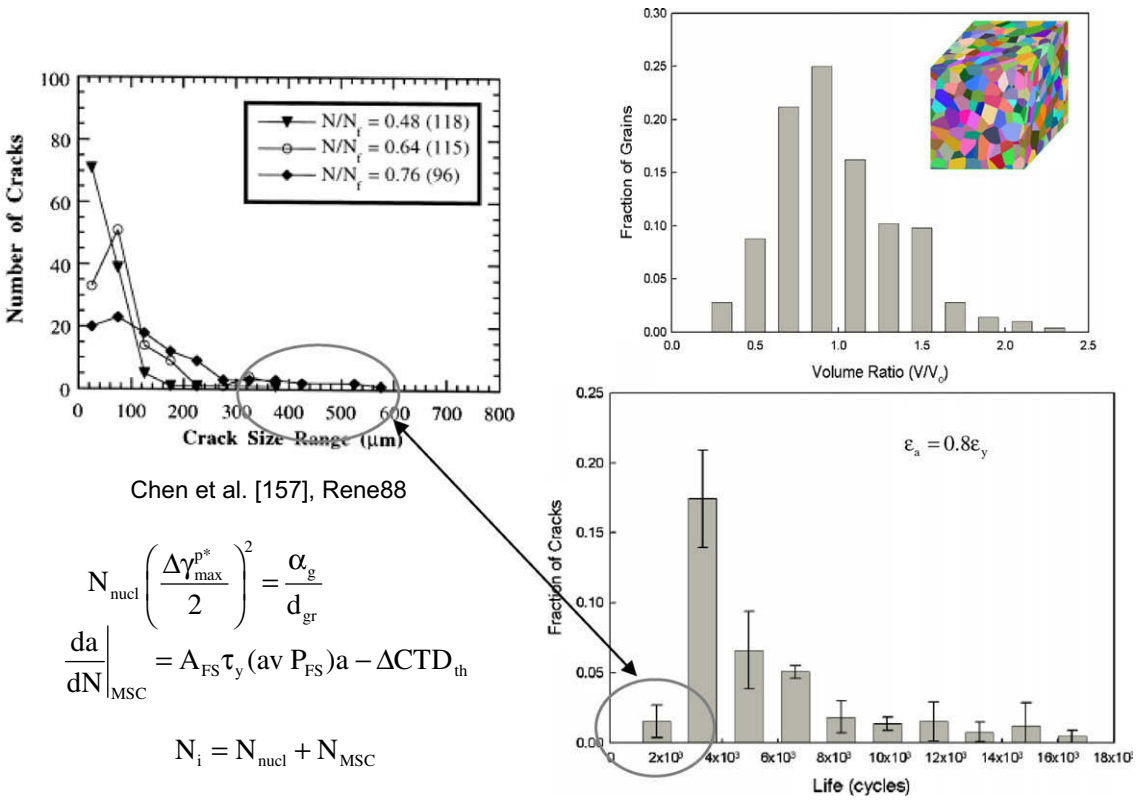

Fig. 4. Estimated distribution fraction of grains with fatigue cracks that reach a length three times mean grain size (40 μm) as a function of applied loading cycles (lower right) for multiple statistical realizations of equiaxed polycrystalline IN 100 microstructures with log normal grain size distribution shown at top right subjected to completely reversed strain-controlled cycling ($R_\varepsilon = -1$) at $T = 650$ °C [124]. Ellipses point to the tails of the distributions that related to the life-limiting crack scenarios. (See above-mentioned reference for further information.)

advanced structural materials. In the final sections we address future needs and directions in companion experimental techniques to support microstructure-sensitive fatigue modeling.

3. Integrated computational and experimental strategies in fatigue modeling

Using FIPs, different microstructures can be compared in terms of their expected values and distributions of driving force(s) to form and grow microstructurally small fatigue cracks. A primary objective of this kind of modeling approach is to estimate the sensitivity of fatigue responses to microstructure variation (either within a given microstructure or among comparison microstructures), thereby using modeling and simulation to substantially leverage costly experimental characterization of the variability of fatigue life or fatigue strength in smooth and notched specimens [107,108,135]. Microslip and its dependence on stress ratio was investigated by Morrissey et al. [132,145] who showed that the onset of local plastic ratchetting, leading to failure for Ti–6Al–4V, depended strongly on stress ratio. Bennett and McDowell [59–61] and Morrissey et al. [132] investigated the role of microstructural heterogeneity on (HCF) using polycrystal plasticity and argued that the degree of heterogeneity of cyclic slip is a key aspect in HCF in steels and Ti–6Al–4V, respectively. The work on cast A356–T6 Al alloys in the USCAR program [62–65] highlighted the multistage framework discussed in Section 2.1, along with multiple fatigue limits associated with nonpropagating cracks. Shenoy at al [146] used similar polycrystal techniques to investigate thermomechanical fatigue in a directionally solidified Ni-based superalloy, embodying a phenomenological creep-fatigue-environment crack initiation model. Studies of fretting fatigue using polycrystal plasticity have been carried out by Goh et al. [122,123], in which grain scale plastic strain and stresses in the vicinity of a fretting contact were examined. Polycrystal plasticity combined with damage evolution equations has been investigated by Dingli et al. [147] for cyclic behavior, and by Ekh et al. [148]. Some of the limitations of conventional crystal plasticity, such as the absence of length scale effects and the simplifications made in incorporating grain boundaries within the models have been addressed by Buchheit et al. [149]. The field of microstructure-sensitive crystal plasticity relations is rapidly evolving with improvements in material models based on the latest experimental studies on advanced alloys (cf. [150,151]).

In the remainder of this section we discuss recent examples of applying the foregoing framework along with microstructure-sensitive cyclic deformation simulations to support understanding of service failures and design of fatigue-resistant microstructures. The scope of these examples is limited principally to crack incubation as defined in Eq. (1), assuming the grain as the fundamental unit of homogeneous lattice orientation and employing FIPs averaged over a volume on the order of a significant fraction of grain size.

3.1. A non-intuitive example: facet fatigue failures in Ti–6Al–4V

Probably the first theoretical attempt at addressing crack nucleation was that due to Stroh [152] who considered a line of dislocations oriented with respect to the remote applied loading and carried out an elastic analysis to determine the stress state local to the line of dislocations. By introducing a fracture criterion, a prediction of the stress required to nucleate a crack was possible. In the context of facet fatigue crack formation within individual grains in titanium alloys, Evans and Bache [153] and Evans [154] interpreted the experimental data in the light of the Stroh [152]

model to postulate that faceting may result from a particularly potent and uncommon combination of hcp crystallographic orientations in adjacent grains with respect to the loading direction [154]. Recent work by Dunne et al. [70,72] and Rugg et al. [69] generalized this and has largely demonstrated that Evans and Bache [153] were correct regarding a particular combination of crystallographic orientations as a necessary but not sufficient requirement for faceting. In particular, a facet crack formation mechanism based solely on combinations of orientation does not explain the dwell dependence of faceting, the more damaging effect of a stress (as opposed to strain) dwell, nor its material volume dependence. Rate effects were addressed in particular by Hasija et al. [79] and Venkataramani et al. [82] and the important phenomenon of *load shedding* was introduced in which stress redistribution occurs from grains well-oriented for slip (e.g., with *c*-axes normal to the load axis) to those less well oriented (*c*-axes parallel with the load axis). In the work by Dunne et al. [70,72], it was shown that a worst case combination of crystallographic orientations exists – termed a rogue grain combination – in which a 'hard' grain is oriented with its *c*-axis parallel to the applied load and adjacent to a 'soft' grain oriented with its *c*-axis normal to the load and an active prismatic slip system at about 70° to the normal to the load. In Rugg et al. [69], the same micromechanical, rate-dependent crystal plasticity model was used to compare strain and stress cycle dwells in the rogue grain combination and it was found that grain boundary stresses were considerably higher in stress-dwell cycles because of the load shedding effect [79]. More details will be provided in Section 3.3.

3.2. Ni-base superalloys

Crystal plasticity modeling techniques have also been brought to bear upon fatigue crack incubation in complex Ni-base superalloys. Dunne et al. [125] carried out low cycle fatigue tests on a model 'two-dimensional' polycrystalline Ni-base superalloy, i.e., a directionally solidified material with near prismatic grains. Grain morphology and orientation were determined using EBSD, and polycrystal plasticity analyses carried out for the characterized microstructure with, in principle, identical conditions to the experiment tests. At the length scale of individual grains, fatigue crack nucleation and growth depends crucially on microstructure features such as grain boundaries, triple points, crystallographic orientation, and inclusions. It was found that crack nucleation occurred at free surface locations where localized slip banding was predicted to develop by the crystal plasticity analyses. Work by Manonukul and Dunne [126] on a similar polycrystalline material also adopted the accumulated plastic strain (i.e., p in Eq. (4)) as a FIP and the model captured the sites for fatigue crack formation in both HCF and LCF regimes.

Results from polycrystal plasticity simulations employing the accumulated plastic strain FIP p are compared with experimental observations for the case of a '2D' directionally solidified polycrystalline nickel alloy sample subjected to $R = 0$ three-point bend fatigue tests. Results are presented only for a small region of the bend sample where stresses are highest; Fig. 2a shows the grain structure and crystallographic orientation in this region. The model test sample was subjected to loading conditions identical to those in the experiments. Experimental sample surface observations revealed the development of surface slip traces, and it was shown [125] that they were found to agree with slip directions obtained by considering the projection of active slip directions corresponding to maximum Schmid factors onto the plane of the sample where the slip traces were observed. We examine, in particular, the evolution of the accumulated plastic strain only within the gage section in Fig. 2b. Considerable slip localization is predicted. The crystal plasticity simulations predict the development of free-surface roughening from which the bands of intense slip emanate. The location of the highest accumulated plastic strain is identified in the figure at the boundary of two grains, precisely where the mid-section fatigue crack was observed to nucleate and grow in experiments. It is argued, therefore, that the experimentally observed cracking occurs within a band of intense slip predicted by the crystal plasticity simulations. Furthermore, crack nucleation occurs first within that slip band with the highest level of accumulated plastic strain.

The free surface (as opposed to mid-section) of the bend test sample was subject to a state of plane stress. The accumulated plastic strain distribution under these circumstances was also modeled and the results and comparisons with experimentally observed cracking are shown in Fig. 3. The model test sample was subjected, in principle, to loading conditions identical to those in the experiments. The resulting free-surface cracking observed in the experiment is shown in Fig. 3a, and the predicted distribution of accumulated plastic strain after one cycle of cyclic plasticity is shown in Fig. 3b. Bands of intense slip are predicted to develop, emanating from the sample free surface at three particular locations. Grain boundary regions (see Fig. 3a for the geometry) seem to correlate with the development of the highest levels of plastic slip. Comparison of the simulated bands of slip localization with the experimentally observed sites of crack nucleation in Fig. 3b on the free surface shows that the cracks which are observed to nucleate and grow lie within the predicted bands. The orientations of the propagating cracks also match those of the predicted slip patterns. However, crack formation was not observed experimentally in the left-most predicted slip band. Overall, the results indicate the importance of slip localization as reflected by a continuum measure of cumulative plastic strain on fatigue crack formation. One caveat is that slip localization is not fully modeled by these kinds of continuum crystal plasticity models; specifically, details of slip band width and spacing are not fully addressed.

These kinds of simulations based on formation of cracks within individual grains can be extended to include growth in the MSC regime. A multistage approach has recently been used along with hierarchical polycrystal plasticity simulations for $\gamma - \gamma'$ Ni-base superalloys [124,155,156] to estimate the formation and growth of distributed small fatigue cracks for a range of IN 100 microstructures as a function of applied strain amplitude to support design of heat treatment (and associated precipitate distribution) for HCF resistance. Fig. 4 illustrates the application of a combined crack nucleation and MSC growth algorithm for IN 100 [124]. A microstructure-sensitive crystal plasticity model was used to explicitly model individual grains and polycrystals, which is then used to explore effects of: (a) grain size distribution and (b) secondary and tertiary coherent γ' precipitate size distributions and volume fractions on the distribution of cyclic inelastic strain. Using multiple statistical volume elements (SVEs) subjected to random periodic boundary conditions to build up statistically significant distributions of cyclic microplasticity, multiaxial fatigue criteria with critical plane approaches were used to estimate the crack initiation life based on a criteria for forming a crack on the scale of the largest grain and then growing to three times the mean grain size. The resulting distributions of cracks were representative of those observed experimentally.

3.2.1. Extreme value statistics

In most fatigue design scenarios the target probability of failure is quite low (<1%). Consequently, the distribution of rare events of fatigue crack formation are of most relevant. However, these tails of probability distributions are quite difficult to characterize experimentally. Przybyla et al. [158] and Przybyla and McDowell [159] have explored the linkage of extreme value distributions of FIPs for Ni-base superalloys and α–β Ti microstructures in terms of key microstructure attributes that are associated with these rare

events. Such an approach seeks to link the distributions of microstructure attributes and correlations between various microstructure attributes to distributions of local response parameters (e.g., FIPs). To this end, marked correlation functions were introduced to explore biased or weighted spatial correlations of microstructure attributes (e.g., grain size and orientation) in the neighborhood of FIP hotspots in Ni-base superalloys. Such weighted probability methods depart from conventional approaches that consider only stereological characterization of attributes and extreme value spatial correlations of such geometric attributes. In other words, it is not enough to simply quantitatively characterize microstructure – companion simulations of responses are necessary to demarcate microstructure attributes particularly relevant to fatigue resistance.

Given a volume window Ω over a microstructure, Przybyla and McDowell [159] define the probability distribution of the extreme valued response parameter α as $F^{ex}(\alpha|\Omega)$, which is the probability that the response parameter of value α is the extreme value for a sampled statistical volume element of microstructure Ω. This follows the ideas of extreme value sampling from classical extreme value statistics of Gumbel [160,161]. Corresponding to the probability distribution of the extreme value response parameter is the extreme value marked radial correlation function, $R^{\max(\alpha)}(\beta, \beta'|r, \Omega)$. We define $R^{\max(\alpha)}(\beta, \beta'|r, \Omega)$ as the probability of finding of a sphere centered at the microstructure attribute β corresponding to the location of the maximum response parameter α in the microstructure window Ω, with microstructure attribute β' at a distance within r to $r + dr$ from β in any direction. Although based on the notion of the marked correlation functions introduced by Pyrz [162], this new construct is fundamentally unique in its framing of extreme value statistics.

This two part statistical construct captures both the extreme value response of the microstructure as represented by the response parameter α and the biased correlations of microstructure attributes between β and β' in the neighborhood of the observed extreme values of α in a microstructure window Ω. In this way, spatial correlations are identified between microstructure attributes that have a high probability of existing in the neighborhood of an extreme value response parameter. This sampling is performed on microstructure window Ω and is expected to depend on the size of Ω. The method requires multiple instantiations of Ω to effectively sample both $F^{ex}(\alpha|\Omega)$ and $R^{\max(\alpha)}(\beta, \beta'|r, \Omega)$ to build up the tail of the probability distribution corresponding to extreme value response neighborhoods. Such sampling can require extensive processing time for both simulations and data analysis depending on the complexity of the models being analyzed. Moreover, the number of samples required depends on the response parameter considered and material being analyzed. Analogous experimental data are typically not available.

Fig. 5 shows extreme values of the Fatemi-Socie (Eq. (5)) FIP for large numbers (25–100) of statistical volume elements of IN100 [159]. The data are plotted to reveal parameters of the extreme value Gumbel distribution, i.e., $F_{Y_n}(y_n) = \exp[-e^{-\alpha_n(y_n-u_n)}]$. These FIPs were fit with high confidence ($R^2 > 0.97$) by the Gumbel distribution. These extreme value distributions of the FIP responses coupled with the extreme value marked correlation functions permit assessment of the distribution of driving force(s) for fatigue damage formation (i.e., crack nucleation and microstructurally small crack growth) in polycrystalline IN100. Moreover, by association of the character of the marked correlation function $R^{\max(\alpha)}(\beta, \beta'|r, \Omega)$ for extreme value events $F^{ex}(\alpha|\Omega)$, Przybyla and McDowell [159] demonstrated that for a given applied stress state, the particular microstructure attributes that affect low probability of failure can be identified. These are often non-intuitive and are essentially inaccessible to experiments unless very large numbers are performed, which is usually impractical. Accordingly, they serve as effective indicators to guide design of extreme value attributes of microstructure that influence HCF resistance.

3.2.2. Surface to subsurface transitions in HCF to VHCF

Primary inclusions are often dominant sites of fatigue crack formation and early growth in high strength steels, powder metallurgy alloys, and casting alloys. Transition from surface-dominated fatigue processes to subsurface failure initiation is often observed in these systems in moving from the HCF (10^6 cycles) to the VHCF regime (10^9 cycles and beyond) [163,164]. Competition between near surface and bulk inclusions is key to this failure mode transition. Cashman [165] studied competing fatigue failure modes for René 95, with nucleation attributed to the presence of small ceramic inclusions; the difference in fatigue lives was an order of magnitude between surface and subsurface initiated modes of failure. Jha et al. [166,167] noted that experimental fatigue life data separates into two distinct populations corresponding to competing surface and bulk initiation at nonmetallic particles, based on data for two aircraft gas turbine engine materials, a titanium alloy, and a Ni-base superalloy. The increased scatter in the experimental life data [168,169] in clean steels at low stress amplitudes is attributed to the competition between surface and internal inclusion failure modes that manifest significantly different fatigue lives.

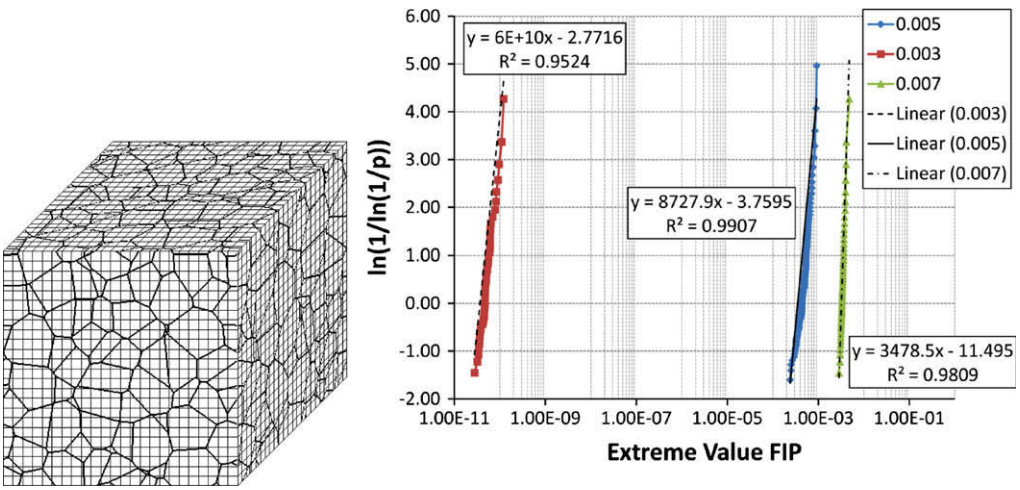

Fig. 5. Example polycrystalline statistical volume element (SVE) (left) and extreme value distribution of the Fatemi-Socie FIP (right) as estimated within most highly activated grains of individual SVEs among a large set for completely reversed simulations cycled at 0.3%, 0.5%, and 0.7% strain amplitude [159].

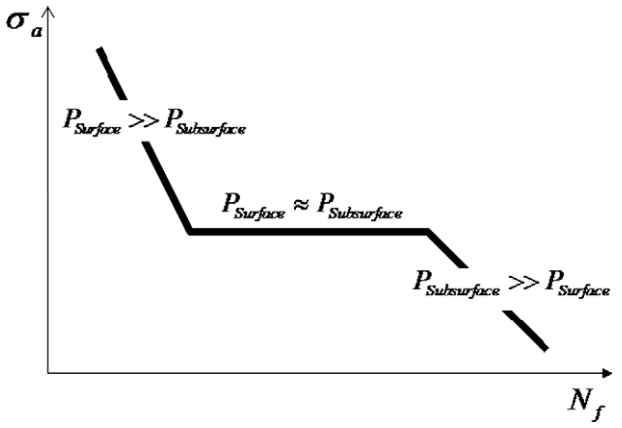

Fig. 6. Relative probabilities of surface and subsurface fatigue crack formation for LCF to HCF/VHCF transition.

Prediction of the ratio of surface to subsurface probabilities for crack initiation demands a probabilistic mechanics framework that incorporates competing effects of local microstructure neighborhoods, proximity to the surface, inclusion size and shape, and interaction with surface oxides or other environmental effects. As the applied stress amplitude decreases, the influence of microstructure attributes becomes pronounced since localized microplasticity dominates. The probability of life-limiting hotspot microstructure attributes occurring in the bulk of the specimen for fatigue crack formation and early growth increases with decreasing applied stress even though the bulk to surface volume remains constant. As the applied stress amplitude decreases, the number density of microstructure hotspots that can produce sufficient driving force for fatigue crack formation in the surface region decreases and so does the probability of a hotspot located near the surface. The essential notion used to describe the stress amplitude dependence of the failure mode transition from HCF to VHCF regimes is the weighting of the probability of finding microstructure

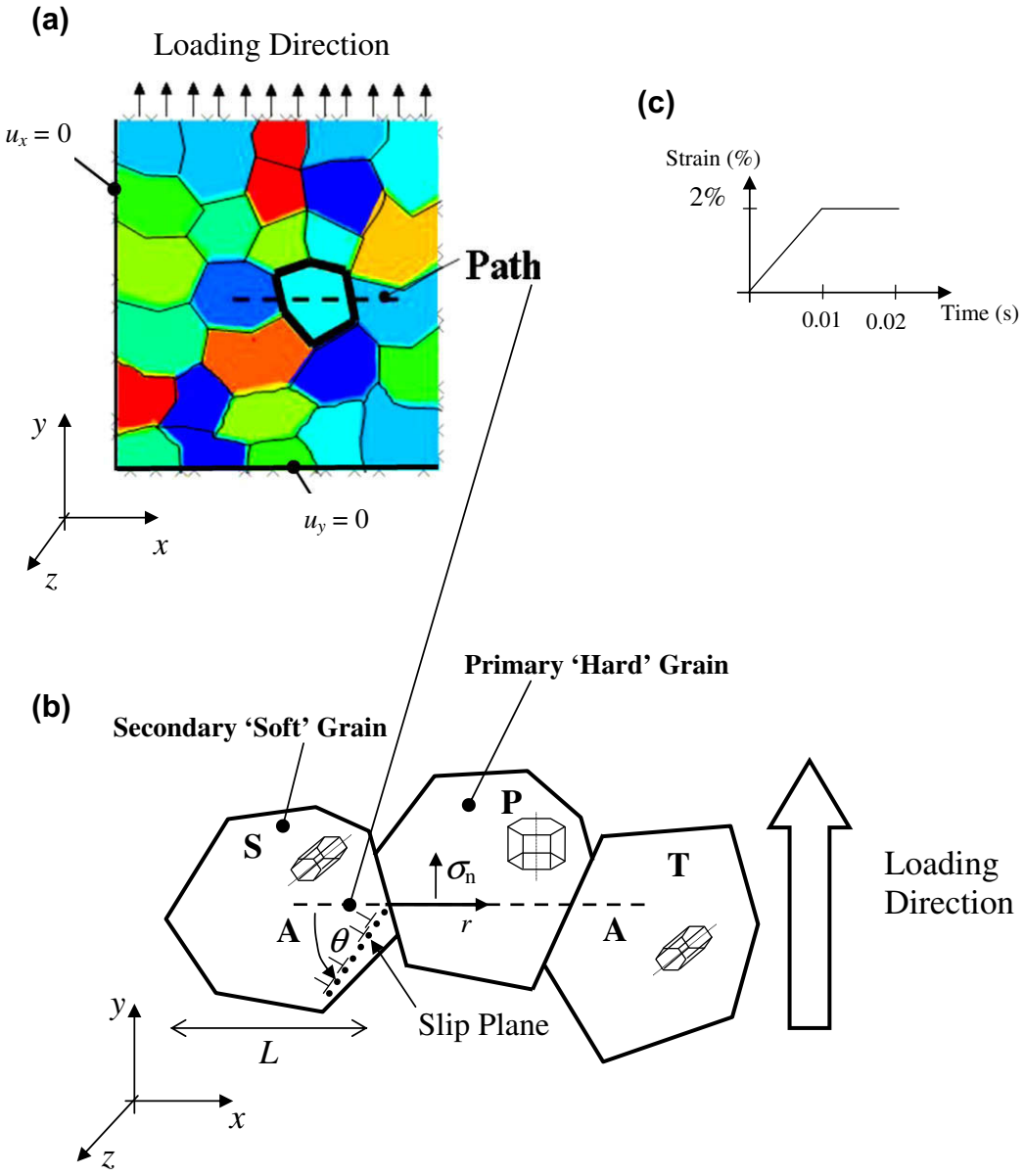

Fig. 7. (a) Schematic polycrystal showing the path through three grains along which stresses are determined and the boundary conditions, (b) representative crystallographic orientations of the three (primary, secondary and tertiary) grains, and (c) the displacement-controlled loading applied at the top boundary of the polycrystal shown in (a).

attributes of a certain size, shape, and spatial correlation with other microstructure attributes by the corresponding potency for forming fatigue cracks, using a nonlocal average FIP parameter from numerical simulations. In effect, this is entirely analogous to the use of the marked correlation function described in the last section to identify the extreme value statistics for HCF in microstructures with complex, multivariate interactions. Work is underway to pursue the description of the HCF to VHCF failure mode transition illustrated schematically in Fig. 6 [158].

3.3. Ti–6Al–4V and α–β Ti variants

Facet fatigue crack nucleation in titanium alloys, discussed in Section 3.1, is becoming increasingly well understood with assistance from polycrystal plasticity modeling. Fig. 7a shows a polycrystal model comprised of 27 grains with different crystallographic orientation. Three grains, however, have had their crystallographic orientations specified, namely the primary, secondary and tertiary grains through which a path has been drawn in Fig. 7a, as schematically shown in Fig. 7b. The displacement-controlled loading applied to the polycrystal is shown in Fig. 7c in terms of strain versus time; the yy stresses developed at a time of 0.01 s (Fig. 7c) are given in Fig. 8 for a range of orientations of the secondary, soft, grain, for fixed orientations of the primary and tertiary grains. At the primary – secondary grain boundary, the orientation variation of the secondary grain leads to a stress variation of about 120 MPa. Work by Dunne et al. [70] showed that there exists a worst case combination for hcp crystals; as shown schematically in Fig. 7b, this worst case corresponds to a primary grain with *c*-axis near-parallel to the loading direction adjacent to two (secondary and tertiary) grains with *c*-axes near-normal to the loading direction together with an active slip system in the secondary grain making an angle

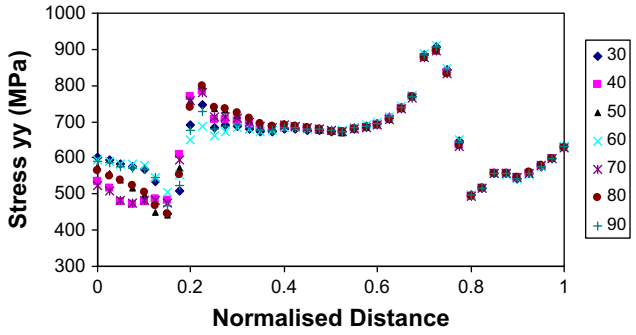

Fig. 8. Normal stress component yy along the path shown in Fig. 7 through the primary, secondary and tertiary grains for the in-plane orientations of grain S (denoted by θ in Fig. 7b).

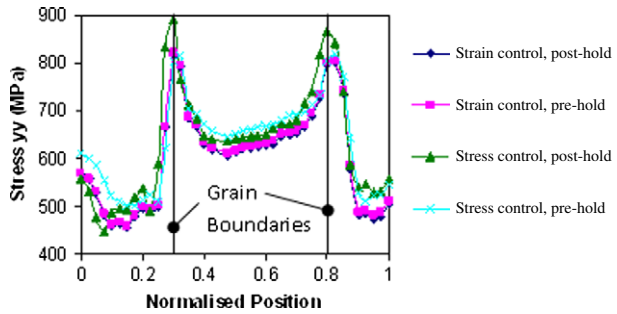

Fig. 9. The local yy normal stress component along the path shown in Fig. 7a and b through the rogue grain combination.

of approximately 70° to the normal to the loading direction. This rogue grain combination gives rise to the highest grain boundary stresses between the primary hard grain and the secondary soft grain.

The polycrystal in Fig. 7a has also been subjected to strain- and stress-controlled loading with and without a strain or stress dwell period, respectively. The local stresses along the path shown in Fig. 7 are given in Fig. 9 for both displacement/strain- and load/stress-controlled histories at both the post-hold and pre-hold points in the loading. Under strain-controlled conditions, the stresses both before and after the dwell period are quite similar, although in the soft, secondary and tertiary grains (shown schematically in Fig. 7), some stress relaxation is observed following the dwell period. However, for the case of stress-controlled loading, at the grain boundaries, the stresses can be seen to increase significantly after the dwell. This occurs because during the stress dwell, the softer (secondary and tertiary) grains creep, leading to local stress relaxation. The requirement to maintain the applied stress therefore results in the hard (primary) grain carrying a higher stress. This effect has been termed load-shedding by Hasija et al. [79], but a comparison of responses obtained under load- and displacement-controlled deformation had not been addressed. It is of considerable significance that a load-controlled dwell leads to notably higher stresses within the primary grain, close to the boundary, relative to those obtained under displacement-controlled loading, since facet formation under cyclic loading containing a dwell period has been observed in experiments to be much more likely for the load-controlled case.

Sinha et al. [170] have carried out load-controlled dwell-fatigue tests on a near-α titanium sample for which microstructural examination revealed the nucleation of a facet, shown in Fig. 10a. Detailed SEM and EBSD with serial sectioning enabled determination of the location of facet formation, and the orientations of the grain in which faceting occurred and surrounding grains. The basal orientation distribution in a sample section (normal to the loading direction) [170] is shown in Fig. 10a together with the faceted grain. The facet was found to occur in a grain with basal plane oriented nearly normal to the loading direction and adjacent grains had *c*-axes nearly normal to the faceted grain. This is precisely the worst combination of orientations predicted by crystal plasticity modelling and indeed for the loading shown in Fig. 10b, the modeling techniques were able to predict the formation of a facet precisely where it was observed in the experiment, shown in Fig. 10c and d.

Bridier et al. [171,172] considered the spatial and orientation distributions of cyclic slip on various slip systems and found that parameters that combine effects of plastic shear strain range with normal stresses on such planes (e.g., FS parameter in Eq. (5)) are useful to identify individual grains where cracks form in duplex Ti–6Al–4V, using microstructure-sensitive constitutive models for Ti-64 [173,174]. In particular, it is observed that cracks form at within mesoscopic bands of preferred crystallographic texture in grains with high FS FIPs; such micro-textures are important in controlling minimum fatigue life in α–β Ti alloys [172]. It is noted that standard crystal plasticity models typically predict too many operative slip systems for this class of alloys, so provision must be made for preferred softening of initially activated systems due to breakdown of short range order [172,174]. In addition, this high degree of slip planarity promotes formation of shear bands; as shown in Fig. 11, an explicit strategy for allowing shear to localize in bands is necessary to both model progressive cyclic softening for single crystals in different orientations and to properly localize cyclic plastic strain for purposes of modeling the driving force for fatigue crack formation [175]. This demonstrates the importance of constitutive modeling in applying these types of FIP-based algorithms.

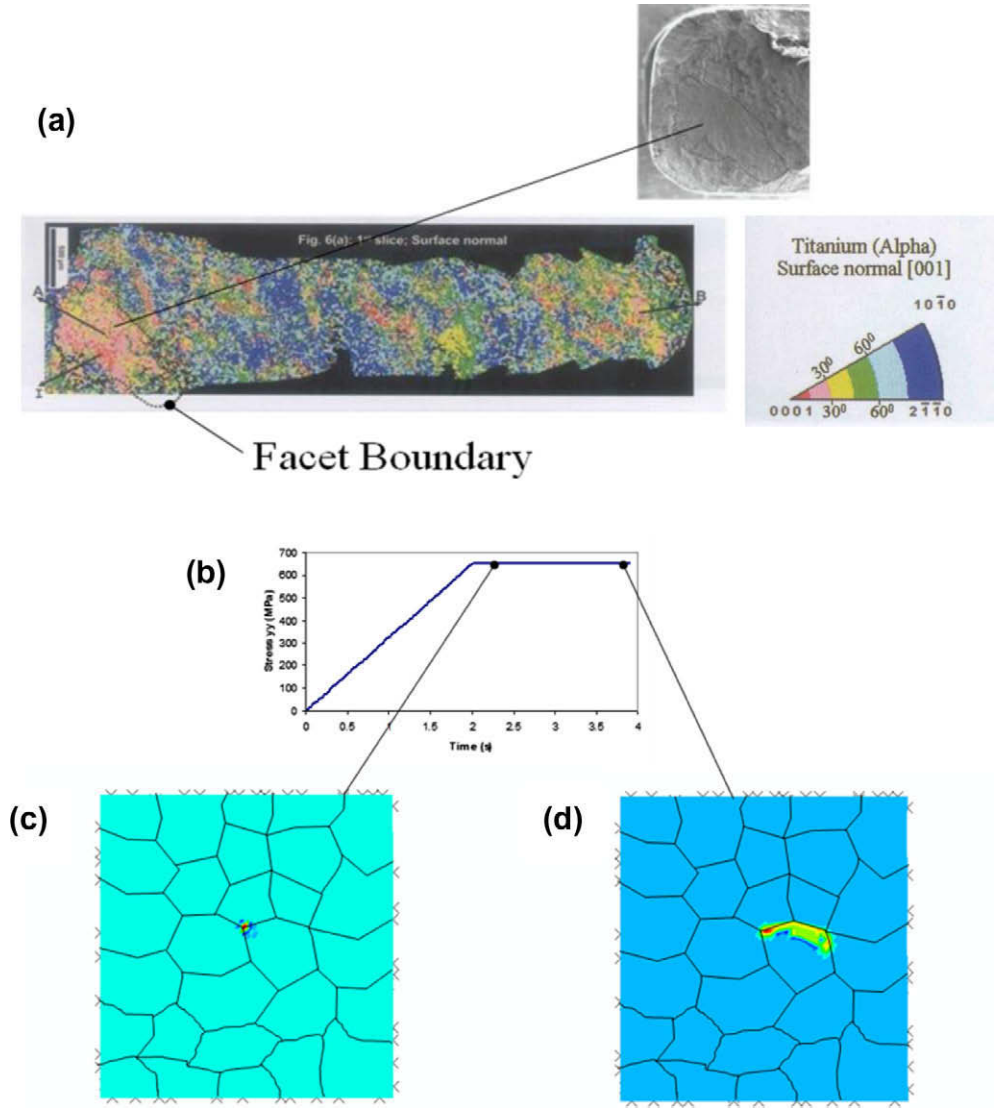

Fig. 10. (a) Experimentally determined crystallographic orientations (courtesy of [170]) used in the modeling, (b) the load-controlled history (σ_c = 1200 MPa) with a stress dwell leading to (c) the initial formation of the facet in the rogue grain combination early in the dwell period, followed by (d) full facet formation at the end of the dwell period. In (c) and (d), any color other than that of the background indicates that the cleavage failure criterion has been achieved and that at that point, the material has no stiffness.

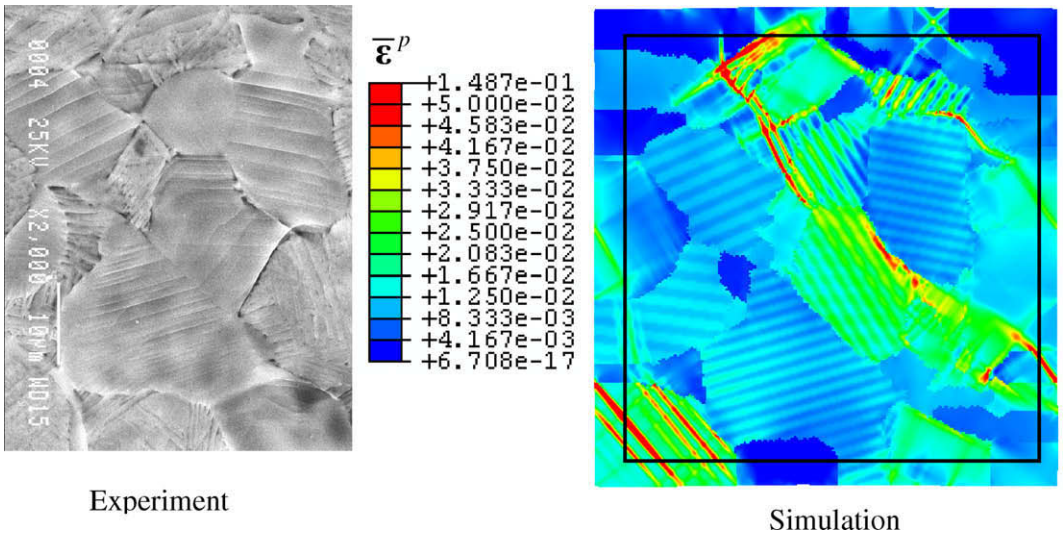

Fig. 11. Comparison of experimentally measured slip traces with predicted cumulative plastic strain distribution at an applied strain ε_t = 2% in Ti–6Al–4V [175].

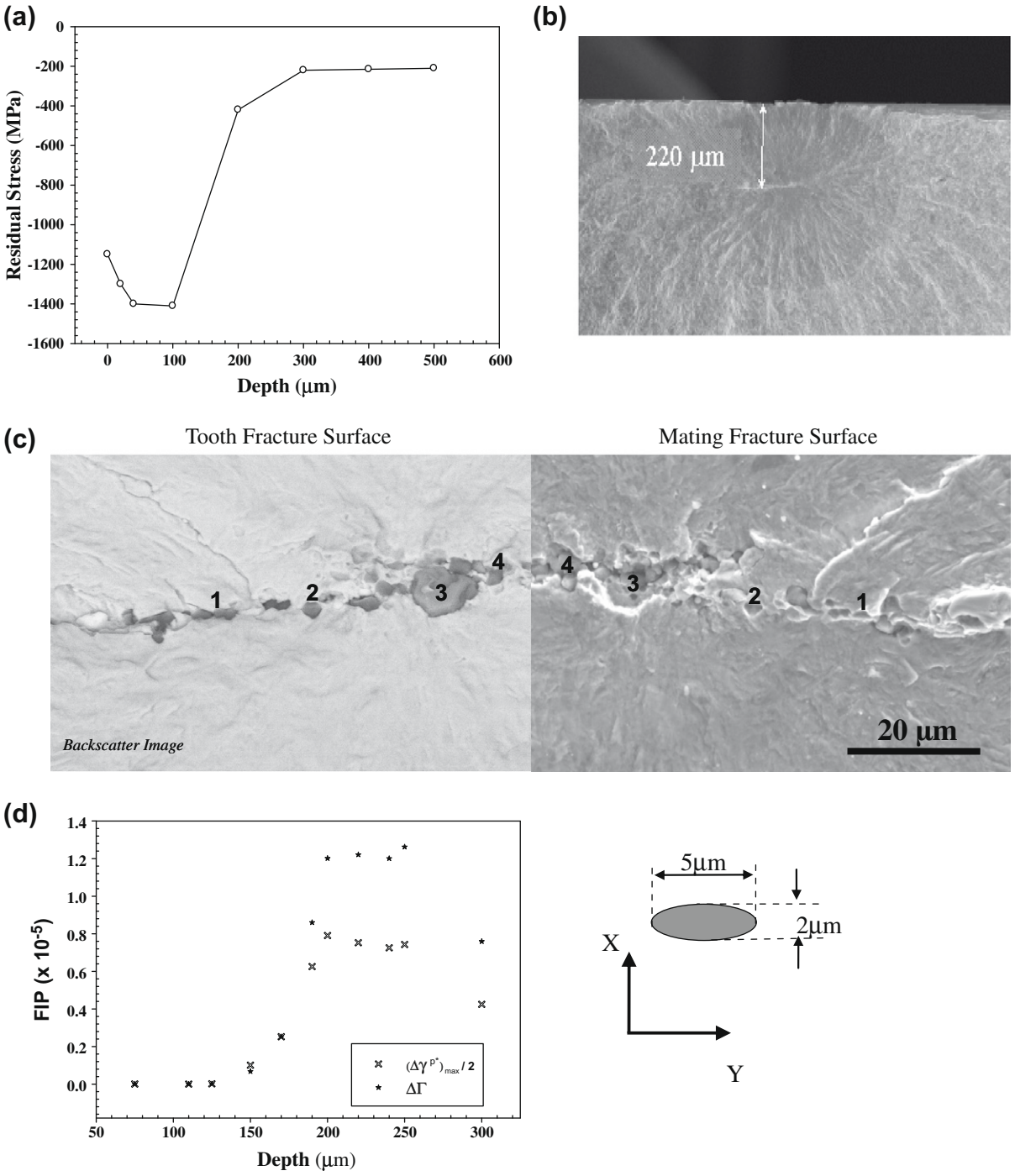

Fig. 12. Variation of nonlocal maximum cyclic plastic shear strain amplitude and FS parameter $\Delta\Gamma$=P_{FS} with depth for single partially debonded particle in martensitic gear steel. Remote uniaxial cyclic loading direction is parallel to *Z*-axis.

3.4. Martensitic gear steels strengthened by carburization and shot peening

High strength martensitic gear steel is a viable candidate material for high performance, reliable transmission systems in aerospace and automotive applications. Microstructure at different length scales (inclusions, precipitates, and composition gradients) affects fatigue performance of martensitic steels [176–180]; however, efforts to develop computational models that correlate these attributes with variability in fatigue crack formation and microstructurally small crack growth have been limited. Additionally, processing steps such as carburization and shot peening play a crucial role in improving the HCF resistance of martensitic steels. Due to the hierarchical microstructure of martensite [181–185] and the scales over which process-induced strengthening effects are realized in components, it is quite challenging to develop models that couple process effects and microstructure attributes at different length scales. A hierarchical approach is most suitable and computationally conducive to investigate the coupling of process route with grain scale cyclic plastic deformation phenomena in components.

In a study of Ferrium® C61 alloy gear steel, a carburized, fully lath martensitic steel [186] developed by Questek Innovations LLC [187], Prasannavenkatesan et al. [188] and Zhang et al. [189]

developed simulation strategies that account for the effect of the gradient of carbon content on mechanical properties and the effects of shot peening on subsurface residual stresses in the vicinity of intact, cracked and partially debonded primary Al_2O_3 inclusions and inclusion clusters.

The measured residual stress profile after shot peening is shown in Fig. 12a. Under reversed bending stress with $R = 0.05$, it is observed that fatigue cracks form at a depth of approximately 200–270 μm below surface, as shown in Fig. 12b. The location of crack formation is not within the tensile residual stress zone of the shot peening-affected region. SEM analysis of the fracture surface and its mating surface in Fig. 12c indicates that the cracks are formed at clusters of debonded Al_2O_3 inclusions (particles 1, 2, 3 and 4) on the tooth fracture surface [186]. The location of subsurface fatigue crack formation is accurately predicted using either the two parameter FIP in Eq. (5) or the cyclic plastic shear strain range $\Delta\gamma^{p*}_{max}/2$, both averaged over 1 μm^3 at the micronotch root. The simulation results indicate a strong propensity for crack formation at subsurface depths in accordance with experiments. By varying the initial condition of the interface between primary inclusion and the matrix (debonded versus intact, as well as cracked particles), Prasannavenkatesan et al. [188] and Zhang et al. [189] showed that residual stresses following shot peening are sensitive to inclusion interface conditions. The gradient of material properties, applied stress, and distribution of residual stress can cooperatively affect subsurface fatigue crack formation, as can alignment of inclusion stringers relative to the free surface and orientation of primary applied stress.

4. Companion experimental techniques and studies

Modeling techniques are now capable of providing support in the development of mechanistic understanding of material behavior at the length scale of grains and below in polycrystals. However, micromechanical testing is crucial to the development of mechanistic understanding and support of models. In this section, we identify some important experimental and characterization techniques that should be employed both for the calibration and validation of modeling techniques.

There remain substantial hurdles to the development of realistic microstructure-level models for fatigue crack formation and early growth. These include the paucity in understanding of grain boundaries and slip transfer, the development of highly localized planar slip which is characteristic of metals with low to moderate stacking fault energy, and the development of dislocation substructures within grains. A further practical problem is that most current modeling strategies neglect initial residual stress, which can substantially affect HCF response. An immediate complexity, even with respect to a 'simple' single phase metal, is the three dimensionality of the grain structure. One way to simplify is to consider pseudo two-dimensional grain structures, both in experiments and modeling, but this is strictly limited to directionally-solidified materials, for example. Another model simplification is to mesh 2D representations of 3D microstructures (e.g., cutting planes). In this case, not only is the constraint problematic, but the 3D nature of the material is not fully considered, including more complex interactions of grains/phases. Nonetheless, such 2D idealizations provide significant simplification and can enable larger parametric studies. The increase in computing time when moving from 2D to 3D microstructures is often several orders of magnitude, and such computations are highly intensive even in 2D. Although 3D data would inherently seem preferable, a *statistically significant set* of quantitative 3D microstructure data are often limited for a given material. Moreover, in exploring virtual microstructures, such data do not exist. For microstructurally small cracks, very few studies in the literature have attempted to measure the 3D nature of fatigue cracks and sequence of formation and propagation events; what appears to be crack formation at the surface may sometimes correspond to subsurface formation and growth to the surface, for example. The nature of the crack front is not captured unless some type of tomographic imaging is used. There is a tremendous need for experimental strategies that facilitate selective formation of cracks that are indistinguishable from naturally occurring cracks, and to track them through the MSC growth in the first few grains in 3D manner rather than just relying on optical surface measurements [190].

Much recent work has focused on the development of microtesting methods. For example, Gong and Wilkinson [191] have developed techniques for micro-milling cantilever beams of length about 20 μm using a FIB. Nano-indentation is then used to apply loading at the free end. The cantilevers may be single crystal or may contain a single grain boundary. Careful choice of the location for FIBbing enables control of the particular crystallographic orientation(s) of the single or bi-crystal. In this way, it is possible to contrive slip to occur on very particular slip systems and it is feasible that this experimental technique could provide valuable information about slip transfer across a grain boundary. It also potentially provides information about highly localized planar slip. These sorts of experiments, probably combined with discrete dislocation modeling, can potentially enable the development of 'rules' for slip transfer (dependent on combinations of crystallographic orientations and grain morphologies) that can be employed in crystal plasticity. Mechanistic understanding and validation could be obtained through post-processing of tested samples using TEM and X-ray synchrotron diffraction techniques.

A higher length scale pertains to an aggregate of say 10–20 grains. Here, there is a need for experimental techniques to determine grain-level deformation (e.g., using samples with grids or employing digital image correlation) and pre- and post-test EBSD that provides information regarding lattice rotation. In addition, EBSD techniques developed by Wilkinson et al. [192] also enable the direct determination of lattice curvature (although not out-of-plane) from which estimates of densities of geometrically necessary dislocations can be made; this can reinforce the results from discrete dislocation simulations and can provide further validation for the dislocation-based hardening rules implemented in the crystal plasticity model. Measurement of deformation and lattice curvature at scales involving hundreds of grains is presently problematic.

From a practical perspective, variation of composition in alloys can have a profound effect on local strength and ductility. It is rarely characterized experimentally. Initial dislocation density is typically not well characterized to provide initial conditions and calibration for microstructure-sensitive crystal plasticity models. Residual stresses are often neglected in experiments, as is characterization of initial texture or texture gradients. All of these aspects play a first order role not only in calibrating and validating models, which is the usual context in which they are mentioned, but also in proper interpretation of experimental data. In other words, pursuit of a strategy for microstructure-sensitive fatigue modeling relies heavily on updating testing and characterization protocols to provide more details of the state of the material, particularly if the goal is to predict the fatigue life distribution; this is the current state of affairs.

5. Opportunities for next generation simulation-based fatigue

With increased emphasis on reducing materials development and insertion cycle times and design of reliable fatigue resistant materials, microstructure-sensitive modeling and simulation come

to the forefront. Achieving enhanced predictive capability is a major current research driver for simulation-based design. There are some areas in which crystal plasticity models need to improve for modeling cyclic plasticity. For example, low symmetry crystal structures often exhibit both slip and twinning. Heterogeneity of slip and twinning at the grain scale is typically not considered in crystal plasticity, but would be relevant to crack formation. As highlighted in Fig. 11, nonlocal models capable of predicting localization of shear at the mesoscale, calibrated or validated by experiments, is an emerging frontier. Another area is the treatment of grain boundaries in mediation of slip. Much recent interest has focused on the role of grain boundaries in mediating plastic deformation [193–196] and how this may contribute to fatigue crack formation and early growth [197]. The issue of how much fidelity is necessary in models to resolve grain level response is greatly tempered by the reality that our present state of modeling is lacking in realism in capturing slip transfer reactions at grain and phase boundaries. Frankly, this is enough of a concern that it dampens the urgency of methods for smooth topological meshing of grains in 3D polycrystals until it is properly addressed.

Several compelling aspects requiring future development are listed below:

- Amplitude, stress state, and material-specific predictive relations are lacking for fatigue crack nucleation. In spite of considerable literature regarding dislocation substructure formation in fatigue, crack nucleation is a very complex multiscale phenomenon, still very much in the early stages of modeling. It seems to us incontrovertible that unless mechanistic understanding of material behavior at length scales appropriate to crack nucleation is better developed and captured by the modeling techniques, prediction of nucleation will remain elusive. As mentioned before, various nucleation models in the existing literature appeal to energetics of fracture processes with evolving irreversibility and are not of predictive nature [119,120]. Kirane and Ghosh [83] have recently proposed an approach for fatigue crack nucleation based on the observed similarities between crack evolution at the tip of a crack and a dislocation pileup. The nucleation model is calibrated and validated using data available from acoustic microscopy though real time monitoring of crack evolution in dwell fatigue experiments. Sauzay and Gilormini [198] have considered the role of the free surface on nucleation of fatigue cracks in slip bands. The roles of free volume and related atomistic aspects have not yet been fully woven into mesoscale criteria or models.
- Crack growth is related to irreversibility of slip arising from environmental interactions with slip, interaction of point and line defects with microstructure, and internal stresses that evolve with dislocation structure and modify the crack tip driving force, yet continuum crystal plasticity slip measures do not reflect this irreversibility nor do they employ any predictive means to account for it, particularly for realistic microstructures. Phenomenological models have been introduced [199,200], including extensions of fracture mechanics concepts that consider microstructure [201] or models based on continuously distributed dislocations [202]. Discrete dislocation models offer a more predictive pathway to understand amplitude, *R*-ratio and overload/underload effects but are presently highly idealized in terms of slip mode, geometry and interaction with surrounding microstructure. The use of combined strategies of discrete dislocation models with mixed mode cohesive zone strategies may offer qualitative description of trends and phenomena [104–106]; it remains to be seen if the basic physics of fatigue crack growth is adequately treated by such idealizations to offer predictive capability in the context of hierarchical microstructure.
- Crack growth relations from micron-scale inclusions or pores within the microstructure do not typically address the important role of discrete dislocations at such scales. Microstructurally small cracks growing from heterogeneities such as inclusions are subject to consideration of the scale of dislocation spacing relative to mesh size in continuum relations, and hybrid discrete dislocation models may be useful to pursue [106].
- As mentioned above, grain boundaries are treated largely as compatibility surfaces (mechanical effects of misorientation) without acknowledging effects of their structure on dislocation mediation. Grain boundary engineering is appealing as a context for design using microstructure-sensitive fatigue. Gao et al. [197] have shown, for example, that GB-engineered polycrystals of ME3 Ni-base superalloy can achieve reduced average crack growth rates in the MSC regime compared to as-received material. Existing methods to account for grain boundaries are of simplified nature and lack predictive quality.
- Strain localization processes associated with dislocation substructure formation (e.g., slip bands) are not naturally treated in the local continuum representation of slip. The relative ratios of transgranular and intergranular crack nuclei cannot presently be predicted, nor can the fractions of transgranular and intergranular growth paths in the MSC regime. Calibration is necessary. For example, some promising recent work is devoted to understanding the role of cyclic softening in strain localization [203,204] in martensitic steels.
- HCF and particularly VHCF are characterized as extreme value problems in terms of the relevant statistics that govern reliability. Extreme value statistics are necessary to address these issues, and are not presently well developed, particularly with regard to the common case of low probability of failure [159].
- Characterization of scatter in fatigue via modeling is a promising future trend for microstructure-sensitive fatigue simulation [1,107,108,205,206] in view of its practicality and potential for augmenting and reducing the number of required experiments.
- Methods for accelerating simulations [84] to capture responses of polycrystals over tens or hundreds of thousands of cycles are presently not well developed and would be of substantial utility for evolving residual stresses and cumulative plastic deformation, particularly for metastable microstructures (e.g., cyclic softening or hardening).

6. Conclusions

The development of microstructure-sensitive computational methods for fatigue crack formation in polycrystalline microstructures over the past few decades is reviewed. The concept of microplasticity within individual grains is introduced as a key driving force parameter for fatigue crack formation, and associated fatigue indicator parameters (FIPs) are introduced that relate to grain scale fatigue crack formation and microstructurally small fatigue crack growth. Strategies are discussed which employ explicit 2D representations of a set of experimentally characterized surface grains, as well as 3D statistical volume elements that are constructed by sampling spatial statistics of microstructure attributes. The former are used to understand mechanisms of cyclic plastic deformation and fatigue crack formation and to validate models, and the latter are used to support design of fatigue-resistant microstructures and build up statistics of failure probability. One may pursue multiple pathways in designing fatigue-resistant microstructures. One is to reduce nucleation probability though refinement and strengthening of microstructure, or to decrease the number density of nucleation sites by controlling morphology. Another is to increase the threshold for MSC propagation by reducing barrier spacing, promoting extension of Stage I propagation, or increasing barrier strength.

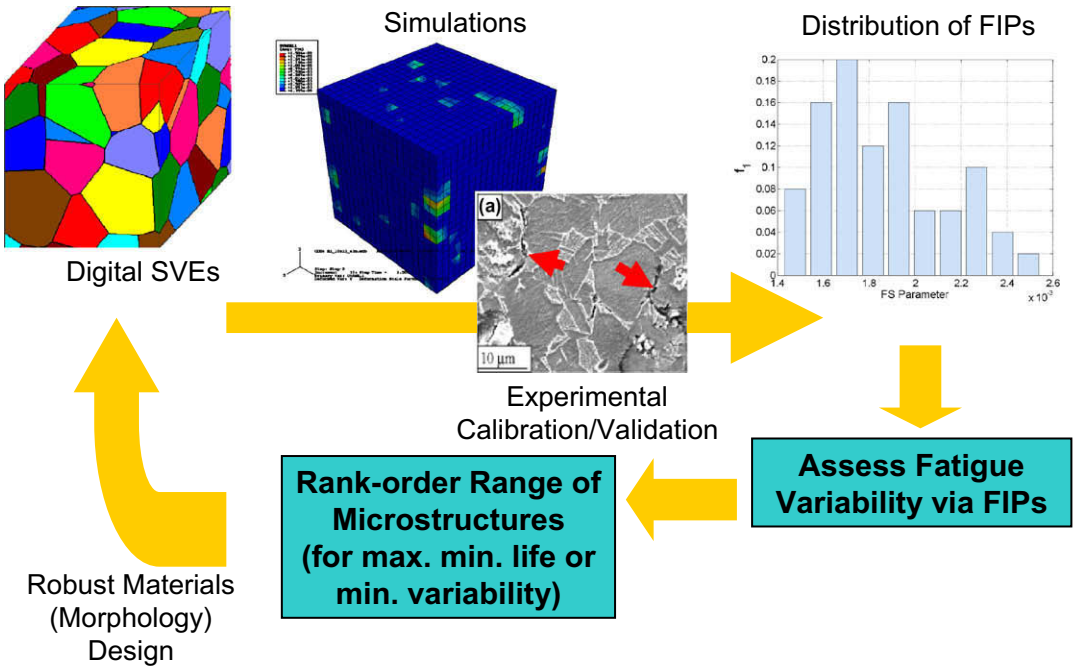

Fig. 13. Using microstructure-sensitive simulations to "close the loop" in rank ordering microstructures for fatigue resistance, including design for desired failure probability (courtesy of C. Przybyla, Georgia Tech).

From a "top-down" perspective, the methodology of quantifying the effects of microstructure morphology on the distribution of fatigue response is a logical component of microstructure-sensitive design and prognosis strategies. Fig. 13 provides a philosophical construct for using computational micromechanics to relate variation of microstructure (within a single sample or a population) to variability in fatigue response (or properties). We note that although a given simulation is deterministic, statistics are compiled by simulating a population of microstructures (SVEs) and related attributes. In the absence of robust and reliable damage state detection methods capable of sensing and distinguishing small fatigue cracks with dimension on the order of microstructure (e.g., grain size, phase size), this kind of scheme is able to deliver information related to the expected distribution of cracks that would propagate to detectable lengths. Moreover, such approaches can be pursued to explore effects of microstructure attributes that give rise to extreme value fatigue responses associated with the tails of probability distributions of potential surface and subsurface fatigue crack formation sites, including transitions between modes of crack formation, surface to subsurface transitions, and so forth.

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