A LARGE SCALE COMPUTATIONAL STUDY OF FATIGUE HOT-SPOTS

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A LARGE SCALE COMPUTATIONAL STUDY OF FATIGUE HOT-SPOTS

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...let’s go exploring!

Bill Watterson
For my grandfathers.
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Summary

Formation of a fatigue crack at the subgrain scale is a statistically rare event, as plastic deformation at the microscale ranges from highly heterogeneous at low strain to homogeneous at high strain. Improvements in computational resources and methodology coupled with experimental validation and calibration offer a promising alternative to explore fatigue response of a material with substantial time- and cost-savings. Such efforts require hierarchical, multiscale models that incorporate the material physics at each length scale of interest, from subgrain up to macroscale material properties. These models must also be coupled with a statistical approach that compiles the relevant microstructure statistics in order to study the rare event nature of fatigue crack formation. This requires creating programmatic workflows to handle the large dataset generated from a large scale computational study of structure-property response of fatigue.

This thesis considers Fatigue Indicator Parameters (FIPs) for Ti-6Al-4V, which are computed using crystal plasticity finite element modeling of uniaxial cyclic straining of ensembles of statistical volume elements for a range of distinct microstructures at several strain ranges and mean strain conditions. The selection of FIPs is informed by prior experimental studies. The sites of extreme value (EV) FIPs that are most likely to form and grow a fatigue crack are identified in these simulations, and 2-point spatial correlations are applied to investigate the higher dimensional influence of microstructure attributes in the neighborhood of these fatigue hot-spots. To reduce the high dimensionality of the associated 2-point correlations, principal component analysis is applied. A reduced-order model using an artificial neural network is used to classify EV FIP locations based on these neighborhood spatial correlations.

The conclusions of this work include the rank ordering of 12 microstructures of Ti-6Al-4V under High Cycle Fatigue (HCF) and transition fatigue regimes. Then, the grain attributes of EV FIP locations are thoroughly investigated for trends related to fatigue crack formation. By including 1st nearest-neighbor grains and applying neighborhood spatial
correlations, the reduced order PC components, when used as inputs for the neural network, show a promising ability to classify EV FIP grains based on neighborhood information.
1.1 Motivation

Traditionally, materials design has followed a deductive path by selecting a material for a given set of performance criteria from experimentally established properties resulting from conventional processing methods [1]. This deterministic approach allows for limited material exploration as it relies heavily on time- and cost-expensive experiments to validate material structure, properties, and performance. To meet the stated goals of the Materials Genome Initiative [1] of decreasing the time required to bring new materials to full manufacturing development, inductive design methods show promise for rapid materials exploration and deployment. Inductive design uses performance requirements as objectives or targets, and identifies potential structure and process paths that deliver properties that meet those requirements, subject to various constraints [2]. Developing these inductive linkages is a complex task, requiring new data science-based computational methods that allow for rapid exploration of materials with minimal experimental validation and calibration [3–7]. Within current materials design approaches, mapping the complex process-structure-property-performance (PSPP) relationships of a material requires multiscale modeling methods that include top-down information as well as bottom-up information [8]. In this work, we will focus on elucidating the microstructure attributes or combination of attributes that drive fatigue crack formation and early growth in polycrystalline metal alloys with strong isotropic behavior and microstructure heterogeneity at multiple length scales.

For metals used in aerospace applications, one of the primary performance requirements is the fatigue lifetime, or number of loading cycles to failure [9]. Fatigue life predictions first linked the applied stress amplitude to the number of cycles to failure, known
as S-N curves [10]. Basquin [11] fit these curves with a power law rule to interpolate over the applied stress range to provide predictive fatigue life estimates. Coffin and Manson proposed a strain life relation that includes material constants, which require post facto calibrations; these fatigue life correlations do not provide sufficient predictive support for design or selection of fatigue resistant microstructures for a given alloy system [12]. Fracture mechanics-based strategies have employed remote applied stress and information regarding cracked component geometry to quantify local driving forces for fatigue (e.g., \( \Delta K \), \( \Delta J \)-integral, \( \Delta CTOD \)). However, these approaches typically ignore details of material microstructure and are no longer useful when a crack has all dimensions less than 5-10 grains, a so-called microstructurally small crack (MSC), which is well below current commonly employed non-destructive evaluation techniques [13, 14]. For example, in the high cycle fatigue (HCF) regime of Titanium alloys, which can mean applied loading cycles of more than \( 10^6 \), formation and early growth of MSCs can consume up to 85% of the total fatigue lifetime [14].

1.2 Problem statement

Under high cycle fatigue (HCF), the material experiences a predominantly elastic, homogenized mechanical strain response, with some localized plastic deformation due to the anisotropy and heterogeneity at the grain scale [15–17]. For low cycle fatigue (LCF), an increasingly more uniform distribution of grains within the polycrystalline metal alloy undergo localized plastic deformation, resulting in a more homogeneous but still microstructure-dependent material response [18]. This localized deformation resulting from microstructure inhomogeneity drives local crack formation, and these embryonic cracks may propagate through favorably oriented neighboring grains or arrest at the first obstacle encountered [19, 20].

Experimental HCF tests have been used to characterize mean fatigue life and scatter as a function of microstructure, but are extremely expensive and time consuming, even with
recent developments of ultrasonic testing methods [21]. These costs to estimate variance of fatigue behavior are much larger than for effective material properties, as the formation and growth of microstructurally small fatigue cracks is an extreme event and statistically rare, requiring a greater number of physical experiments to determine fatigue properties. Thus, computational methods have been developed to combine microstructure effects with physically-based micromechanical models to decrease the reliance on experimental testing and improve understanding of the deformation and fatigue mechanisms of different microstructures [22]. These microstructure-sensitive models still rely experimental methods for validation and calibration, but show promise for identifying correlations between mechanisms of fatigue crack formation and, separately, fatigue crack growth, facilitating parametric explorations related to the probability of fatigue failure. Moreover, they are objective and can be used to screen performance of various microstructures for improved fatigue resistance. It is critical that current, state-of-the-art research utilize a microstructure-sensitive based approach to improve inductive design exploration of fatigue behavior.

Determining combinations of microstructure attributes that correlate with fatigue crack formation and early growth is critical to improving materials selection and design for fatigue resistance. In the HCF regime, localized reversed cyclic slip and cumulative cyclic plastic strain result in “hot-spots” with higher probability of fatigue crack formation and early growth. Naturally, crack formation also depends on specific mechanisms of intergranular and transgranular fatigue type, both of which may be present in a given metal or alloy and act as threshold barriers for crack growth. For polycrystalline metal alloys, fatigue crack formation at these local material hot-spots is influenced by coupled microstructure neighborhood attributes and their interactions (e.g., grain size, shape, orientation, interface character, etc.). These spatial correlations between microstructure attributes for crack formation and early growth, once found, can be used to explore candidate fatigue-resistant microstructures.
1.3 Research objectives

A statistically-based computational methodology is first outlined as a template for large-scale computational studies of extreme, statistically rare fatigue crack formation behavior of materials. As high performance computing resources are increasingly available, a roadmap must be laid out to fully utilize these resources, while reducing the number of time- and cost-prohibitive experiments to validation and verification of computational methods. Working within current limitations on available computational resources requires a statistically-based approach to compromise between the size of material able to computationally modelled and current programmatic workflows to handle such large data sets.

The first research objective addressed with this methodology will utilize a microstructure-sensitive multiscale computational approach to investigate structure-property linkages between fatigue crack formation and early growth and the local microstructure attributes in the vicinity of fatigue hot spots. This will be accomplished through use of fatigue indicator parameters (FIPs) that are manifested by the primary deformation mechanisms of Ti-6Al-4V. These FIPs may be regarded as surrogate measures of the driving forces for crack formation and early growth. Ti-6Al-4V is selected as an example polycrystalline metal alloy due to its widespread use in aerospace and automotive industries and its highly anisotropic material behavior. For the simulations in this work, the large size of a representative volume element (RVE) for fatigue behavior is prohibitively expensive. Instead, ensembles of statistical volume elements (SVEs) will be instantiated using Dream.3D [23], with relevant grain size distributions, orientation distributions, and phase volume fraction as inputs. FIPs are computed from crystal plasticity finite element model (CPFEM) simulations of cyclic loading of SVEs, and the extreme value (EV) distribution of maximum FIP values are identified for each ensemble of SVEs for a given applied loading condition, using the peaks-over-threshold (POT) methodology.

To link these extreme FIP values to fatigue crack formation and behavior, a number
of challenges must be addressed. First, the extreme value FIPs must be characterized according to the grain in which the maximum FIP occurs, along the neighboring grains and associated attributes. Data related to grain/phase sizes, orientations, and FIP distributions of those neighboring grains will be collected. Neighborhood spatial statistics will be applied to these attributes referenced to the hot spot sites (i.e., spatial correlation functions) to quantitatively compare their effect on extreme FIP values. As one primary novel outcome of this work, this is expected to elucidate probability distributions regarding combinations of microstructure attributes that correlate with fatigue crack formation.

A second primary anticipated advance of this work is to pursue these grain neighborhood correlations combined with reduced order modeling (ROM) to increase understanding of nearest-neighbor effects on highly localized strain responses of grain or grains.

1.4 Significance of research

The research presented here lies at the intersection of integrated computational materials engineering (ICME) and materials data science and informatics (MDSI). By combining several ICME tools for computationally efficient microstructure generation and simulation, a much larger dataset can be generated to investigate structure-property relationships of a material. As the size of the dataset increases, the importance of introducing data science techniques to address big data problems becomes increasingly critical to these studies. The significance of this research includes

(i) Combining simulated statistical microstructure representations in DREAM.3D with an ensemble SVE approach and CPFEM ABAQUS [24] UMAT to compute FIPs using POT EV theory for 14,400 microstructure instantiations modeling 6.5 million grains of Ti-6Al-4V.

(ii) Rank-ordering 12 Ti-6Al-4V microstructures for fatigue resistance over a range of applied strain amplitudes that capture HCF, transition from HCF to LCF, and LCF
regimes, using POT EV theory for two FIPs and two strain ratios.

(iii) Novel application and convolution of masked and padded neighborhood spatial correlations surrounding fatigue hot-spots for investigating fatigue crack formation and early growth as identified by experimental literature and our computational methodology.

(iv) Applying a feed forward Neural Network with variational Bayesian inference to classify the reduced order models of fatigue hot-spots associated with EV FIP grain neighborhoods.

1.5 Dissertation structure

Chapter 2 lays out the background of current fatigue crack formation research of Ti-6Al-4V, and the history of the methodologies used to statistically represent a simulated microstructure. It also covers the kinetics and kinematics of the crystal plasticity finite element model (CPFEM) used to describe the material deformation under loading, and introduces fatigue indicator parameters (FIPs) and extreme value (EV) theory for fatigue crack probability. A short background on materials informatics is presented as well. Chapter 3 outlines the computational workflows for batch generating and processing a large data set using ensembles of statistical volume element (SVE) instantiations. Chapter 4 focuses on rank-ordering of 12 different Ti-6Al-4V microstructures for resistance to fatigue crack formation of the two primary transgranular deformation mechanisms, and considers several loading conditions that span from high cycle fatigue (HCF) to low cycle fatigue (LCF) regimes. Chapter 5 presents grain neighborhood spatial correlations at locations of EV FIPs identified by our computational approach and from experimental literature, to identify the microstructure attributes from 1st nearest-neighbor (NN) grains. Reduced order modeling is also used to train a neural network to predict these EV FIP locations. Then the conclusions and recommendations for future work are presented in Chapter 7.
CHAPTER 2
BACKGROUND

2.1 Introduction

Chapter 2 reviews the relevant topics that follow throughout this dissertation, including titanium alloys and specifically Ti-6Al-4V (Section 2.2), statistical methods of representing microstructures of a material (Section 2.3), crystal plasticity finite element modeling (Section 2.4), fatigue of Ti-6Al-4V (Section 2.5), and finally materials data science and informatics (Section 2.6).

2.2 Titanium alloys

Titanium alloys are commonly used in aerospace applications due to their high strength-to-weight ratio and high temperature performance [25]. Ti-6Al-4V is one of the most commonly used alloys and has a wide range of possible microstructures depending on material composition and processing route. These range from near-\(\alpha\), \(\alpha + \beta\), to near-\(\beta\) alloys, and result in a large variety of macroscale mechanical responses [26]. Duplex \(\alpha + \beta\) Ti-6Al-4V morphologies are relatively equiaxed, with a high volume fraction of primary \(\alpha\) grains with a diameter of \(~5-20\,\mu m\) in conventional product forms like sheet, plate, and forgings. Due to the higher number density of grain boundaries in the former, equiaxed Ti-6Al-4V shows increased resistance to formation and growth of small fatigue cracks, whereas lamellar Ti-6Al-4V provides higher resistance to growth of long fatigue cracks [27]. Bimodal duplex Ti-6Al-4V consists of primary globular \(\alpha\) grains with lamellar colonies of secondary-\(\alpha\) embedded as laths within \(\beta\)-grains, offering a promising combination of small- and long-crack fatigue resistance to improve overall fatigue behavior.

The \(\alpha\)-phase of titanium has hexagonal close packed (HCP) crystal structure, and \(\beta\)-
phase has body centered cubic (BCC) crystal structure. The primary active slip system types of the α-phase HCP structure are \{0001\}{⟨11\bar{2}0⟩} basal slip, \{10\bar{1}0\}{⟨11\bar{2}0⟩} prismatic slip, \{10\bar{1}1\}{⟨11\bar{2}0⟩} pyramidal ⟨a⟩ slip, and \{10\bar{1}1\}{⟨11\bar{2}3⟩} pyramidal slip ⟨c + a⟩. The relative slip system strengths of each HCP slip type is still a matter of much debate [28]. Recently, Dawson and coworkers [29] used a combination of high-energy x-ray diffraction (HEXD) and finite element simulations to conclude that the ratios of flow stress of slip systems from basal to prismatic to first-order pyramidal is 1:1.2:1.7. This is in agreement with experimental observations that the basal slip plane in α-Ti experiences higher accumulated plastic strain [30, 31], and is more likely to form continuous slip bands across microtextured regions [32]. The BCC phase contains up to 48 slip systems, but only the 12 \{001\}{⟨111⟩} are assumed to be activated for the homogenized colonies, along with 12 basal, prismatic, and ⟨a⟩ pyramidal slip from the α-phase. Details on the homogenization scheme of the α + β colonies can be found in Ref. [33]. The α + β laths follow the well-defined Burgers orientation relationship (BOR) of (110)β||{(0001)α & [1\bar{1}1]β||[1\bar{1}20]α for the colony grains [34].

2.3 Statistical representations of microstructure

2.3.1 Representative vs. statistical volume elements

The concept of a Representative Volume Element (RVE) has been historically useful for evaluating the properties of a microstructure using computational simulation methods such as CPFEM [35]. Selection of an RVE for a desired property or response of a given material requires that the volume element size is sufficiently large to capture the homogenized material response of interest. If properly selected, that associated response will not be sensitive to further increases of RVE size or translations within the microstructure. Although the concept of a RVE [35] is useful for certain properties, the size of a RVE necessary to capture the statistics of rare event responses such as VHCF fatigue crack formation would be untenably large for computation via CPFEM. Indeed, it is even too large for laboratory
samples, since experiments reveal statistical scatter in VHCF. Kanit et al. [36] proposed the use of an ensemble of smaller statistical volume elements (SVEs) to compile cumulative statistics. This approach requires that the number of instantiations in an ensemble of SVEs is large enough to capture an unbiased statistical representation of the microstructure feature distributions of interest, and the SVE volume size itself is large enough to capture the relevant microstructure spatial correlations of interest. In particular, the SVE size should be larger than the maximum correlation length of key microstructure features that influence fatigue crack formation and early growth. By using a statistical ensemble of SVE instantiations, the collective fatigue properties of the overall microstructure can be accumulated, subject to the caveat that longer wavelength spatial correlations are neglected.

The responses of SVEs exhibit variability, and therefore a sufficient number of SVEs of required to generate ensemble statistics as necessary to converge to a reasonable estimate of the extreme value distribution statistics of interest [4, 36–38]. For our purposes, SVE ensembles are used to compare extreme value distributions of various microstructures, so convergence to RVE scale simulations is not essential so long as rank-ordering of microstructures is preserved. Each generated microstructure SVE instantiation for Ti-6Al-4V is a two-phase material system containing approximately 300 grains/phases, which is the minimum required for Ti-6Al-4V to converge to the homogenized stress-strain response of a material over an ensemble of SVEs [39, 40]. Przybyla and McDowell [41–43] investigated the SVE size for extreme value fatigue behavior of Ti-6Al-4V and polycrystalline Ni, and concluded that the minimum SVE size is determined by the spatial correlations of microstructure attributes of interest in the neighborhoods of maximal FIP values. This includes nearest-neighbor grain data and often second-nearest-neighbor grains. As found in Ref. [40], an average of more than 5 grains per edge of a cubic SVE is considered large enough for Ti-6Al-4V specifically; the current work captures 6 grains per edge.
2.4 Crystal plasticity finite element modeling

2.4.1 Material deformation kinematics

Crystal plasticity is implemented in the user material (UMAT) subroutine model for ABAQUS [44], following a fully implicit integration scheme [24]. Modeling material response to an applied loading begins with the multiplicative decomposition of the deformation gradient tensor, which describes the deformation from an undeformed reference configuration to the current configuration, decomposed into two parts, i.e.,

\[ F = F^e \cdot F^p \]  

(2.1)

where \( F^e \) is the elastic deformation tensor that accounts for elastic lattice distortion and rotation, and \( F^p \) is the plastic deformation gradient tensor that accounts for combined effects of dislocation glide along slip systems [45]. The mapping \( F^p \) corresponds to an isoclinic intermediate configuration, which forms the updated reference state for the elastic deformation of the lattice, as shown in Figure 2.1. The concept of an isoclinic intermediate configuration in the multiplicative decomposition of the deformation gradient into elastic and plastic parts comes in useful for commonly used finite element analysis software that uses displacement-based analysis.

For a given material orientation (e.g., lattice orientation in metals), if a director vector is attached to the lattice substructure, the plastic part of the deformation tensor then describes the shearing deformation, analogous to a deck of cards. This deformation still allows the director vectors to remain the same from the reference to the intermediate configuration, while accounting for the plastic deformation of the material. Therefore, though the material may have spin at the continuum scale, there is no spin with respect to an observer attached to the lattice, as no elastic deformation or lattice rotation is captured in the intermediate configuration. This means no rigid body motion is captured in the intermediate configura-
Figure 2.1: Multiplicative decomposition of deformation gradient tensor.
tion, allowing the intermediate configuration to then serve as the ‘reference’ configuration for any thermoelastic deformation that results in the current configuration.

Modern descriptions of material deformation using crystal plasticity models employ internal state variables (ISVs) which are conjugate to the thermodynamics forces and used to describe nonequilibrium, irreversible evolution of microstructure. McDowell [46] outlines the derivation of the thermodynamic equations underlying ISV theory consistent with the physically-based kinetics and kinematics.

This isoclinic intermediate configuration is fundamental to the crystal plasticity implementation; all the evolution equations of internal state variables and slip system shearing rates are written in this configuration. The Cauchy stress tensor is based on a push-forward of the 2nd Piola-Kirchhoff stress tensor from the isoclinic configuration. In the intermediate configuration, the plastic deformation is fully captured via slip without any lattice spin effects; the slip direction \( s^\alpha_0 \) and normal \( n^\alpha_0 \) of slip system \( \alpha \) remain unaltered from the reference configuration, as shown in Figure 2.1. Transforming \( s^\alpha \) and \( n^\alpha \) from the intermediate configuration to the current configuration \( s^\alpha \) and \( n^\alpha \) is accomplished by applying \( F^e \),

\[
    s^\alpha = F^e \cdot s^\alpha_0 \tag{2.2}
\]
\[
    n^\alpha = s^\alpha_0 \cdot (F^e)^{-1} \tag{2.3}
\]

Assuming small elastic strains, the 2nd Piola-Kirchhoff stress tensor, which is calculated with respect to the intermediate configuration is computed simply using linear elasticity, and is then pushed forward to the current configuration (see Equation 2.1) to obtain the Cauchy stress tensor. The internal state variable evolution laws, are numerically integrated using a fully implicit formulation in the intermediate configuration for each strain increment (and corresponding time increment(s)) in the displacement-base finite element
implementation. The plastic deformation gradient evolves according to

\[ \dot{F}_p = L_0^p \cdot F^p \]  

(2.4)

where \( L_0^p \) is the plastic velocity gradient in the intermediate configuration. In the continuum representation, incompressible plastic shear due to the applied stress is resolved onto individual active slip systems [47]. The plastic velocity gradient is written as

\[ L_0^p = \dot{\gamma}^\eta (s_0^\eta \otimes m_0^\eta) \]  

(2.5)

where \( \dot{\gamma}^\eta \) is the slip system shearing rate for slip system \( \eta \), \( s_0^\eta \) and \( m_0^\eta \) are unit vectors in the slip direction and slip plan normal direction for slip system \( \eta \), respectively. Vectors \( s_0^\eta \) and \( m_0^\eta \) are defined in the reference configuration. The elastic deformation gradient intermediate to current configuration is calculated via

\[ F^e = F^p \cdot F^{-1} \]  

(2.6)

In the intermediate configuration, the elastic Green strain tensor, \( E^e \), is then calculated from

\[ E^e = \frac{1}{2} [(F^e)^T \cdot F^e - I] \]  

(2.7)

where \( I \) is the second rank identity tensor. The conjugate stress tensor to the Green strain is the symmetric second Piola-Kirchhoff stress tensor \( \sigma_{ij}^{PK2} \), obtained via linear elasticity under the assumption of small elastic strain as

\[ \sigma_{ij}^{PK2} = C_{ijkl} E^e_{kl} \]  

(2.8)

Here, \( C_{ijkl} \) is the fourth rank elasticity tensor. The Cauchy stress tensor, \( \sigma \), in the current configuration is obtained by pushing \( \sigma_{ij}^{PK2} \) forward from the intermediate to the current
configuration, i.e.,
\[
\sigma = \frac{1}{\det(F^e)} F^e \cdot \sigma^{PK2} \cdot (F^e)^T
\]  
(2.9)

The resolved shear stress on each active slip system in the current equation can be found from
\[
\tau^\eta = \sigma^{PK2} : (s^\eta \otimes n^\eta)
\]  
(2.10)

The elasticity tensor, \(C_{ijkl}\), is subject to considerations of crystal and stress-strain symmetry that reduces the tensor components to 36, and can be represented using Voight notation as a 6x6 matrix with reduced indices, \(C_{ij}\) where \(i=1,2,\ldots,6\) and \(j=1,2,\ldots,6\) [48]. The HCP structure of the primary \(\alpha\)-phase has the crystal symmetry shown below,

\[
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{66} & \\
sym. & C_{44} & 0 & \\
\end{bmatrix}
\]  
(2.11)

The BCC \(\beta\)-phase has greater symmetry than the HCP phase,

\[
\begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & \\
sym. & C_{44} & 0 & \\
\end{bmatrix}
\]  
(2.12)
2.4.2 Material deformation kinetics

This microstructure-sensitive model has evolved from the early work of Mayeur and McDowell [33] on Ti-6Al-4V, who first introduced the model to investigate slip effects in 3D, which are critical for Ti-6Al-4V because of its highly anisotropic material response. The model was calibrated by Mayeur and McDowell to uniaxial loading experiments, and further expanded by Zhang et al. [49] to capture the material deformation response to cyclic loading, as well as probability distributions of microstructure features, notably grain orientation. Bridier et al. [50] then adapted the constitutive model to account for HCF loading of Ti-6Al-4V and elucidate the progressive occurrence of slip activation between different slip types. The dominance of slip along basal and prismatic planes agreed well with experimental results. In the present work, the slip system flow rule of slip system $\eta$ is given by

$$
\dot{\gamma}^\eta = \dot{\gamma}_0 \left( \frac{|\tau^\eta - \chi^\eta| - \kappa^\eta}{D^\eta} \right)^M \text{sgn}(\tau^\eta - \chi^\eta)
$$

(2.13)

where $\dot{\gamma}_0$ is the reference shearing rate, $\tau^\eta$ denotes the resolved shear stress, $\chi^\eta$ is the back stress, $\kappa^\eta$ is the threshold stress, $D^\eta$ is the drag stress of slip system $\eta$, respectively, and $M$ is the inverse strain rate sensitivity parameter. The initial resolved shear stress and back stress are taken to be zero at the beginning of the simulation without any prior loading history. In this model, slip systems are considered ‘active’ once the initial threshold stress $\kappa^\eta$ is reached by the magnitude of overstress, $|\tau^\eta - \chi^\eta|$. Material parameters $\dot{\gamma}_0$ and $M$ are taken from Bridier et al. [50]. For the back stress evolution, a typical Armstrong-Frederick hardening law is employed to account for direct hardening and dynamic recovery, i.e.,

$$
\dot{\chi}^\eta = h^\eta \dot{\gamma}^\eta - h_D \chi^\eta |\dot{\gamma}^\eta|
$$

(2.14)

Back stress is not a substantial contributor to the response of Ti-6Al-4V. The threshold stress $\kappa^\eta$ is expressed as a combination of a Hall-Petch initial strength term and a softening
term $\kappa_s^\eta$ with that evolves with inelastic deformation, i.e.,

$$\kappa^\eta = \frac{\kappa_y}{\sqrt{d}} + \kappa_s^\eta$$  \hspace{1cm} (2.15)

Here, $\kappa_y$ is the Hall-Petch slope, $d$ is the mean free slip distance, taken to be the grain diameter for primary $\alpha$ grains and the width of the laths within $\alpha/\beta$ colonies. The Hall-Petch strengthening term does not evolve, but the threshold stress softens from an initial value $(t = 0)$ of $(\kappa^\eta_s)_{t=0}$ according to

$$\dot{\kappa}^\eta_s = -\mu \kappa^\eta_s |\dot{\gamma}|$$  \hspace{1cm} (2.16)

where $\mu$ is the softening rate coefficient [51]. It is assumed that the drag stress does not evolve [50], $\dot{D}^\eta = 0$.

2.5 Fatigue of Ti-6Al-4V

Fatigue is a major design concern for engineering applications of metallic alloys. Failure from fatigue is the result of accumulated plastic deformation and damage, which form cracks in a given microstructure where localization of strain fields increases around heterogeneities or defects. Fatigue life traditionally is defined by either crack growth up to a pre-determined final crack size or length, or by crack growth until complete failure of a structural component or specimen. Nondestructive evaluation (NDE) methods can be used to evaluate fatigue cracks that have grown large enough to be detected, but the propagation of such long cracks represents a small portion of the total fatigue life. The term crack formation is used to encompass the collective processes of crack nucleation and early growth at the grain scale, which is typically several orders of magnitude below NDE detection limits. Given the increase in computational power over the last several decades, methodologies utilizing high-performance computing resources are a promising field for developing fatigue crack formation, and eventually fatigue life, predictions to fill that knowledge gap.
Traditionally, fatigue life corresponding to some final crack size or length, or complete failure of a structural component or specimen, is separated

\[ N_{total} = N_i + N_p \]  

(2.17)

where \( N_i \) is the number of cycles to fatigue crack initiation and \( N_p \) is the number of cycles to propagate a fatigue crack. However, in high cycle fatigue,

\[ N_{total} \approx N_i \]  

(2.18)

which necessitates further decomposition for the number of cycles to form a fatigue crack. McDowell and coworkers [52] decompose this into

\[ N_{total} = N_{inc} + N_{MSC} + N_{PSC} + N_{LC} \]  

(2.19)

where \( N_{inc} \) is the number of cycles to incubate a crack, \( N_{MSC} \), \( N_{PSC} \), and \( N_{LC} \) are the number of cycles of crack propagation in the microstructurally small, physically small, and long crack regimes from McDowell [22]. The MSC regime comprises roughly 3-10 grains (including plastic zone), PSC is up to 1mm, and LC is the remainder of crack life, where linear elastic fracture mechanics sufficiently describes crack growth. Figure 2.18 that the division into regimes allows for models to address the varying physical mechanisms that carry plastic deformation over a range of scales with suitably chosen computational models. Moreover, the definition of initiation fatigue life to be defined by each user according to the appropriate stage or crack size of interest. The remainder of \( N_{total} \) then is attributed to (long) crack growth. Typically, \( N_p \) is estimated based on fracture mechanics methods. Stein et al. [53] outline some of the specific complications of modeling fatigue crack initiation in nickel-based superalloys. Hochhalter et al. [54] found that orientation has a strong influence on microstructurally small fatigue cracks for AA7075-T651 using crystal
plasticity modeling couple with a study of fatigue damage parameters. The nucleation of cracks was shown to be able to be predicted from statistical distributions of microstructure features and localized strains for the same material by Hochhalter et al. [55].

For total fatigue life on the order of $10^6 - 10^8$ cycles, conducting experimental tests may be infeasible due to the time required to run such a long experiment, so computational methods for studying fatigue life represent an attractive alternative and/or augmentation of information to traditional testing, especially for high cycle fatigue (HCF) or very high cycle fatigue (VHCF). The models used for testing HCF or VHCF must incorporate the necessary structure-property relationships as described previously in order to provide significant meaning and insight. This is due to the low strain amplitudes applied for HCF, where most of the material is in the elastic regime, with select few favorably oriented grains or other local stress raisers experiencing plastic deformation.

Fatigue is a complex evolutionary process depending on a hierarchy of microstructure attributes that influence the stages of crack formation and growth. Fatigue life variability is directly related to the coupling of crack driving and resisting forces to the material microstructure. This complexity is amplified for two-phase Ti-6Al-4V due to the highly elastic and plastic anisotropic material deformation response of its HCP primary $\alpha$ grains, especially the variability of slip system plasticity. Experimental testing of fatigue behavior in bimodal Ti-6Al-4V shows a range of several orders of magnitude of fatigue life for a range of applied stress amplitude, as shown in Figure 2.2. Understanding the influence of neighboring microstructure attributes that drive localized cyclic plastic deformation is of critical importance in the HCF regime, when only select few favorably-oriented grains undergo strain localization that lead to fatigue crack formation and early growth.
2.5.1 Fatigue crack formation mechanisms

From previous experimental and computational studies, two dominant fatigue cracking mechanisms have been identified for $\alpha + \beta$ Ti-6Al-4V. The first is transgranular slip band formation due to dislocation pileup on basal planes aligned nearly perpendicular to the applied loading axis in favorably crystallographic oriented “soft” primary $\alpha$ grains [57–61]. Bridier et al. [62] used EBSD to experimentally investigate slip system activation in near-$\alpha$ Ti-6Al-4V, and found a predominance of slip activation on basal and prismatic slip systems. Fatigue cracks formed on both basal and prismatic planes but cracks both formed and propagated more quickly along basal slip planes that experienced a combination of high shear stress on and peak normal stress to basal planes owing to the crystallographic anisotropy range of HCP $\alpha$-Ti-6Al-4V [63].

The second primary cracking mechanism is transgranular cracks arising from dislocation pileup within slip bands at the grain boundary associated with positive loading stress or strain ratios. A fatigue crack nucleation criterion based on the stress developed by such
a dislocation pileup was first derived by Stroh [64], who showed that the highest stress parallel to the loading in the hard grain occurred for one slip plane orientation. Dunne et al. [59] employed a CPFE model to investigate possible grain orientation combinations of rogue grain pairs, and found that a large range of orientations resulted in dislocation pileup along and high normal stress to basal slip planes, concluding that those conditions alone are not sufficient to predict fatigue crack formation. Later, Bache et al. [65] used a similar CPFE model and a non-local failure model to investigate quasi-cleavage fracture on the basal plane of near-\(\alpha\) Ti-685, and predicted crack growth into neighboring favorably oriented prismatic slip planes of neighboring grains. It was found that the resulting accumulated strain correctly predicted crack nucleation and subsequent growth direction. Zheng and coworkers [66, 67] used discrete dislocation plasticity models to study load shedding in near-\(\alpha\) Ti alloys to validate Stroh’s original proposal that dislocation pile-up in a grain can cause crack nucleation in a neighbor of that grain [64]. Ghosh and coworkers [60, 68] employed both polycrystalline and two grain, hard-soft, CPFEM simulations to show a strong correlation between fatigue crack formation and the surface area fraction of soft grains surrounding each hard grain. This work was then expanded to create a unified constitutive model and flow rule for polycrystalline CPFEM simulations of Ti-7Al and experimentally validated [61, 68, 69].

2.5.2 Fatigue Indicator Parameters (FIPs)

Dunne’s recent review of fatigue crack formation [70] identifies the critical need for development of multiscale models for fatigue crack formation which are continuum-based but mechanistically informed in order to understand the driving force for slip transfer. Fatigue Indicator Parameters (FIPs) have been introduced [71–74] as part of a multiscale modeling approach to capture relevant microstructure driving forces for fatigue crack nucleation and to facilitate parametric studies on the effects of relevant microstructure attributes on fatigue resistance. FIPs can be approximately divided into the categories of strain-, stress-
and energy-based concepts, depending on the deformation mechanisms active in a given material and stress/strain state. For Ni-base superalloys, Stinville et al. [75] studied low cycle fatigue using digital image correlation and found a strong correlation between the crack initiation site and the highest cyclic uniaxial strain localization. Similarly, Naragani et al. [76] found, under micro-tomography, a gradient of strain magnitude is present across a crack formation site located at a non-metallic inclusion in RR1000 under uniaxial cyclic loading. After finding a link between crystallographic slip planes and fracture surface orientation, Proudhon et al. [77, 78] used resolved shear stress damage indicator to predict propagation and distance along a inserted crack front of a near-β titanium alloy. Ozturk and coworkers [61] proposed a FIP based on a mixed-mode stress intensity factor for fatigue crack formation at grain boundaries for α-titanium. However, Chen et al. [79] investigated an inclusion within the nickel-matrix and observed that slip was a necessary but not sufficient condition for actual crack formation. Dunne and coworkers [79, 80] argue for a stored energy criterion over stress- or strain-based criteria to predict crack formation in nickel-based superalloys. Approaches based on geometrically necessary dislocations and discrete dislocation dynamics to predict fatigue crack formation [13, 69, 81–85] have also been developed.

In the HCF regime, total fatigue life ranges from $10^5$ – $10^8$ cycles and beyond, and is characterized by primarily elastic response of the bulk material with few favorably oriented grains experiencing heterogenized plastic deformation. For HCF of Ti-6Al-4V, the majority of the total fatigue life occurs during the crack incubation, initiation, and subsequent growth to the first grain boundary, as the first grain boundary encountered represents the largest obstacle to crack growth. This heterogeneous plastic deformation is a direct result of the local microstructure attributes and variations (e.g., grain size, grain orientation), both individually and as combinations; it results in heterogeneous local stress and strain states, depending on the material of interest. Additionally, internal gas pores and shrinkage pores can also drive crack initiation [86]. When the cyclic plastic deformation is irreversible and
accumulates enough localized damage, a crack is formed, which may or may not propagate to the next grain due to dislocation pinning [87]. For example, for Ti-6Al-4V, up to 85% of the total fatigue life within HCF is occupied in this regime [14]. Therefore, in order to predict failure for materials loaded in HCF, improving FIP correlations for microstructures of interest is necessary.

FIPs must be carefully selected to capture the primary deformation mechanisms of interest in a material for transgranular crack formation and growth. For duplex Ti-6Al-4V, the Fatemi-Socie FIP (FIP_{FS}) [71, 88] has been extensively used in conjunction with computational simulations to capture both HCF and LCF for multiaxial fatigue [89], i.e.,

\[
FIP_{FS} = \frac{\Delta \gamma_p^{\star \max}}{2} \left( 1 + k \left\langle \frac{\sigma_n^{\star \max}}{\sigma_0} \right\rangle \right)
\]  \hspace{1cm} (2.20)

Here \(\Delta \gamma_p^{\star \max}\) is the maximum cyclic plastic shear strain range, \(\sigma_n^{\star \max}\) is the maximum stress normal to the plane of maximum cycle plastic strain, \(\sigma_0\) is the macroscale yield strength of the material, and \(k\) is a material constant with typical values between 0.5 and 1. The \(\star\) indicates that volume averaging must be performed to regularize mesh sensitivity effects in simulations, and to enforce a finite damage process zone size that accords with physics.

Within a SVE instantiation, the local FIP_{FS} is calculated for every mesh integration point in the ABAQUS mesh in post-processing. Previous volume averaging studies for the FIP_{FS} by McDowell and coworkers [90–92] have used grain volume, Gaussian kernels, cubic volumes, and approximate slip band averaging. The type of banding used for the FIP_{FS} is referred to as stacked or layered banding, and divides the elements within a grain along bands parallel to the slip planes of the grain with respect to the loading direction [92, 93]. Band averaging was introduced to be consistent with the physical mechanisms of irreversible slip and represent the fatigue damage process zone. This subgrain approach has been shown to be a good compromise between mesh sensitivity effects of elemental averaging versus grain averaging, which does not capture the variation of FIP_{FS} values within
a grain [91] on a given slip band. Notably, Castelluccio and McDowell [91] found that the orientations of surrounding grains affect the variability of maximum stacked band-averaged FIP\textsubscript{FS} by a factor of 2-3 and nearest neighbor orientation by about 30\%. Given these results and the crystallographic dependence of fatigue crack formation and early growth in Ti-6Al-4V, stacked band-averaged FIP\textsubscript{FS} are well-suited to elucidate correlations of local microstructure fatigue behavior.

Variations on the Fatemi-Socie FIP have been introduced to capture different deformation mechanisms using as similar physics-based approach. For bimodal Ti-6Al-4V, internal cracks at colony boundaries are driven by discontinuous slip on prismatic slip planes, leading to dislocation pileup at grain boundaries [56, 94, 95]. With regard to cases involving mean stress (but not dwell fatigue per se), the grain boundary impingement FIP (FIP\textsubscript{GBI}), developed by McDowell and coworkers [22], accounts for dislocation pileup that drives formation of crystallographic fatigue cracks that stem from grain or phase boundaries disrupted by the pileup, and is defined by

\[
FIP_{GBI} = \gamma_{net}^p \left(1 + k \frac{\sigma_{GB}^n}{\sigma_0} \right)
\]

where \(\gamma_{net}^p\) is the net plastic shear strain at a grain boundary, \(\sigma_{GB}^n\) is the maximum stress normal to that grain boundary, \(\sigma_0\) is the macroscale yield strength of the material, and \(k\) is a material constant with typical values between 0.5 and 1. The \(^\ast\) indicates the volume averaging must be performed to minimize any mesh sensitivity effects for simulations, and also to consider a physically-consistent fatigue damage process zone size.

This second transgranular fatigue crack formation mechanism correlates more with dislocation slip that impinges on a phase boundary. It is noted that some studies have been devoted to understanding interactions between hard-soft grain pairs and dislocation pileups that accumulate under elevated temperature dwell fatigue, which involves time-dependent deformation [70, 96, 97] in the load shedding process from soft to hard grains. Here,
the focus on a different set of loading conditions and manifestation of dislocation pileups, namely corresponding to continuous cycling with a tensile mean stress under low to moderate high cycle fatigue or transition fatigue cyclic stress and strain ranges; we consider that progressive accumulation of localized shear deformation due to unbalanced ratcheting is associated with dislocation pileups that impinge on phase boundaries with disorientation, eventually resulting in image forces that work together with lattice disruption at/near the interface owing to higher slip irreversibility to form transgranular cracks near the boundary, i.e., a Zener-Stroh mechanism [98, 99].

2.5.3 Extreme value statistics of FIPs in fatigue

Variability of fatigue life is primarily due to the statistical occurrence of extreme values of configurations of microstructure attributes that combine to drive fatigue crack formation and early growth. Extreme value statistics consider the extreme value tails of quantities of interest. For this work, FIPs calculated from CPFEM simulation results are the quantity of interest to investigate correlations between microstructure features and fatigue cracks. To characterize the nature of the tail of the maximum FIP probability distribution, the individual maximum FIP values per \( n \) SVEs, \( X_1, X_2, \ldots, X_n \) are used to find the maximum of all responses, or

\[
Y_n = \max(X_1, X_2, \ldots, X_n)
\]  

where the probability of finding \( Y_n \) within a given set of SVEs that is less than \( y \) is found from the cumulative distribution function of the generalized extreme value distribution (GEVD),

\[
F_{Y_n} \equiv P(Y_n \leq y) = P(X_1 \leq y, X_2 \leq y, \ldots, X_n \leq y)
\]  

For the GEVD, there are three possible options for the tail behavior that can converge [100], the Gumbel distribution (Type I), the Fréchet distribution (Type II), and the Weibull distribution (Type III). Of these three, the Gumbel EVD is primarily used in this work,
as the larger the number of samples of interest, the better the Gumbel EVD converges to
the FIP extreme maximum distribution [101], and has been previously used by McDowel-
well and coworkers [39–42, 51, 90, 101–103]. Fréchet EVD will be used as well. Current
attempts to link fatigue life to the extreme value statistics are limited to distributions of
single a microstructure attribute of interest such as inclusions, grain size, and stress corro-
sion, as reviewed by Atkinson and Shi [104]. These methods lack critical interaction ef-
fects between microstructure attributes and resultant changes in the extreme value response
distributions. As discussed previously, fatigue response in Ti-6Al-4V requires including
interaction effects, which means spatial correlations must be taken into account for fatigue
crack formation and early growth. Pyrz [105] first introduced marked correlation func-
tions (MCFs) to investigate the relationship between the mean value of a distribution of a
variable and spatial correlations between microstructure attributes, i.e.,

\[ M(r) = \frac{h(r)}{g(r)} \]  

(2.24)

where \( g(r) \) is the pair distribution probability density function, such that \( g(r)dr \) is the
probability of finding a point whose center lies between two concentric spheres of radii \( r \)
and \( r + dr \) about another point. A value of \( M(r) = 1 \) indicates no correlation between
marked attributes, with a positive value indicating positive correlation and a negative value
indicated negative correlation.

Przybyla and coworkers [39, 41, 42] expanded the use of MCFs to investigate extreme
value fatigue behavior of polycrystalline metal alloys. Similar to n-point statistics, extreme
value marked correlation functions (EVMCFs) capture information regarding microstruc-
ture local states and potential correlations between multiple local states but are explicitly
defined to address the statistically rare sites where cracks are expected to form. EVMCFs
describe the probability of finding correlated local microstructure attributes at the same lo-
cation as where the extreme value response is located for a given volume. Given a particular
instantiation of the ensemble set of SVEs, Ω, and the probability distribution of a response of interest parameterized by α, the EVMCF is defined as a radial distribution probability density function, i.e.,

\[ R^{\text{max}}(\alpha)(h, h'|r, \Omega) \]

where \( R^{\text{max}}(\alpha)(h, h'|r, \Omega) \) is the probability of finding local state \( h \) coincident at spatial location \( x \) to the maximum response of \( \alpha \) and a second local state \( h' \) within \( r \) to \( r + dr \) from \( x \) in any direction for a given microstructure volume \( \Omega \). In this work, the material responses of interest represented by \( \alpha \) are the locations of maximal FIPFS and FIPGBI calculated from CPFEM simulations results. By determining the EVMCF, the extreme value distribution response is also found, and is related to the probability density of the GEVD discussed above. Finding EVMCFs using this method allows identification and characterization of the correlated local states (e.g., combinations of microstructures attributes) that have a high probability of existing in the neighborhood of maximum FIP values, and thus, fatigue hotspots within a given material.

2.5.4 Microstructurally small fatigue crack growth and arrest at the first grain boundary

Elucidating the structure-property relationships for fatigue failure is a complex proposition as fatigue crack formation and growth is a cascade of processes that occur at multiple hierarchical material scales [19, 21]. These processes span effects ranging from first principle-based atomistics through macroscale plasticity, encompassing a wide range of experimental methodologies and computational models, cf. Figure 2.3; most of these models are developed with respect to one specific length/time scale and currently are limited in terms of ability to inform models at other scales.

Further complicating the study of fatigue failure is the occurrence of multiple, often competing plastic deformation mechanisms and potential crack formation within a material. Thus, this variability in fatigue behavior is correlated not only to the type of cracking mechanism but also to probability of an embryonic crack propagating through or arrest-
Figure 2.3: Hierarchy of length scales critical to crack formation and growth processes [89].

As outlined earlier, McDowell and coworkers [22, 107] provide a decomposition of total fatigue life into regimes. Fatigue crack formation occurs within the first grain or phase, microstructurally small fatigue crack growth continues across roughly 5-10 grains, then physically small fatigue crack growth from this point forward until similitude conditions of long crack growth are met, where the crack front is large enough to effectively sample enough grains to homogenize any variability in microstructure attributes. This latter regime is effectively addressed by linear elastic fracture mechanics (LEFM) or elastoplastic fracture mechanics (EPFM). These classical fracture mechanics approaches correlate parameters such as stress intensity factor range ($\Delta K$), $\Delta J$-integral range, and crack tip displacement range ($\Delta CTD$) to the local driving force for fatigue crack growth [108–110]. However, these approaches fail at a length scale smaller than some characteristic length related to the microstructure heterogeneity and contrast [20, 111, 112]. To bridge between fatigue crack formation and growth into the adjacent phase/grain, probabilistic models and
predictive models were introduced. Early statistical approaches attempted to link fatigue
damage to Coffin-Manson and Palmgren-Miner laws for total fatigue lifetime [113]. More
recent probabilistic models focus on slip irreversibility and resulting fatigue damage pro-
cess zones [114–116], including using extreme value statistics of FIPs.

Recent efforts towards identifying and tailoring microstructures for increased fatigue re-
sistance have focused on microstructure-sensitive fatigue analysis [22, 41, 89], and suggest
that the heterogeneity of cyclic plastic deformation can be used to distinguish between the
high cycle fatigue (HCF) and low cycle fatigue (LCF) regimes of material microstructure.
The HCF regime corresponds to highly heterogeneous microplasticity at stress amplitudes
below macroscopic yield yielding, and the bulk of the material experiences primarily elastic
deformation. As applied stress amplitudes increase, the transition to the LCF regime occurs
upon widespread plastic deformation, leading to more homogeneously distributed plastic-
ity throughout the bulk material. Due to this increasingly uniform distribution of plasticity,
fatigue behavior in the LCF regime exhibits less variability than in the HCF regime.

Fatigue crack formation arises from the accumulation of irreversible slip dislocation
under cyclic loading [117, 118]. This is associated with strain localization occurring at
spatial locations corresponding to previously described soft oriented grains, load shedding
of hard-soft grain combinations, or due to other material inhomogeneities such as inclu-
sions or voids as a result of processing techniques. Persistent slip bands (PSBs) have long
been associated with sites of fatigue crack formation in metal alloys [119–122], either
within a PSB or at grain/boundary interfaces, particularly for surface grains due to the de-
velopment of extrusions and intrusions at the free surface. Surface crack initiation sites are
more common in the LCF regime than the HCF regime, in which internally-formed cracks
increasingly trigger life-limiting events. The applied stress amplitude decreases into the
HCF regime; the increase in variability of fatigue behavior is due to the influence of the
attributes of grain/phase boundaries, or other obstacles that may arrest crack growth [19,
20]. Compared to a long crack, a MSC has far less driving force to overcome microstruc-
ture thresholds; thus, the accumulation of fatigue damage and a resultant crack formation event may or may not correspond to a life-limiting event [119].

2.5.5 Rank-ordering microstructures in terms of FIPs for fatigue response

The motivation to develop a methodology for rank ordering microstructures for fatigue response for a given loading condition lies in providing decision support for engineering material selection. Bulk properties, such as Young’s modulus and yield strength are fairly straightforward to obtain, but any non-homogenized structure-property response has historically been quite difficult, due to the time and cost associated with experimental efforts to make such a comparison. The statistically rare, extreme event, nature of fatigue crack further adds complication to generating such rankings, given that the heterogeneity of crack initiation and early growth are still not fully understood at each of the length scales that affect such an event, from atomistic through continuum scales. McDowell [22] described the characterization of these mechanisms as nascent in 2007. Extreme value theory began to be incorporated soon after, to capture distributions of the far right tail of fatigue indicator parameters. Przybyla et al. [41] first looked at the number of SVE instantiations to converge to the Gumbel extreme value distribution (EVD) for IN100. Taking this further, Przybyla and McDowell [40, 42] then compared Gumbel EVDs to rank order between maximum applied strains for IN100, and for Ti-6Al-4V, they rank ordered 4 different microstructure, comparing coarse vs. fine grain size and high vs. low α volume fraction, using the FIP\textsubscript{FS}, the cumulative effective plastic strain, and maximum plastic shear strain. Przybyla and coworkers [101] also investigated various volume averaging schemes for computing EV FIPs. See the review paper by Pineau et al. [123] for further discussion.

More recently, work done by Stopka and McDowell [93, 124] has shown the validity of EV statistics of FIPs for rank-ordering of rolled vs. random microstructure for surface vs. subsurface crack initiation of Al7075 and Ti-6Al-4V, and for uniaxial, equibiaxial, simple shear, and pure shear of those materials as well. Zhang et al. [125] looked at using EV
fits of geometrically necessary dislocation dislocations of Ti-6Al-4V to rank-order fatigue resistance with varying $\alpha$-phase volume fraction, $\alpha$-lath width, and average grain size. Uncertainty quantification work done by Whelan and McDowell [126] on this approach established upper and lower uncertainty limits on EV statistics of FIPs and CPFEM model form and parameters for four Ti-6Al-4V textures. There have also been efforts at creating reduced order linkages of the structure-property relationships of fatigue, with the intent of reducing the need for CPFEM modeling requirements, considering at 12 synthetic $\alpha$-titanium microstructures under HCF and transition fatigue [127, 128].

2.6 Materials informatics

2.6.1 2-point spatial correlations

Traditional quantitative metrics of microstructures have been used to convey statistical information about microstructure information, such as grain size distribution, distribution of misorientation angles between grains, or volume fraction of phases present [129, 130]. PyMKS has been used to construct structure-property linkages/correlations for a material, and is built on the framework of Adams [131–133]. The microstructure function $m(h, x)$ represents the probability density of finding local state $h$ at spatial location $x$, given that both $h$ and $x$ are continuous variables. In this context, local state can refer to either the microstructure instantiation built by DREAM.3D before applied loading or the CPFEM simulation results after applied loading. By discretizing the microstructure and binning the spatial domain and local state space, the microstructure can be described by

$$m(h, x)dhdx \approx \sum_{n=1}^{N} \sum_{s=1}^{S} M^n_s \chi_n(h) \chi_s(x)$$

(2.26)

where $M^n_s$ is the discretized microstructure function, and $\chi_i()$ are indicator functions defined as 1 if the argument belongs in the bin labeled $i$ and 0 otherwise, and $dh$ and $dx$ are measures of the bin sizes. $M^n_s$ in this context represents the volume fraction of the material.
belonging to bin \( n \) that also belongs to bin \( s \).

This discretized representation of the microstructure is more desirable in practice, as the data used from experimental characterization are inherently discretized by its scale limitations of the technique used, in addition to the SVE instantiations for FEM simulations requiring mesh discretization. A modification to the microstructure function above was made to account for discretization and then extended by Paulson et al. [134] to account for crystal orientation for metals, using generalized spherical harmonics (GSH) for hexagonal crystal structures [135]. Kalidindi and coworkers [136–138] have demonstrated the viability of a materials knowledge system (MKS) approach for setting up a universal framework (with respect to length and structure scales) using principal component analysis (PCA) and n-point spatial statistics combined with molecular dynamics and phase-field simulations.

To represent digital microstructures, the discretized microstructure function \( M^n_s \) from Eq. 2.26 is of limited use as a single point descriptor which only provides information on volume fraction of the particular microstructure local state of interest [102, 128, 134, 139]. To capture higher order coupling between local states, correlation functions and statistics must be introduced. The most systematic and general approach to characterize the heterogeneity and spatial arrangement of microstructure attributes is through n-point spatial correlations [140–142]. The simplest form of n-point statistics is 2-point statistics, formally expressed as

\[
f(h, h' | \mathbf{r}) = \frac{1}{\text{Vol}(\Omega_r)} \int_{\Omega_r} m(h, \mathbf{x})m(h', \mathbf{x} + \mathbf{r})d\mathbf{x} \tag{2.27}
\]

In Eq. 2.27, \( f(h, h' | \mathbf{r}) \) is the conditional probability density of finding local states \( h \) and \( h' \) at the spatial locations \( \mathbf{x} \) and \( \mathbf{x} + \mathbf{r} \), respectively, separated by a vector \( \mathbf{r} \). The volume \( \Omega_r \) is dependent on the selection of \( \mathbf{r} \) due the need to know a priori the local states at \( \mathbf{x} \) and \( \mathbf{x} + \mathbf{r} \). This integral can be discretized as

\[
f(h, h' | \mathbf{r})dhdh'd\mathbf{r} \approx \sum_{p=1}^{N} \sum_{n=1}^{N} \sum_{t=1}^{S} F_{t}^{np} \chi_n(h) \chi_p(h') \chi_t(\mathbf{r}) \tag{2.28}
\]
where $F_{np}^t$ is the probability of finding local states $n$ and $p$ in spatial bins separated by vector $t$. The discretized microstructure is related to the 2-point spatial correlations through the probability $F_{np}^t$,

$$F_{np}^t = \frac{1}{|S_t|} \sum_{s=1}^{S_t} M_s^n M_{s+t}^p$$

(2.29)

where $|S_t|$ is the total number of spatial bins of multidimensional array $s$, and under periodic boundary conditions, $S_t$ is reduced to $S$, the number of spatial bins in the microstructure. 3-point and higher order correlations can also be utilized if needed. However, the dimensionality of even 2-point statistical correlations can still be very high, and do not provide information on which coupled microstructure features show the largest variance with respect to fatigue behavior. The calculation of the complete representation of the discretized 2-point statistics in Equation 2.29 requires calculating $F_{np}^t$ for all $t$, $n$, and $p$, which is on the computational order of $O(S^2)$. By invoking the convolution theorem and using discrete Fourier transforms (DFT), fast Fourier transforms (FFT) can be employed to reduce computational time to $O(S \log S)$ [4, 133]. In DFT space, Equation 2.29 becomes

$$f_{np}^k = \frac{1}{S} m_k^n \odot m_k^p f_{np}^k = \mathcal{J}(F_{np}^t), m_k^n = \mathcal{J}(M^n_s)$$

(2.30)

where $\odot$ is the element-wise operator, $*$ denotes the complex conjugate, and $\mathcal{J}(\cdot)$ denotes the DFT transformation into frequency space $k$. PCA applied to the 2-point statistical correlations reduces the dimensionality by finding and ordering the orthogonal and linear combinations of microstructure feature data from highest to lowest variance.

Jha and coworkers [143] recently proved the viability of this approach by applying PCA to slip and grain neighborhood metrics of near $\alpha$-Ti and showed strong correlation between higher FIP$_{FS}$ values and principal components. 2-point statistics may not be sufficient to capture possible longer-range effects of microstructure, but represent improvement on 1-point statistical attempts to predict fatigue behavior, such as volume fraction or average grain size. Furthermore, it is likely that the SVE size required to capture such higher-order
statistics will be computationally infeasible with current computational tools, even with an ensemble approach.

Adapting the above approach to non-periodic microstructures requires an additional step of applying ‘padding’ to the discretized microstructure representation to ensure that vectors larger than the 2-point vectors of the microstructure can wrap around any edge of the volume. In a non-periodic microstructure, $S_t$ can no longer be reduced to $S$. For a three dimensional SVE of volume $S^3$, by adding pads of width $T$ so that the SVE side is now $(S + T)$. Very high values of $T$ can result in meaningless answers, so for this work, $T < \frac{S}{2}$. Let this padded microstructure be denoted by $\tilde{M}_n^s$. This allows use of DFTs to compute $\tilde{m}_k^n = \mathcal{J}(\tilde{M}_n^s)$ where the padding is essentially an additional phase where all of the microstructure values are 0. By padding the microstructure, non-periodic boundary conditions can be accounted for while meeting the requirements to calculate the spatial correlations in DFT space [144]. The concept of padding a microstructure can be further extended to ‘masking’ the microstructure by any set of criteria a researcher could design. A masked region can be defined within the existing region, with the areas of interest masked in the same way that padding is applied, given that the spatial correlations of the unmasked volume are properly normalized. Padding still must be applied to masked microstructure to enforce periodic boundary conditions for DFT calculations.
CHAPTER 3
A GENERAL METHODOLOGY FOR LARGE SCALE COMPUTATIONAL STUDIES USING SVE ENSEMBLES

3.1 Introduction

With the advent of increased computational resources developed over the past several decades, there has been a marked need for developing methodologies to improve the capabilities of computational materials science. These methodologies allow for supplementing time- and computationally-expensive experimental tests, though they cannot replace experimental testing entirely. Computational models still rely on experiments for critical verification and validation. Simulated microstructure representations have also greatly improved, increasing in fidelity from simplistic 2D isotropic material models to 3D anisotropic models that include statistical distributions of microstructure attributes. The coupling of improved models with higher fidelity microstructure representations allows for rapid exploration of microstructure-property relationships for both bulk material response as well as rare event responses, such as fatigue crack formation.

3.2 Microstructure morphologies and design of experiments

As the example material selected for developing computational methodologies and workflows for studying fatigue response, Ti-6Al-4V provides a large variety of possible microstructure morphologies, depending on the thermomechanical processing parameters. Ti-6Al-4V can range from near-α equiaxed with a high volume fraction of α-phase grains to fully lamellar α+β colony grains, with grain size ranging over several orders of magnitude from ~10 µm-1 mm. Some examples of these morphologies are shown below in Figure 3.1.
Figure 3.1: Various microstructure morphologies of Ti-6Al-4V based on processing route [145].

The statistically rare event nature of fatigue crack formation further complicates the study of Ti-6Al-4V fatigue behavior. Even when a singular processing path is selected for investigation, fatigue life variability can still range over several orders of magnitude, especially for the low applied strain amplitudes associated with High Cycle Fatigue (HCF) or Very High Cycle Fatigue (VHCF) regimes. At such small cyclic strain ranges, any plastic deformation in the material is highly heterogeneous, and generally occurs only in favorably oriented ‘soft’ grains for activated basal slip systems. As the strain increases through the transition to the Low Cycle Fatigue (LCF) regime, the plastic deformation becomes increasingly homogeneous, but fatigue life can still vary even at higher cyclic strain ranges.
Figure 3.2: Stress-life plot showing fatigue life, defining failure as specimen in two pieces, variability over a range of stress amplitudes [146].
3.2.1 Microstructures under consideration

Given these complexities of morphology and fatigue life prediction, elucidating the microstructure property relationships of Ti-6Al-4V requires a large design of experiments to account for the variables of interest. The grain size of primary $\alpha$ grains is expected to play a role in fatigue crack formation due to the increase in mean free slip distance in abnormally large grains. Texture and microtexture effects also result in fatigue life variability, as grain orientation is critical because of the anisotropy resulting from the hexagonal close packed (HCP) structure of $\alpha$-Ti-6Al-4V. For bimodal $\alpha + \beta$ Ti-6Al-4V, the phase volume fractions of $\alpha$ and colony grains can range from ratios of 30% $\alpha$-70% colony to 60% $\alpha$-40% colony.

With these microstructure attributes of concern, experimental data of a microstructure of Ti-6Al-4V was provided by collaborators at AFRL, shown below in Figure 3.3 [147]. The average grain size from the data is 10.9 µm, with a maximum grain size of around 20 µm. Fitting the grain size data to a log-normal distribution, the standard deviation ($\mu_1$) is 3.7 µm.

Given this data and the concern of outlier large primary $\alpha$ grains, the average grain size was kept at 10.9 µm with the standard deviation of 3.7 µm, and the maximum grain size was then limited to either twice (2x) or three times (3x) the average grain size, 21.8 µm and 32.7 µm, respectively. Two phase volume fractions were selected to represent the range of phase volume fractions of duplex Ti-6Al-4V, 30% $\alpha$-70% colony to 60% $\alpha$-40% colony. By selecting the outlying phase volume fractions, the intent is to investigate the largest possible effect that phase can have on Ti-6Al-4V fatigue behavior.

Crystallographic texture has a first order influence on the microstructure-sensitivity of the EV FIP distributions for low symmetry phases such as HCP $\alpha$-Ti [93, 102, 124, 134, 148, 149]. Accordingly, we introduce a range of feasible textures to facilitate comparison of fatigue behavior among candidate microstructures with the same composition and different thermomechanical process paths. The first texture data is taken from EBSD data provided by AFRL from HCF experimental data, T1. The remaining textures are texture 2 (T2),
Figure 3.3: 2D cross-sectional SEM micrograph of duplex Ti-6Al-4V. Dark grey is $\alpha$-phase, light grey is transformed $\beta$-phase [147].
using basal/transverse Ti-6Al-4V data for primary $\alpha$ grains (B), with rolled texture for colony grains (D). Texture 3 (T3), using strong transverse Ti7Al texture for primary $\alpha$ grains (C) with rolled texture for colony grains (D). Simulated inverse pole figures (IPFs) for the three microstructures are shown below in 3.4, 3.5, and 3.6.

Figure 3.4: Inverse pole figures (IPFs) generated by Dream.3D of the simulated microstructure of texture 1 (T1).

In total, with these variations on microstructure morphology, there are then 12 microstructures to be investigated for developing microstructure-property relationships for fatigue behavior of Ti-6Al-4V, summarized in Table 3.1.
Figure 3.5: Inverse pole figures (IPFs) generated by Dream.3D of the simulated microstructure of texture 2 (T2).

Figure 3.6: Inverse pole figures (IPFs) generated by Dream.3D of the simulated microstructure of texture 3 (T3).
Table 3.1: Simulated microstructures for duplex Ti-6Al-4V, textures correspond to IPFs in Figure 2. Each microstructure condition is designated according to texture (T), maximum grain size (2x or 3x), and primary \( \alpha \) volume fraction.

<table>
<thead>
<tr>
<th>Micro.</th>
<th>Grain size ((\mu m))</th>
<th>Texture</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Avg.</td>
<td>Std. Dev.</td>
<td>Max.</td>
</tr>
<tr>
<td>T1 2x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T1 2x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T1 3x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
<tr>
<td>T1 3x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
<tr>
<td>T2 2x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T2 2x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T2 3x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
<tr>
<td>T2 3x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
<tr>
<td>T3 2x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T3 2x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>21.8</td>
</tr>
<tr>
<td>T3 3x 30</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
<tr>
<td>T3 3x 60</td>
<td>10.9</td>
<td>3.7</td>
<td>32.7</td>
</tr>
</tbody>
</table>

3.2.2 Mechanical loading conditions under consideration

Fatigue experimental data is available for a number of strain ranges (0.4%, 0.6%, 0.8%, 1.0%, and 1.2%) for uniaxial loading conditions, see Figure 3.7, but only three strain ranges (0.4%, 0.8%, and 1.2%) are selected for an optimal number of total configurations for simulation while covering the largest possible range of applied strain. Lastly, two strain ratios (\( R_\varepsilon = \frac{\varepsilon_{\text{min}}}{\varepsilon_{\text{max}}} \)) are selected. The first is fully-reversed cyclic loading (\( R_\varepsilon = -1 \)) is chosen following previous work with the CPFE models focusing on fully-reversed cyclic loading, and the second is a positive strain ratio loading (\( R_\varepsilon = 0.1 \)), chosen to approximate real world loading conditions.
3.2.3 Design of experiments

Based on the microstructure and mechanical loading conditions outlined above, the full-factorial design of experiments consists of 72 configurations. Due to the statistically rare nature of fatigue crack formation, a large number of SVE ensembles is desirable to capture an unbiased statistical representation of the features of interest of the microstructure regarding the response of interest. For this work, an ensemble of SVE instantiations was defined as 200 instantiations. This results in each configuration’s ensemble modeling roughly 600,000 grains. To facilitate comparison between the two strain ratios of interest, SVE ensembles were generated for 36 of the configurations, a total of 7,200 SVE instantiations. These same ensembles were cyclically loaded in ABAQUS CPFEM for both the $R_\varepsilon = -1$ and $R_\varepsilon = 0.1$ strain ratios, for a total of 14,400 CPFEM simulations. Using parallel processing and the PACE high performance computing cluster at Georgia Institute of Technology [150], completing the 7,200 $R_\varepsilon = -1$ simulations took roughly four months, and the 7,200
\( R_e = 0.1 \) took a month, due to the much smaller strain amplitude for the positive strain ratio simulations.

### 3.3 Crystal plasticity finite element modeling

The current version of the CPFEM model was implemented in an ABAQUS user subroutine material model, most recently for rank-ordering fully lamellar Ti-6Al-4V [90, 103]. The microstructure morphology of fully lamellar Ti-6Al-4V is substantially different than equiaxed bimodal Ti-6Al-4V, which is the material of focus in this project. Lamellar grains within Ti-6Al-4V are formed when the previous \( \beta \)-grains follow a processing route that nucleates secondary-\( \alpha \) lathes within these grains. Due to the length scale difference between these lathes and the grain sizes typically being several orders of magnitude, the lathes are not explicitly modeled in the CPFEM framework, and these lamellar grains are hereafter referred to as colony grains, in reference to the homogenization scheme [33].

#### 3.3.1 CPFEM model

The first task of adapting the CPFEM constitutive relations to duplex bimodal Ti-6Al-4V was incorporating grain size effects of the primary \( \alpha \) grains. To do so, the drag stress was calibrated to the experimental macroscale cyclic stress-strain data, and the pipeline was adapted to pass in the grain size of each \( \alpha \) grain in the SVE instantiation. By computing the threshold stress using the grain size as the mean free slip distance \( d \) in 2.15 for primary \( \alpha \) grains, the yield strength now exhibits grain size effects, Figure 3.8. This means each primary \( \alpha \) grain has a different threshold.

For the colony grains, the mean free slip distance is set to 5 µm, since the lathes break up the free slip distance of a colony grain, and due to the model displaying too strong of sensitivity for slip distances substantially below 2 µm. From the SEM data, the lamellae are closer to 2 µm in width, but 5 µm is deemed a reasonable compromise.
3.3.2 CPFEM model calibration

Model calibration was performed twice. One set of model calibration data were provided by AFRL and the second were taken from work done for Boeing, Ref. [90, 103]. AFRL provided monotonic and cyclic stress-strain results ($R_\varepsilon = -1$ and $R_\varepsilon = 0.1$) in addition to the EBSD and SEM data described above. The fully-reversed ($R_\varepsilon = -1$) cyclic simulations were run in ABAQUS with the model parameters from Smith and coworkers [90, 103], referred to below as Set 1. The $R_\varepsilon = 0.1$ cyclic simulations were run using Set 2 elastic constants. All of the remaining model parameters were held the same, as listed in Table 3.2. The primary difference between the two parameter sets are the elastic constants shown in Table 3.3. These parameter sets were calibrated for room temperature and a quasi-static strain rate of $0.0005 \text{ s}^{-1}$.

Calibrated cyclic stress-strain curves fit to experimental data are shown below for the
Table 3.2: Model parameters held constant for both model parameter sets.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{basal}^{0}$</td>
<td>340 MPa</td>
<td>$h$</td>
<td>8000 MPa</td>
</tr>
<tr>
<td>$D_{prism}^{0}$</td>
<td>365 MPa</td>
<td>$h_D$</td>
<td>8000 MPa</td>
</tr>
<tr>
<td>$D_{pyr}^{\langle a \rangle}^{0}$</td>
<td>450 MPa</td>
<td>$d_{colony}$</td>
<td>5 µm</td>
</tr>
<tr>
<td>$D_{pyr}^{\langle a+c \rangle}^{0}$</td>
<td>550 MPa</td>
<td>$\mu$</td>
<td>2</td>
</tr>
<tr>
<td>$(\kappa_n^0)_{t=0}$</td>
<td>40 MPa</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.3: Difference in elastic constants for the two model parameter sets at room temperature.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Set 1 (for $R_e = -1$)</th>
<th>Set 2 (for $R_e = 0.1$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>172.8 GPa</td>
<td>165.8 GPa</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>97.9 GPa</td>
<td>93.6 GPa</td>
</tr>
<tr>
<td>$C_{13}$</td>
<td>73.4 GPa</td>
<td>70.2 GPa</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>192.2 GPa</td>
<td>183.9 GPa</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>49.7 GPa</td>
<td>47.5 GPa</td>
</tr>
</tbody>
</table>

AB AQUS user material subroutine for both sets of model parameters, Figure 3.9 and Figure 3.10. The calibration for model parameter set 1 shows good agreement with experimental data, with full experimental details available in Ref. [103]. The calibration for model parameter set 2 shows some discrepancies between experimental data and calibration. The yield strength and Young’s modulus were the primary calibration foci for model parameter set 2, as the constitutive flow rule and evolution equations as chosen were selected to capture material hardening behavior, unlike the near elastic-plastic transition shown by the experimental data. Additionally, there is a mismatch between strain values, as there was some residual strain in the sample due to previous cyclic loading at a lower nominal peak strain, so the residual strain was subtracted from the strain data from cyclic loading to 1.0% strain. The residual strain may also have impacted the elastic-plastic transition.

Simulated polycrystalline uniaxial stress-strain curves for each of the microstructures in Table 3.1 are shown below, monotonic results in Figure 3.11 and Figure 3.12, and cyclic results in Figure 3.13 and Figure 3.14. It is noted that, while the two model parameter sets
Figure 3.9: Calibrated polycrystalline uniaxial cyclic stress-strain curves using model parameter set 1 ($R_e = -1.0$), simulated microstructure SVE instantiation contains \(~300\) grains.
Figure 3.10: Calibrated polycrystalline uniaxial cyclic stress-strain curves using model parameter set 2 ($R_e = 0.1$), simulated microstructure SVE instantiation contains ~300 grains.
differ, the Young’s modulus and yield strengths differ very little and would be well within experimental variability, allowing for direct comparison between the two model parameter sets.

![Model parameter set 1](image)

Figure 3.11: Simulated polycrystalline uniaxial monotonic stress-strain curves using model parameter set 1, simulated microstructure SVE instantiations each contain ~300 grains.

Model set 1 parameters were calibrated to 0.2% cyclic yield stress of 955 MPa and a Young’s modulus of 122 GPa. Model set 2 parameters were calibrated to 0.2% cyclic yield stress of 930 MPa and a Young’s modulus of 116 GPa. Young’s modulus values between the two parameter sets are within 1% of experimental values for texture T3, 5% for T2, and 10% for T1, Table 3.4. There is small variation of yield strength and Young’s modulus within each texture, and therefore comparison can be made directly between the fully-reversed and positive strain ratio results. Monotonic results are shown up to 1% strain, as the parameter sets were calibrated to cyclic data at 1% nominal peak strain.
Figure 3.12: Simulated polycrystalline uniaxial monotonic stress-strain curves using model parameter set 2, simulated microstructure SVE instantiations each contain ~300 grains.

Table 3.4: Young’s modulus from monotonic CPFEM loading for set 1 and set 2 parameters.

<table>
<thead>
<tr>
<th>Micro.</th>
<th>Young’s modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Set 1</td>
</tr>
<tr>
<td>T1 2x 30</td>
<td>131.7</td>
</tr>
<tr>
<td>T1 2x 60</td>
<td>131.5</td>
</tr>
<tr>
<td>T1 3x 30</td>
<td>131.2</td>
</tr>
<tr>
<td>T1 3x 60</td>
<td>130.7</td>
</tr>
<tr>
<td>T2 2x 30</td>
<td>124.8</td>
</tr>
<tr>
<td>T2 2x 60</td>
<td>123.7</td>
</tr>
<tr>
<td>T2 3x 30</td>
<td>127.0</td>
</tr>
<tr>
<td>T2 3x 60</td>
<td>126.6</td>
</tr>
<tr>
<td>T3 2x 30</td>
<td>122.3</td>
</tr>
<tr>
<td>T3 2x 60</td>
<td>122.8</td>
</tr>
<tr>
<td>T3 3x 30</td>
<td>120.5</td>
</tr>
<tr>
<td>T3 3x 60</td>
<td>120.1</td>
</tr>
</tbody>
</table>
Figure 3.13: Simulated polycrystalline uniaxial cyclic stress-strain curves using model parameter set 1, simulated microstructure SVE instantiations each contain ~300 grains.
Figure 3.14: Simulated polycrystalline uniaxial cyclic stress-strain curves using model parameter set 2, simulated microstructure SVE instantiations each contain \( \sim 300 \) grains.
3.4 Statistical microstructure distributions

As in prior works [40–43, 90, 101, 103], a substantial number of SVEs is employed to estimate the probability distribution of extreme value FIPs in large SVE ensembles of grains. To instantiate the SVEs for the CPFEM simulations, Dream.3D is used due to its open source nature and large suite of tools for digitally reconstructing various microstructures [23]. Dream.3D has been utilized to capture the statistical distributions of interest in its generated microstructure instantiations, including grain size, grain orientation, misorientation, and volume fraction for titanium alloys [68, 69]. Volume fraction is entered into DREAM.3D for each phase as a discrete value.

A dataset of duplex bimodal Ti-6Al-4V EBSD data was provided by AFRL, and grain sizes were obtained. From the EBSD dataset, 2D equivalent sphere diameters were converted to 3D average grain size (assuming spherical grains) using the transfer function technique outlined by Gerlt et al. [151]. The average grain size will be kept constant at 10.9 µm, and the maximum value of the grain size distribution is set to either two or three times the average grain size (21.8 µm or 32.7 µm), to investigate the effect of maximum vs. average grain size on FIP response. Two volume fractions are selected to encompass the range of bimodal Ti-6Al-4V: 60% primary α grains and 40% α + β colony grains; and 30% primary α grains and 70% α + β colony grains.

Simulated microstructures for the 12 configurations considered in this project are generated using DREAM.3D [23] using a pipeline consisting of the StatsGenerator and Write DREAM.3D Data File filters. In StatsGenerator, the user first adds a primary phase, designating the appropriate crystallographic symmetry and volume fraction, which is then generated. Here, the primary phase is the HCP primary α phase, with a volume fraction of either 30% or 60%. More phases can be added with their respective crystal structure and phase fraction, and are added either as another primary phase, or a precipitate or matrix phase type. The colony grains for Ti-6Al-4V are added as a hexagonal primary phase.
with phase fraction of 70% or 40%. Once the required number of phases are generated, the user moves to entering the grain size distribution of each phase in Equivalent Sphere Diameter (ESD), which is in a log-normal distribution where the average feature ESD and standard deviation is input in μm. Here, the average feature ESD is 10.9 μm with a standard deviation of 3.7 μm as computed from EBSD measurements. Then the maximum and minimum grain size cut offs are entered, and the bin step size of the distribution is adjusted to ensure a reasonable number of bins. For this dataset, the minimum cut off was set to twice the standard deviation, resulting in lower limit of 5.5 μm, and a maximum cut off of 2.04 times the standard deviation for a maximum of 21.8 μm for the 2x grain size ratio, a maximum cut off of 3.232 times the standard deviation for a maximum of 32.7 μm for the 3x grain size ratio. Grain size is entered as the average and standard deviation values for a log-normal distribution for each phase of the microstructure, limiting its ability to fully capture the tail, or extreme, behavior of the distribution. This is a sizable concern with respect to Ti-6Al-4V, as outlying large primary α grains have the largest available mean free slip distance. Both phases were set to the preset statistic model of primary equiaxed.

Next, the orientation distribution functions were defined for both phases. Grain angles and weights were loaded from experimental data and input by Euler angles, weight, and spread. Once the statistical representation of the microstructure is complete, the data is saved in a .dream3d file format.

Orientation distribution functions can be imported directly from EBSD data or approximated by entering a range of Euler angles and weights. The average and standard deviations of 10.9 μm and 3.7 μm are input into DREAM.3D, with the maximum values cut off at either 21.8 μm (2x) or 32.7 μm (3x), Figures 3.15 and 3.16.

Once the microstructure statistics are written into the .dream3d file container, a Python pipeline developed by Kern [152] to batch generate the ensembles of SVE instantiations, apply meshing and boundary conditions, upload to Georgia Tech’s PACE computing cluster, run ABAQUS simulations and download post-processing files is utilized. The pipeline
Figure 3.15: DREAM.3D input for 2x maximum grain size.

Figure 3.16: DREAM.3D input for 3x maximum grain size.
is summarized in Figure 3.17. The user input parameters consist of setting the loading direction(s), stress or strain amplitude, strain rate, overload (if relevant), stress or strain ratio, and number of loading cycles. The number of SVE instantiations is also defined, along with SVE size and number of elements per SVE side. The ABAQUS mesh type is defined as either voxel or tetrahedral, and the desired ABAQUS version is entered, along with the initial, minimum and maximum step sizes, which must be selected to ensure convergence of the CPFEM model.

Figure 3.17: Schematic of Python pipeline for generating microstructure instantiations and running CPFEM simulations via ABAQUS.

The microstructure.py step reads the Dream.3D statistics container, where the grain locations for each phase are generated and the subsequent phase and orientation (in Bunge-
Euler angles) are stored with the location data. Resampling is performed to reduce data density and to voxelate the instantiation. Then, the `meshing.py` step transitions the voxelated microstructure to a mesh as required by FEM. A voxelated mesh can be defined directly from the voxelated microstructure representation and SVE instantiation size information. The user directly inputs the size (defined in mm per side) and shape (number of mesh elements per side) of a cubic SVE instantiation. An ABAQUS C3D8R reduced integration element is then overlaid on each voxel.

Next, the `simulation.py` step executes the FEM simulations after the generated microstructure has been suitably meshed. A loading file is generated which contains the applied loading steps and boundary conditions, as well as specifying the output requests. Here, displacement controlled loading is used under periodic boundary conditions, and the displacement loadings are applied to the outermost nodes of the mesh, as shown by V000, V001, V010, V011, V101, V110, and V111 in Figure 3.18. The origin node, V000, has 0 displacement and V001, V010, V100 have 0 displacement out of axis to eliminate rigid body modes. The boundary conditions are defined using additional node sets for the opposing face and edges and are labeled following Ref. [101]. The pipeline supports periodic, free and flat boundary conditions. Here, periodic boundary conditions are set to enforce equal displacements across opposing faces using the ABAQUS boundary conditions standard of zero-valued linear systems of equations. This ensures the displacements are periodic as the deformed volume is tessellated in the chosen loading direction.

Lastly, the `post_process.py` module allows users to define the desired outputs from the CPFEM simulations. In this case, the stress and strain values at the peak minimum and maximum strains in a loading cycle are output for every C3D8R element node. The four above modules are wrapped by `pipeline.py` which executes the entire pipeline for each SVE instantiation as defined by the user.

The maximum to minimum applied strain ratio, or \( R_\varepsilon \)-value of the simulated loading conditions will be \( R_\varepsilon = -1 \), or fully reversed loading, and \( R_\varepsilon = 0.1 \). It is expected that com-
Figure 3.18: Node sets used for defining boundary conditions and applied loads.
paring the effect of both negative and positive strain ratios will help predict the degree of normalization between the two FIPs of interest, as the grain boundary impingement FIP is expected to have a higher likelihood of maximal FIP values as the strain ratio increases. Three orientation distribution functions are prescribed: T1, taken from HCF program experiments from AFRL and used for both primary α and colonies; T2, consisting of Ti-6Al-4V basal and transverse rolling texture for primary α, with a simulated rolling texture for colonies provided by AFRL; and T3, consisting of Ti7Al strong transverse α for primary α, with a simulated rolling texture for colonies provided by AFRL.

3.5 Fatigue Indicator Parameters subgrain volume averaging

For each SVE instantiation, the local FIP<sub>FS</sub> is computed for every mesh integration point in the ABAQUS C3D8R (reduced integration) mesh in post-processing. Previous volume averaging studies for the FIP<sub>FS</sub> by McDowell and coworkers [90–92] have used grain volume, Gaussian kernels, cubic volumes, and approximate slip band averaging. The type of banding used here for the Fatemi-Socie FIP is referred to as stacked or layered banding, which divides the elements within a grain along bands parallel to the slip planes of the grain with respect to the loading direction. Band averaging was introduced to be consistent with the physical mechanisms of irreversible slip in representing the fatigue damage process zone. The band averaging volume approach has been shown to be a good compromise between mesh sensitivity effects of element level averaging versus grain level averaging, as the latter does not capture the variation of FIP<sub>FS</sub> values within a grain on a given slip band. Notably, Castelluccio and McDowell [91] found that the orientations of 2<sup>nd</sup>-nearest neighbor grains affect the variability of maximum stacked band-averaged FIP<sub>FS</sub> values by a factor of 2 to 3, and nearest neighbor orientation by about 30%.

For the FIP<sub>FS</sub>, each grain is banded along the basal plane and three prismatic planes following Ref. [93, 124]. Pyramidal and BCC planes were not utilized as fatigue crack formation is primarily expected to form on ‘soft’-oriented basal planes. Bands must be
greater than one element wide, so that there are no gaps between band elements. Grains are banded starting from the grain centroid and extending out in layers to the grain boundaries. If a given banding width leaves any layers with less than five elements, that layer is added to the next layer, again to ensure continuity. A mesh convergence study of the banded FIP\textsubscript{FS} was performed, and a band width of 4 \( \mu \text{m} \) was selected as the appropriate band width, giving about three bands per grain. Given these results and the crystallographic dependence of fatigue crack formation and early growth in Ti-6Al-4V, layered band-averaged FIP\textsubscript{FS} are well-suited to elucidate correlations to local slip behavior.

To capture the underlying physical mechanisms that drive dislocation pileup on a grain boundary, for the FIP\textsubscript{GBI}, first, the elements in the grain are banded along the basal plane. The elements in each basal plane band that intersect with grain boundary elements are found, and the band with the highest number of intersecting elements then has the strain of those basal band elements averaged for the net plastic strain on the grain boundary of interest. Then, the stress normal to the grain boundary is averaged over the elements located on that grain boundary. The band of elements is 4 \( \mu \text{m} \) wide, again to ensure continuity of the band. Mesh elements on the grain boundary that share a boundary with only two grains are included in the stress averaging, since the CPFE model does not explicitly incorporate triple point junctions. There is also a minimum number of elements for the stress averaging. A study was done to determine the minimum number of elements on the grain boundary; a minimum of five elements is required. If there are less than five elements that border only two grains on a grain boundary, the FIP\textsubscript{GBI} value associated with that specific grain boundary is taken to be zero. Once these conditions are satisfied, the FIP\textsubscript{GBI} is then calculated from the band averaged element strain values, and grain boundary element stress values. This averaging approach differs from the FIP\textsubscript{FS}, which computes the integration point FIP\textsubscript{FS} values before volume averaging, whereas the FIP\textsubscript{GBI} is computed after averaging over the respective volumes for plastic strain and stress.
3.6 Mesh convergence studies

A critical concern of using this methodology is mitigating any mesh sensitivity effects that may arise from the ABAQUS mesh overlaid on the simulated microstructures. The size of a SVE instantiation is largely determined by the size required to contain a minimum of $\sim 300$ grains to converge to the macroscale stress-strain response of the material. However, there still remains the issue of an appropriate mesh size at several scales. First, the mesh size must converge for the target grain size distribution, as a mesh that is too large may skew the distribution towards larger grains, and a mesh that is too fine may require significantly more computational power. An optimal balance between the two is sought, to have a mesh size just small enough to capture the target grain size distribution with the least use of computational resources. Similarly for the macroscale stress-strain response, the meshing must also be optimized to eliminate mesh sensitivity effects while minimizing computational requirements. Lastly, mesh convergence also has to be studied for each of the FIP responses, specifically with regards to the tail behavior of the FIP distributions. Essentially, mesh size has to be investigated at each scale of the study in order to maintain a balance between incorporating as much of the underlying physics as possible with reducing the computational load that arises from higher density meshes. It is always a trade-off between model fidelity and mesh fidelity, but for the specific fatigue responses studied here, the plastic deformation zone of fatigue crack formation occurs within an averaged subgrain volume. This is important to identify the size and number of SVE instantiations in an ensemble that can be used to compare EVDs of FIPs among various microstructures. Increasing mesh fidelity by increasing density is less important that balancing the computational cost, since the response of interest is essentially ’smeared’ over the averaging voxels.
3.6.1 Grain size study

The previously identified requirements of determining SVE size are as follows: it should contain over 300 grains to approximate the macroscale stress-strain response, with a minimum of 5 grains per edge. Further, for the selected FIPs, 2\textsuperscript{nd} nearest neighbor grains should be included to capture higher order effects of fatigue response. Given this set of conditions and an average grain size of 11 \( \mu m \), a SVE size of 75 \( \mu m \) per side (421,875 \( \mu m^3 \)) was selected, ensuring at least 6 grains per edge of the SVE instantiation, and an average of over 300 grains per cubic volume. This size also ensures 2\textsuperscript{nd} nearest neighbor grains for at least the average grain size. To study what size the mesh voxels should be, three different sizes were selected, 29, 33, or 37 elements per SVE side. The odd numbers are selected with future spatial correlation work in mind, as the 2-point correlations work best with an odd number of discretized elements. Given that two maximum grain sizes are investigated, the mesh convergence has to satisfy both conditions. First, the Kullback-Leibler Divergence test for grain size distribution was applied to 25 SVE instantiations at each maximum grain size and number of elements per SVE side. As can be seen in Figure 3.19, clear divergence is shown for 29\textsuperscript{3} elements for both maximum grain sizes, while the remaining two grain sizes converge for both mesh sizes. Due to the discretized nature of the KL Divergence test, the divergence values will always be greater than zero. Next, the Kolmogorov-Smirnov distance test was applied to the same 25 SVE instantiations for grain size distributions, Figure 3.20. This time, there is strong convergence for 29\textsuperscript{3} elements and 33\textsuperscript{3} elements, and less convergence for 37\textsuperscript{3} elements. Similar to the KL test, the KS distance will also always be greater than zero. Given these two tests, it appears a mesh size of 33\textsuperscript{3} elements is sufficient to capture the grain size distribution as described by the target log-normal distribution. The target and actual grain sizes are shown below in Figure 3.21, and show good agreement between the two. However, given that the maximum grain size is a concern for fatigue crack formation, the right hand tail of the grain size is more critical to capture than the average parts of the distribution. The same data presented above was plotted in a cumulative distri-
Figure 3.19: KL Divergence study for SVE mesh size with respect to maximum grain size.

Figure 3.20: KS Distance study for SVE mesh size with respect to maximum grain size.
Figure 3.21: Probability distribution function of log-normal target and actual SVE grain size distributions for 2x maximum grain size.

This function was used to prove that this distribution adequately captures the largest grain sizes as well as the average grain sizes, Figure 3.22.
Figure 3.22: Cumulative distribution function of log-normal target and actual SVE grain size distributions for 2x maximum grain size.

3.6.2 Polycrystalline stress-strain study

Next, for mesh convergence to the homogenized polycrystalline stress-strain response of the material, the same element options were investigated. 25 SVE instantiations of microstructure T1 2x 30 were generated for each element size option, and CPFEM simulations run for 3 cycles of fully-reversed cyclic loading at the calibration strain amplitude of 1.0% strain, Figure 3.23 below. From this figure, it’s clear that any size above $29^3$ elements is sufficient to converge on the cyclic uniaxial stress-strain response of Ti-6Al-4V.
Figure 3.23: Meshing convergence study to polycrystalline fully-reversed cyclic stress-strain at 1.0% peak strain.

3.6.3 Extreme value Fatigue Indicator parameters study

Lastly, the fatigue response must also show mesh insensitivity, especially as both FIPs are averaged over subgrain volumes. Both FIP\textsubscript{FS} and FIP\textsubscript{GBI} values were computed for the simulations run in the above section, as well as a 41\textsuperscript{3} element option. These distributions were then plotted on a log-normal scale due to the majority small values of FIPs expected for non-fatigue hot-spots, Figures 3.24 and 3.25. Once again, for FIPs, the primary concern is the right hand tail behavior of such a distribution, and convergence around the average is far less critical than convergence at the extreme. These same plots were adjust to the 90\% CDF to show convergence at the tail. For the FIP\textsubscript{FS} distributions all mesh sizes converge well for the tail, extreme values, but for FIP\textsubscript{GBI}, the 29\textsuperscript{3} elements does not appear to converge. In summary, for the conditions outlined above for selecting an appropriate mesh size at each length scale of simulation, 33\textsuperscript{3} elements represents the best compromise between
Figure 3.24: Cumulative distribution function of FIP_{FS} values for SVE mesh size options.

Figure 3.25: Cumulative distribution function of FIP_{GBI} values for SVE mesh size options.
Figure 3.26: 90% tails of cumulative distribution function of $FIP_{FS}$ values for SVE mesh size options.

Figure 3.27: 90% tails cumulative distribution function of $FIP_{GBI}$ values for SVE mesh size options.
model fidelity and computational resources, Table 3.5.

Table 3.5: Results of mesh convergence studies.

<table>
<thead>
<tr>
<th>Mesh study</th>
<th># of mesh elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain size</td>
<td>$33^3$</td>
</tr>
<tr>
<td>CPFEM</td>
<td>$29^3$</td>
</tr>
<tr>
<td>FIP$_{FS}$</td>
<td>$29^3$</td>
</tr>
<tr>
<td>FIP$_{GBI}$</td>
<td>$33^3$</td>
</tr>
<tr>
<td>Conclusion</td>
<td>$33^3$</td>
</tr>
</tbody>
</table>

3.7 Summary

A statistically-based methodology for investigating microstructure-property relationships of fatigue for large computational datasets is presented in this chapter. The design of experiments was selected to cover a range of microstructure attributes and loading conditions used in common applications of Ti-6Al-4V. This represents the first such attempt at such a large DOE for a computational study for any material, which has only been made possible recently due to advances in high-performance computing resources and the advent of programmatic workflows for handling such large datasets. Next, the adaptations made to the CPFE model are presented, primarily the adaptation to ensure that the model captures grain size effects on the yield strength of bimodal Ti-6Al-4V. The model was calibrated using an auto-calibration tool developed by Tallman [153] for two sets of parameters for the two experimental data sets obtained. The microstructure statistics of interest, e.g., grain size distribution, texture, misorientation, etc., must be captured by whichever method is used to generate simulated microstructure instantiations. The volume averaging of both FIP$_{FS}$ and FIP$_{GBI}$ is discussed to best capture the local deformation zone of each of those transgranular deformation mechanisms within a grain. Lastly, mesh convergence studies are done for each step of this process, to ensure that any mesh effects are mitigated, and the statistics all converge to their respective values.
CHAPTER 4
RELATIVE MICROSTRUCTURE RANKING FOR FATIGUE RESPONSE

4.1 Introduction

High Cycle Fatigue (HCF) behavior of metallic systems is linked to the stochastic, heterogeneous nature of hot spots associated with high local driving forces for fatigue crack formation. Under HCF loading conditions, these hot spots exhibit strong spatial heterogeneity and rare event character over significant volumes, which necessitate the use of extreme value statistics. The probability distribution of these high local Fatigue Indicator Parameters (FIPs) is affected both by microstructure attributes and loading conditions. The rare event nature of HCF results in a significant scatter of the overall fatigue life for a material for a set of specimens [154]. Thus, rank-ordering the FIP distributions for different microstructures in terms of relative fatigue resistance must address this variability.

Transition and low cycle fatigue (LCF) regimes in metallic systems are characterized by increasingly homogeneous plastic deformation throughout the bulk material, as compared to high cycle fatigue (HCF) [26]. In this transition fatigue regime of practical importance to applications, the probability of fatigue crack formation is highly sensitive to local microstructure environments that promote enhanced cyclic plastic strain, necessitating the use of extreme value theory to capture the tails of probability distributions of the driving force to form fatigue cracks. As in high cycle fatigue (HCF), combinations of microstructure attributes contribute to the high driving forces for fatigue crack formation at these local fatigue hot-spots that are correlated with these extreme value probabilities.

Microstructure-property relationships that probabilistically assess driving forces for fatigue crack formation for engineering alloys in the HCF and VHCF regimes can provide decision support for the selection of processing routes that improve fatigue resistance. Ti
alloys commonly used in aerospace applications exhibit substantial scatter in fatigue life and have a wide range of accessible microstructures based on thermomechanical process path. This variability in fatigue response presents a challenge to reliable life prediction for Ti components. Early computational works on local fatigue processes in polycrystals appeared some 40 years ago [52, 155–157]. Microstructure-sensitive computational approaches can reduce the burden on costly and time-consuming experimental studies by augmenting with Fatigue Indicator Parameters (FIPs) from simulations. These FIPs can then be used to construct probability distributions to enable comparisons of likelihood to form fatigue cracks among microstructure morphologies and inform the probability of occurrence of a life-limiting fatigue failure within a given volume of material. Further exploration of the microstructure in the vicinity of these highest FIP values (i.e., “hot spots”) can provide insight to complement understanding gained from cost-limited experimental observations regarding characteristic neighborhoods of microstructure attributes that relate most closely to fatigue crack formation and early growth.

In this chapter, the effects of phase volume fraction and texture on the VHCF, HCF and LCF regimes were studied for $\alpha + \beta$ Ti-6Al-4V by utilizing mesoscale FIPs that capture two primary mechanisms that drive localized plasticity and related modes of transgranular crack formation. A crystal plasticity finite element model (CPFEM) was used to simulate the polycrystalline response to cyclic fatigue loading via a user-defined material subroutine in ABAQUS [24]. Ensembles of statistical volume element (SVE) microstructure instantiations were generated using DREAM.3D [23]. Consistent with experimental measurements, crystal orientation and distribution of each phase, phase volume fraction, grain size, and synthetic orientation distribution functions were input to DREAM.3D [90, 103]. FIPs were calculated from CPFEM results, and the extreme values were determined using the peaks-over-threshold (POT) extreme value (EV) approach; these values were then fit to the Generalized Pareto Distribution (GPD) to enable rank-ordering of microstructures in terms of resistance to form fatigue cracks for each failure mode under different loading condi-
tions. Lastly, FIP distributions were characterized by the phase of grains/grain boundaries where extreme values occur, and EV FIP grains were compared in terms of orientation, phase, FIP value, and grain size.

4.2 Fatigue regimes of Ti-6Al-4V

Fatigue is a complex, multiscale, hierarchical process influenced by a range of microstructure attributes that contribute to fatigue crack formation and subsequent growth through various stages that depend on the ratio of crack size to characteristic microstructure sizes and applied loading conditions. The early stages of fatigue crack formation and growth past the first grain/phase boundary encountered [89]. Elucidating the influence of microstructure on fatigue crack formation and early growth within the nucleant grain/phase is particularly challenging for Ti-6Al-4V, given the highly anisotropic material deformation response of Ti-6Al-4V and low crystallographic symmetry of the HCP structure of the α-phase.

Transgranular slip bands have been shown to form cracks in primary α grains with favorably ‘soft’ oriented basal planes under reversed cyclic loading [57–61, 158]. This mechanism is typically favored when the c-axis of the grain is relatively well aligned with the loading direction, resulting in high normal stress acting on basal planes that experience significant cyclic slip as shown experimentally [159–161]. Dislocation pileup is more commonly associated with positive strain ratios, as an active dislocation source emits multiple dislocations that impinge on a grain boundary when the strain ratio is not reversed sufficiently to allow the dislocation to release back towards the source [70, 97, 162]. For Ti-6Al-4V, this commonly happens between neighboring hard-soft grain pairs, where increased plastic deformation of the soft grain leads to stress redistribution onto the adjacent hard grain [96, 163].

In the transition and LCF regimes, plastic deformation is much more widely and uniformly distributed through the microstructure than in HCF, where the bulk material response is primarily elastic with only preferably oriented ‘soft’ grains experiencing signif-
icant localized plastic deformation. As the applied strain increases, interaction effects between grains undergoing localized plastic deformation increases and become more critical to understanding fatigue crack initiation. At strains high enough to induce LCF response in Ti-6Al-4V, nearly all grains in the sample or volume element experience plastic deformation.

4.3 Ti-6Al-4V microstructure and digital reconstruction

A total of 12 duplex bimodal Ti-6Al-4V microstructures are modeled in this effort. SEM micrographs and EBSD angle measurements were provided by AFRL to inform microstructure selection and reconstruction [147]. Three textures were selected: texture one (T1), making use of EBSD measurements for primary $\alpha$ and colony grains; texture 2 (T2), using basal/transverse Ti-6Al-4V data for primary $\alpha$ grains with rolled texture for colony grains; and texture 3 (T3), using strong transverse Ti7Al texture for primary $\alpha$ grains with rolled texture for colony grains. The average grain size was held constant at 10.9 µm for a log-normal distribution with a standard deviation of 3.7 µm. The maximum grain size allowed was either 21.8 µm (twice average grain size) or 32.7 µm (three times average grain size) within that log-normal distribution. Two volume fractions, representing the extremes considered to be bimodal, were considered, 30% volume fraction primary $\alpha$/70% colony grains or 60% volume fraction primary $\alpha$/40% colony grains. The simulated microstructures are summarized in Table 4.1 and pole figures for textures are shown in Table 4.2.

For the mechanical loading conditions, all simulations are conducted under uniaxial strain-controlled cycle for 3 cycles, loading to a peak nominal strain of either 0.4%, 0.8% or 1.2% strain at a strain rate of $5 \times 10^{-4} \text{ s}^{-1}$ at room temperature, at strain ratios ($R_\varepsilon = \varepsilon_{\min} / \varepsilon_{\max}$) of $R_\varepsilon = -1$ and $R_\varepsilon = 0.1$. All SVEs have fully periodic boundary conditions, simulating the bulk subsurface material, and are loaded in the 33- or z- direction, corresponding to the normal direction of the material (with regard to the pole figures for texture), with zero net traction acting on faces normal to the other two directions. FIPs are computed using
Table 4.1: Simulated microstructures for duplex bimodal Ti-6Al-4V.

<table>
<thead>
<tr>
<th>Micro.</th>
<th>Grain size (µm)</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Avg. Std. Dev.</td>
<td>Max. α% colony %</td>
</tr>
<tr>
<td>T1 2x 30</td>
<td>10.9 3.7</td>
<td>21.8 30 70</td>
</tr>
<tr>
<td>T1 2x 60</td>
<td>10.9 3.7</td>
<td>21.8 60 40</td>
</tr>
<tr>
<td>T1 3x 30</td>
<td>10.9 3.7</td>
<td>32.7 30 70</td>
</tr>
<tr>
<td>T1 3x 60</td>
<td>10.9 3.7</td>
<td>32.7 60 40</td>
</tr>
<tr>
<td>T2 2x 30</td>
<td>10.9 3.7</td>
<td>21.8 30 70</td>
</tr>
<tr>
<td>T2 2x 60</td>
<td>10.9 3.7</td>
<td>21.8 60 40</td>
</tr>
<tr>
<td>T2 3x 30</td>
<td>10.9 3.7</td>
<td>32.7 30 70</td>
</tr>
<tr>
<td>T2 3x 60</td>
<td>10.9 3.7</td>
<td>32.7 60 40</td>
</tr>
<tr>
<td>T3 2x 30</td>
<td>10.9 3.7</td>
<td>21.8 30 70</td>
</tr>
<tr>
<td>T3 2x 60</td>
<td>10.9 3.7</td>
<td>21.8 60 40</td>
</tr>
<tr>
<td>T3 3x 30</td>
<td>10.9 3.7</td>
<td>32.7 30 70</td>
</tr>
<tr>
<td>T3 3x 60</td>
<td>10.9 3.7</td>
<td>32.7 60 40</td>
</tr>
</tbody>
</table>

Table 4.2: Simulated (0001) pole figures generated for DREAM.3D SVE instantiations.

<table>
<thead>
<tr>
<th>Phase</th>
<th>T1</th>
<th>T2</th>
<th>T3</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>colony</td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
</tbody>
</table>
simulation results over the 3rd cycle of loading. For the $\alpha$-phase slip systems, the initial threshold stress values vary from 127-221 MPa for the maximum grain size of 21.8 µm, and 111-221 MPa for 32.7 µm. The colony phase threshold stress values are either 221 MPa for most slip systems, with a value of 276 MPa for the basal and prismatic slip systems parallel to the laths of the colony.

4.4 Fatigue Indicator Parameters

FIPs have previously been introduced to serve as a measure of surrogate driving force for fatigue crack formation and early growth, to link the mesoscale plastic damage zone to the macroscale material deformation. FIP selection is based on the relevant damage mechanisms of a material, and can be computed from stress-, strain- or energy-based criterion. In this work, the Fatemi-Socie FIP ($\text{FIP}_{FS}$) is selected to capture the transgranular slip band formation mechanism; it is computed using the plastic shear strain range on a slip band and the peak stress during a cycle normal to that band [71]. A related FIP proposed by McDowell [22], the grain boundary impingement FIP ($\text{FIP}_{GBI}$), is chosen to capture the dislocation impingement on grain boundaries that results from positive strain ratio loading and is computed from the net plastic strain on a grain boundary and the stress normal to that grain boundary. The volume averaging scheme used in this work first computes the $\text{FIP}_{FS}$ for each ABAQUS mesh element, following which, each grain is banded along the three basal planes and the prismatic plane. The computed $\text{FIP}_{FS}$ values are then averaged, with the highest average value from each of the 4 planes taken to be the $\text{FIP}_{FS}$ for the grain. As for $\text{FIP}_{FS}$, volume averaging is performed as for $\text{FIP}_{GBI}$, but the averaging approach differs. The macroscale yield strength is taken to be 930 MPa from experimental data, and $k$ and $k_{net}$ were taken to be 0.5, though it should be noted that these material parameters can take on distinct values for the respective FIPs.

The Fatemi-Socie and grain boundary impingement FIPs are computed from crystal plasticity finite element modeling (CPFEM) simulation stress-strain results. Full details on
the CPFEM model are outlined in Chapter 3. $\text{FIP}_{FS}$ is computed for each C3D8R voxel in the meshed microstructure, and then those values are averaged over 4 µm wide subgrain band volumes corresponding to the basal and prismatic planes of HCP Ti-6Al-4V [92, 149]. The highest $\text{FIP}_{FS}$ value out of the four slip planes is assumed to be the slip plane experiencing the largest amount of plastic deformation, and only one maximum $\text{FIP}_{FS}$ value from the subgrain band volumes is considered in the extreme value FIP distribution, since it is assumed that a crack would form on the slip band within a grain that has the maximum $\text{FIP}_{FS}$ value. $\text{FIP}_{GBI}$ is computed differently, first averaging the plastic strain over a 4 µm wide subgrain band along the most active basal slip system of the grain. Then the stress is averaged over the volume elements on the grain boundary, neglecting any elements that border three or more grains, since the CPFEM model does not explicitly capture triple junction behavior [90, 103]. The $\text{FIP}_{GBI}$ value is calculated this way for each grain boundary within each grain over the entire SVE. Here, both FIPs are computed from crystal plasticity finite element modeling (CPFEM) simulation stress-strain results. Full details on the CPFEM model using ABAQUS [24] user material subroutine and parameters are published in Ref. [164]. $\text{FIP}_{FS}$ is computed for each C3D8R voxel in the meshed microstructure, and then those values are averaged over 4 µm wide subgrain band volumes corresponding to the basal and prismatic planes of HCP Ti-6Al-4V [92, 149]. The highest $\text{FIP}_{FS}$ value out of the four slip planes is assumed to be the slip plane experiencing the largest amount of plastic deformation, and only one maximum $\text{FIP}_{FS}$ value from the subgrain band volumes is considered in the extreme value FIP distribution, since it is assumed that a crack would form on the slip band within a grain that has the maximum $\text{FIP}_{FS}$ value. $\text{FIP}_{GBI}$ is computed differently, first averaging the plastic strain over a 4 µm wide subgrain band along the most active basal slip system of the grain. Then the stress is averaged over the volume elements on the grain boundary, neglecting any elements that border three or more grains, since the CPFEM model does not explicitly capture triple junction behavior [90, 103]. The $\text{FIP}_{GBI}$ value is calculated this way for each grain boundary within each grain over the entire SVE.
4.5 Extreme value statistics of Ti-6Al-4V fatigue

4.5.1 Statistical volume elements

For certain bulk material properties, a representative volume element (RVE) of limited dimension may suffice to capture the relevant spatial statistics of microstructure. However, given the statistically rare event nature of fatigue crack formation, such a RVE element is computationally infeasible. An alternative approach was proposed by Kanit et al. [36], using ensembles of statistical volume element (SVE) instantiations, which are a feasible size for computational modeling efforts. Various recent studies have employed this strategy of building up spatial statistics and measures of variability of fatigue resistance based on ensembles of SVEs [40–43, 101]. The SVE size must be suitably larger than the correlation length of dominant spatial heterogeneities that control fatigue variability (e.g., adjacent large grains, favorable orientations, hard-soft grain pairs, etc.), yet small enough to facilitate tractable computation for large numbers of statistical samples, each of which is constructed with nominal RVE level microstructure statistics as targets [40–43, 93, 101, 149]. The number of SVE instantiations necessary in an ensemble must be sufficiently large to facilitate convergence of extreme value distributions of FIPs. In this work, an ensemble of SVE instantiations was defined as containing 200 instantiations per configuration.

SVE ensembles are generated using the open-source program DREAM.3D [23] for microstructure reconstruction, and the resulting SVE instantiations are meshed for ABAQUS. The meshes are then checked for convergence to the target log-normal grain distribution, orientation distribution via inverse pole figures, homogenized stress-strain response, and FIP distributions. A SVE instantiation with a size of 75 µm per side and 33 mesh elements per side was determined to contain approximately 300 grains and exhibit reasonable convergence for the EV FIP GPD, with adequate computational time to facilitate parametric study. Ensembles for each of the 12 microstructures listed in Table 4.1 consist of 200 SVE instantiations. The instantiations are batch-generated using a Python workflow,
then uploaded to the Georgia Tech PACE computing environment [150], simulations run in ABAQUS, and the relevant results files are downloaded for post-processing.

4.5.2 Peaks-over-threshold approach for determining EV FIPs

Due to the statistically inhomogeneous nature of fatigue crack formation under HCF and VHCF conditions, extreme value statistics are necessary to facilitate qualitative comparisons for fatigue resistance of candidate microstructures for low probability of failure design applications. In particular, we focus on compiling extreme value distributions (EVDs) of FIP values. Much of the previous work in characterizing the tail distribution of FIP values has been based on the first theorem of EV theory, the Fisher–Tippett–Gnedenko theorem [85]. This theorem states that the block maxima of a collection of independent and identically distributed random variables converges to one of three EVDs: the Gumbel distribution, the Fréchet distribution, or the Weibull distribution. There are two limitations to this approach when applied to ensemble values of FIPs. First, by selecting only the block maxima value of FIP from each SVE in the ensemble, it is possible that multiple top FIP values occurring at fatigue hot spots located independently in the same SVE instantiation are ignored. The second issue follows this, as then it is possible that when multiple top FIP values do occur in the same SVE instantiation and are ignored, these FIP values are not included in the EVD.

The second theorem of EVT, the Pickands–Balkema–de Haan theorem [165], states that the tail values above an appropriately selected threshold will converge to the generalized Pareto distribution (GPD). This is also referred to as peaks-over-threshold (POT) analysis [165]. The cumulative distribution function (CDF) of the GPD is calculated based on

\[
G_{\xi,\mu,\sigma}(x) = \begin{cases} 
1 & \text{if } \xi \neq 0 \\
1 - \exp\left(-\frac{x-\mu}{\sigma}\right) & \text{if } \xi = 0 
\end{cases}
\]

(4.1)
Here, $\xi$, $\mu$, $\sigma$ are the shape, location, and scale parameters, respectively. The selected threshold serves as the location parameter when calculating the CDF. Donegan and coworkers [166] applied POT analysis to compare the deviation between experimental and simulated grain size distributions and the log-normal distribution, but clarify that POT analysis is a general EV approach and can be applied to any distribution function. The steps for selecting a reasonable threshold were outlined by Ref. [166] and are executed in this work using threshold choice and mean residual life plots for each EVD of ensemble FIP values, instead of grain size distribution. Estimated values of the shape and scale parameters are taken from the threshold choice plots and used to fit the FIP data via the genpareto function of Scipy Stats toolkit [167], which requires a close estimate of shape, location, and scale parameters for accurate fitting. The estimated GPD parameters for each microstructure at the maximum applied strain are provided in Appendix A, as well as the fitted values for comparison. In this work, the POT EV approach is utilized for the first time to investigate fatigue behavior of a material based on FIPs. It addresses the limitations described above, facilitates more robust exploration of the fatigue crack formation mechanisms captured by the selected FIPs, given an appropriately high threshold and a sufficient number of extreme FIP values above the threshold. The block maxima method treats the FIP distribution from each SVE instantiation as separate individual distributions, but with the POT method, all FIPs from the entire ensemble of SVE instantiations are included in the distribution. This aligns better with SVE ensemble sampling methodology, as increasing the number of SVE instantiations in an ensemble increases the convergence to RVE material response provided that correlation lengths beyond the SVE size do not contribute significantly to FIP responses. For brevity, only the $R^2$ fit values are listed in Table 4.3. Though the Gumbel fits are good, there is a clear increase in fit for GPD. This makes the POT characterization of EV FIPs a preferable method for ranking fatigue resistance of Ti-6Al-4V microstructures for ensembles of SVE instantiations.

Given the statistically rare event nature of fatigue crack formation within the bulk mi-
Table 4.3: $R^2$ fit values for Gumbel and GPD EVDs for FIP$_{FS}$ under fully-reversed loading ($R_e = -1$).

<table>
<thead>
<tr>
<th>Micro.</th>
<th>FIP$_{FS}$ $R^2$ values</th>
<th>GPD threshold value ($\mu$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Gumbel</td>
<td>GPD</td>
</tr>
<tr>
<td>T1 2x 30</td>
<td>0.968135</td>
<td>0.997737</td>
</tr>
<tr>
<td>T1 2x 60</td>
<td>0.978103</td>
<td>0.998195</td>
</tr>
<tr>
<td>T1 3x 30</td>
<td>0.950326</td>
<td>0.987870</td>
</tr>
<tr>
<td>T1 3x 60</td>
<td>0.973908</td>
<td>0.995500</td>
</tr>
<tr>
<td>T2 2x 30</td>
<td>0.966574</td>
<td>0.990979</td>
</tr>
<tr>
<td>T2 2x 60</td>
<td>0.977137</td>
<td>0.992722</td>
</tr>
<tr>
<td>T2 3x 30</td>
<td>0.971814</td>
<td>0.996210</td>
</tr>
<tr>
<td>T2 3x 60</td>
<td>0.965969</td>
<td>0.997319</td>
</tr>
<tr>
<td>T3 2x 30</td>
<td>0.956300</td>
<td>0.953066</td>
</tr>
<tr>
<td>T3 2x 60</td>
<td>0.956281</td>
<td>0.998141</td>
</tr>
<tr>
<td>T3 3x 30</td>
<td>0.965815</td>
<td>0.985121</td>
</tr>
<tr>
<td>T3 3x 60</td>
<td>0.968865</td>
<td>0.994495</td>
</tr>
</tbody>
</table>

crostructure in the transition and HCF regimes, it follows that some portion of the SVE instantiations capturing the fatigue response of the bulk microstructure should not contain a fatigue hot spot. By selecting appropriate threshold values for the EV FIP distributions, it was determined that out of 2,400 SVE instantiations, the majority of SVEs do not contain any FIP that could be considered an extreme value, as shown in Figure 4.1 below. Many SVE instantiations contain two or more EV FIPs, including some with more than five EV FIPs. This trend is true for FIP$_{FS}$ under both fully-reversed and positive strain ratio loading, and even to a greater degree for FIP$_{GBI}$ for $R_e = 0.1$.

Additionally, it was found that about 45% of the ensemble of SVE instantiations each contained two or more EV FIP$_{FS}$ and about 25% contained two or more EV FIP$_{GBI}$ values. These multiple extreme values occur in different grains within the same SVE, as the largest FIP subgrain value within a grain is taken as the highest driving force for fatigue crack formation and considered the EV FIP for the grain as a whole.
4.6 Microstructure rank ordering for fatigue response

4.6.1 High Cycle Fatigue Regime

For the HCF regime, the strain ranges in this work were 0.8% for $R_e = -1$ and 0.36% for $R_e = 0.1$, which corresponds to a stress of $\sim 500$ MPa, which is much lower than the 0.2% yield stress of $\sim 930$ MPa of the microstructure of model parameter set 2. These simulations correspond to the strain ranges encountered in the HCF regime of Ti-6Al-4V. Accordingly, our simulations are not intended to pertain to realistic range of fatigue lives, but rather to unambiguously explore the extreme value problem with regard to computed FIPs, irrespective of the physical thresholds for crack formation, which are less well understood. This permits comparison between microstructures based on computed FIPs. First, the fully reversed, $R_e = -1$, cyclic loading GPD probability distributions of EV FIPs are plotted in Figure 4.2. For these probability plots, fatigue resistance decreases as the FIP value increases (along the x-axis); the overall statistical trends of the entire distribution are more important than individual maximum values. Hence, rank ordering of the microstructures studied for each loading condition relies on the cumulative probability of the entire distri-
Figure 4.2: EV FIP$_{FS}$ fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 0.4% for fully-reversed straining $R_{\varepsilon} = -1$. The y-axis has a lower bound of 0.6 for visual clarity.
bution of EV FIPs over the threshold. Texture 3 (T3, gray), strong transverse \( \alpha \), clearly has the highest fatigue resistance (lowest FIP\(_{FS} \)) and the least spread of EV FIP\(_{FS} \) distributions compared with those of the other two textures for 0.4\% applied strain range. The three textures rank differently for grain size ratio and volume fraction variations. Overall, T1 and T2 have a larger spread, showing a higher sensitivity to the microstructure configurations. T1 is the most sensitive to microstructure configurations, with the larger grain size ratio (3x) manifesting the highest FIP values for both volume fractions, and the increased volume fraction of \( \alpha \)-phase exhibiting the least fatigue resistance. At the smaller grain size ratio, an increased volume fraction of \( \alpha \) could lead to more \( \alpha \) grains that experience more distributed plastic deformation than the smaller volume fraction of \( \alpha \), where fewer favorably oriented \( \alpha \) grains and smaller grain size would accumulate lower levels of plastic deformation. T3 shows a similar grain size ratio dependence as T1, where the 3x grain size ratio displays higher FS FIP values, but the opposite volume fraction dependence of T1, with the smaller volume fraction (30\%) having slightly higher values at 3x grain size ratio, and slightly smaller values for 2x grain size ratio. Fitted GPD parameters are given in Appendix A for Figures 4.2-4.4.

For the positive strain ratio loadings (\( R_\varepsilon = 0.1 \)) for a strain range of 0.36\%, Ti-6Al-4V fatigue lifetimes are decreased compared to fully-reversed loading. T3 again displays best fatigue resistance overall for EV FS FIPs compared to the other two textures, Figure 4.3. The FIP values for \( R_\varepsilon = 0.1 \) loadings are generally an order of magnitude smaller than the \( R_\varepsilon = -1 \) FIP values, which is consistent with experimental data for small crack growth of Ti-6Al-4V with significantly faster growth for \( R_\varepsilon = 0.1 \) than \( R_\varepsilon = -1 \) [26, 168]. T2 has a smaller spread than T1, with T1 3x 60 having the least overall lowest fatigue resistance based on the EV FIP\(_{FS} \). For both fully reversed and positive stress loading ratios, a larger grain size and volume fraction \( \alpha \)-phase results in decreased fatigue performance. This is consistent with the results found by Lutjering and Williams [169] for bimodal Ti-6Al-4V.

For the EV FIP\(_{GBI} \) loaded with a positive strain ratio in Figure 4.4, most of the configu-
Figure 4.3: EV FIP$_{FS}$ fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 0.4% for positive strain ratio loading $R_{\epsilon} = 0.1$.

The strain ratios are nearly identical, with the exception of the larger maximum grain size ratio and primary $\alpha$ volume fraction of T1 and T2. The larger grain sizes also show decreased fatigue resistance for the higher volume fraction $\alpha$-phase for T1 and T2, which is expected in the HCF regime [49], as both T1 and T2 have basal/transverse textures. The plastic deformation at this applied strain range is spatially heterogeneous, and any factor that increases the possibility of basal slip in primary $\alpha$ grains (increasing volume fraction $\alpha$-phase and increasing maximum grain size) will decrease fatigue resistance for all microstructures. From the GPD CDF probability plots of the EV FIPs for all 12 cases in Table 4.1, we found that texture 3 (T3, strong transverse $\alpha$) exhibits the best fatigue resistance for both EV FIP$_{FS}$ for both $R_{\epsilon} = -1$ and $R_{\epsilon} = 0.1$ loadings and EV FIP$_{GFI}$ for $R_{\epsilon} = 0.1$ loading. Both types of FIPs capture the experimentally observed effect that increasing maximum grain size and/or volume fraction primary $\alpha$ reduces fatigue resistance.
4.6.2 Transition Fatigue Regime

After CPFEM simulation stress-strain results are extracted, FIPs are computed and then a threshold value is selected for each distribution of FIPs per ensemble of SVE instantiations of the digitally reconstructed microstructure. The FIP values above the determined threshold are considered to be ‘extreme value’ FIPs and are plotted using a cumulative distribution plot fit of the Generalized Pareto Distribution (GPD), which allows for rank-ordering of the microstructures for fatigue response. Decreasing fatigue resistance correlates with higher FIP values along the x-axis. The EV FIP\textsubscript{FS} of the 12 microstructures at a strain range of 1.6% under fully reversed loading conditions (R\textsubscript{e} = -1) are shown in Figure 4.5.

For these loading conditions, texture 1 (T1) exhibits almost no effect on fatigue resistance, with most microstructures for texture 2 (T2) showing similar fatigue resistance. For these loading conditions, T1 shows little differentiation between the microstructure varia-
tions of maximum grain size and phase volume fraction, suggesting that the texture drives fatigue response for these loading conditions, and T1 is the ‘hardest’ of the three textures. The lack of differentiation of T1’s response is likely due to using the same texture for both α- and colony-phases, rendering microstructure effects less pronounced. The primary outlier of T2 is T2 2x 30, which has the highest fatigue resistance of all microstructures for the FIP_{FS} under the specified loading conditions, with microstructure having little effect between the other configurations of T2. Generally, as the FIP_{FS} is formulated to capture slip band formation on soft-oriented, basal slip planes, it follows that microstructure configurations with smaller primary α grains and decreased volume fraction of α-phase would display increased fatigue resistance. Texture 3 (T3) also shows this increased fatigue resistance for its 2x 30 microstructure. There is also a clear secondary effect of volume fraction for T3 as well, with fatigue resistance increasing with decreased α-phase. Overall, T3 has the highest fatigue resistance of the textures when disregarding microstructure effects, with very little difference between T1 and T2 microstructures except for the one outlier previously discussed. The relative clustering of the EV FIP_{FS} distributions for cyclic straining at this peak strain is most likely due to the increased homogeneity of plastic deformation and slip, leading to competing crack formation sites and reducing microstructure effects on fatigue resistance.

For the positive strain ratio (R_ε = 0.1) loading to a strain range of 0.72%, the FIP_{FS} GPDs shown in Figure 2 show increased variation of both microstructure effects and texture effects. Again, T1 shows very little difference of fatigue resistance between its different microstructures, with 2x 30 showing slightly better resistance and 3x 60 showing slightly decreased resistance, as expected. The 2x 60 and 3x 30 distributions are nearly identical for T1 as well as T2, indicating that increasing either maximum grain size or primary α phase volume fraction result in the same decrease in fatigue resistance for these textures. Overall, T2 has the highest fatigue resistance under these loading conditions regardless of microstructure effects. However, T3 has the largest variation in fatigue resistance (extreme
values of FIP$_{FS}$) based on microstructure, with phase volume fraction having the most impact, followed by grain size. Here, the expected trend is reversed, where the smaller grain size shows increased fatigue resistance at each volume fraction, suggesting that increased deformation in large colony grains inhibits slip band formation in primary $\alpha$ grains. There is also a significant shift in fatigue resistance ranking of T3 microstructures from the fully reversed case to the positive strain ratio case, due to the grain phases of the EV FIP$_{FS}$ for each loading. At $R_e = -1$ for T3, the percentage of EV FIP$_{FS}$ grains are mostly colony ($83\%$ and higher, Table 4.5a.), whereas for $R_e = 0.1$ are mostly primary $\alpha$ grains ($84\%$ and higher, Table 4.5b.).

As the FIP$_{GBI}$ is applicable to conditions of positive strain ratio, which produce progressive dislocation pileups on grain boundaries, only $R_e = 0.1$ results are shown in Figure 4.7. It is important to note that, since the FIP$_{GBI}$ is computed from the net plastic strain and the FIP$_{FS}$ is computed from the plastic strain range, the two FIPs are not directly comparable,
Figure 4.6: EV FIP$_{FS}$ fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 0.8% for positive strain ratio ($R_\varepsilon = 0.1$).

and generally the FIP$_{GBI}$ will have higher values under the same loading conditions. T2 and T3 have similarly clustered results for all microstructure effects, which may correlate with having the EV FIP$_{GBI}$ grains occurring mainly in primary $\alpha$ grains, with slightly more colony grains for T1. For all three textures, the 3x 30 microstructures (stars) have the least fatigue resistance, and the 2x 30 (circles) have the highest fatigue resistance for T1 and T2, whereas T3 notably is the second lowest for 2x 30.
4.6.3 Low Cycle Fatigue Regime

At applied loading levels in the LCF regime of Ti-6Al-4V, it is expected that the microstructure will experience more widely distributed plastic deformation of grains than under HCF conditions, regardless of orientation or other microstructure attributes. At these higher strains, there is a larger grain-level contrast in the plasticity properties compared to the elastic properties, and as a result, there are higher texture dependencies in LCF compared to HCF. The FIP_{FS} GPD results for the fully reversed case are plotted in Figure 4.8. At the strain range of 2.4%, for fully-reversed loading (R_{ε} = -1), experiments show a significant amount of material softening which our model cannot capture. Therefore, these results are presented here for completion, but it should be noted that these conditions do not correspond with experimental results at all. Here, fatigue resistance is clearly linked to texture, with T3 having the highest fatigue resistance, T1 having the lowest, and T2 in between. T3
has the most soft grains based on orientation, and T1 has the most hard grains and therefore higher stresses, leading to increased FIP values. The soft grains of T3 may allow for plastic deformation to be more evenly distributed and inhibit fatigue crack formation. Grain size has the next largest impact on fatigue resistance, as within each texture, all of the 3x grain sizes rank lower in fatigue resistance than the respective 2x grain sizes. All three textures show 3x 60 with the lowest fatigue resistance, followed by 3x 30, suggesting plastic deformation in larger grains has a higher likelihood of occurrence under these loading conditions for fatigue crack formation. Both T1 and T2 have 2x 30 exhibiting the highest fatigue resistance, with T3 being the exception with 2x 60 exhibiting the highest fatigue resistance.

Figure 4.8: EV FIP_{FS} fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 1.2% for fully-reversed straining $R_{\varepsilon} = -1$.

However, the rank-ordering by FIP_{FS} is quite different at positive strain ratio loading ($R_{\varepsilon} = 0.1$) at strain range of 1.08%, Figure 4.9. Here, the fatigue resistance of the textures is shifted, with T3 overall having the worst fatigue resistance for the applied loading, T2
having the highest fatigue resistance, and T1 in between. T1 and T2 again rank order along microstructure attributes in the same way, with 2x 30 showing highest fatigue resistance, 3x 30 showing lowest, and 2x 60 and 3x 60 are similar for both textures, suggesting that larger colony grain sizes lead to reduced fatigue resistance in the LCF regime. For T3, the largest effect after texture is volume fraction, followed by grain size.

![Figure 4.9: EV FIP$_{FS}$ fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 1.2% for positive strain ratio ($R_\varepsilon = 0.1$).](image)

The FIP$_{GBI}$ GPDs for rank-ordering for positive strain ratio ($R_\varepsilon = 0.1$) at strain range of 1.08% are shown in Figure 4.10. Here, texture appears to have the least clear effect on fatigue resistance compared to the other loading conditions, though a similar trend is evident to that of FIP$_{FS}$ rank ordered under the same loading conditions. All three textures show a large spread in fatigue response, with T2 and T3 grouping according to phase volume fraction, with lower $\alpha$ showing increased fatigue resistance, and different dependencies on grain size. For T3, the smaller grain sizes show increased fatigue resistance, but for T2, the 2x 60 shows decreased fatigue resistance compared to the 3x 60 microstructure. T1
exhibits different trends, with 3x 30 having the highest fatigue resistance, followed by 2x 60, 2x 30, then 3x 60, so there is no clear trend based on either phase volume fraction or grain size.

Figure 4.10: EV FIP\textsubscript{GBI} fitted to GPD CDF probability scale for the different microstructures subjected to a maximum applied strain of 1.2% for positive strain ratio (R\textsubscript{ε} = 0.1).

### 4.7 Characterization of EV FIP\textsubscript{FS} and EV FIP\textsubscript{GBI} locations by phase/grain boundary

After selecting the appropriate thresholds when employing the POT approach, the EV FIPs can be characterized by the phase of the grain or grain boundary coincident with the location of an EV FIP. For the transgranular EV FIP\textsubscript{FS}, this results in two types, \(\alpha\) or colony. For the EV FIP\textsubscript{GBI}, there are four different types: \(\alpha\)-\(\alpha\), \(\alpha\)-colony, colony-\(\alpha\), and colony-colony, with the first designation referring to the phase of the grain coincident with the progressive slip accumulation that impinges on the boundary and produces the EV FIP\textsubscript{GBI}, and the latter referring to the neighboring grain/phase. The percentage of each type of EV FIP over the selected thresholds was calculated, and the results are summarized in the
following sections.

4.7.1 High Cycle Fatigue Regime

For 0.4% maximum applied strain, all EV FIP\textsubscript{FS} occur in \(\alpha\) grains for all three textures, most likely due to the highly heterogeneous deformation that occurs in Ti-6Al-4V in the VHCF regime. For the slip band formation mechanism that the EV FIP\textsubscript{FS} addresses, only favorably oriented \(\alpha\) grains undergo sufficient localized plastic deformation to result in an EV FIP\textsubscript{FS} in the VHCF regime. This is consistent with experimental observations that cracks tend to nucleate from primary alpha grains irrespective of the constituent volume fraction Pilchak [158].

Table 4.4: a) percentage of EV FIP\textsubscript{FS} grain location types at a maximum strain of 0.4% over selected thresholds for \(R_e = -1\), and b) percentage of EV FIP\textsubscript{FS} and FIP\textsubscript{GBI} grain location types at a maximum strain of 0.4% over selected thresholds for \(R_e = 0.1\).

| a. | EV FIP\textsubscript{FS} | | b. | EV FIP\textsubscript{FS} | EV FIP\textsubscript{GBI} |
|----|-----------------|----||----|-----------------|-----------------|
| \(T1\) 2x 30 | 100% 0% | | \(T1\) 2x 30 | 100% 0% | \(\alpha-\alpha\) 0% 0% 0% 0% |
| \(T1\) 2x 60 | 100% 0% | | \(T1\) 2x 60 | 100% 0% | \(\alpha-col\) 62% 38% 0% 0% |
| \(T1\) 3x 30 | 100% 0% | | \(T1\) 3x 30 | 100% 0% | \(\alpha-\alpha\) 29% 71% 0% 0% |
| \(T1\) 3x 60 | 100% 0% | | \(T1\) 3x 60 | 100% 0% | \(\alpha-col\) 71% 29% 0% 0% |
| \(T2\) 2x 30 | 100% 0% | | \(T2\) 2x 30 | 100% 0% | \(\alpha-col\) 22% 78% 0% 0% |
| \(T2\) 2x 60 | 100% 0% | | \(T2\) 2x 60 | 100% 0% | \(\alpha-col\) 56% 44% 0% 0% |
| \(T2\) 3x 30 | 100% 0% | | \(T2\) 3x 30 | 100% 0% | \(\alpha-col\) 21% 79% 0% 0% |
| \(T2\) 3x 60 | 100% 0% | | \(T2\) 3x 60 | 100% 0% | \(\alpha-col\) 56% 44% 0% 0% |
| \(T3\) 2x 30 | 100% 0% | | \(T3\) 2x 30 | 100% 0% | \(\alpha-col\) 31% 69% 0% 0% |
| \(T3\) 2x 60 | 100% 0% | | \(T3\) 2x 60 | 100% 0% | \(\alpha-col\) 54% 46% 0% 0% |
| \(T3\) 3x 30 | 100% 0% | | \(T3\) 3x 30 | 100% 0% | \(\alpha-col\) 27% 73% 0% 0% |
| \(T3\) 3x 60 | 100% 0% | | \(T3\) 3x 60 | 100% 0% | \(\alpha-col\) 52% 48% 0% 0% |

The EV FIP\textsubscript{GBI} types show a similar overall trend to that of the EV FIP\textsubscript{FS}: all EV FIPs occur in \(\alpha\) grains. At 0.4% maximum applied strain, all three textures favor \(\alpha\) grain locations, with the neighboring location showing volume fraction dependence, due to the larger volume fraction resulting in more grain boundaries of that type surrounding any given \(\alpha\) grain. T1 has the largest volume fraction dependence for \(\alpha-\alpha\) grain boundaries, with T2 the
largest for $\alpha$-colony grain boundaries, followed by T3 for both trends. Consistent with experi-
ments, fatigue crack formation at 0.4% maximum applied strain, EV FIPs occur solely in $\alpha$ grains, regardless of texture, phase volume fraction, grain size, strain ratio, or trans-
granular fatigue mechanism. It is noted that the percentages of each EV FIP$_{FS}$ type are the
same for $R_\varepsilon = -1$ and $R_\varepsilon = 0.1$ (strain ranges of 0.8% and 0.36%, respectively), though this
may just be an artifact of using the same SVE ensembles for the CPFEM simulations at each strain ratio.

4.7.2 Transition Fatigue Regime

In the transition fatigue regime for $R_\varepsilon = -1$, Table 4.5a, each texture shifts towards more
EV FIPs occurring in colony grains compared to the HCF results. T1 exhibits this shift, based on the phase volume fraction, while for T2 $\alpha$ grains still have the largest percentage of occurrence, though with increased number density of colony grain locations for all microstructures and especially higher colony volume fractions. However, T3 drastically shifts of primarily colony location occurrences for EV FIPs. However this does not indicate that, for the fully reversed case, as the applied strain increases, fatigue crack formation transitions from primary $\alpha$ grains to colony grains depending on the texture. Fatigue crack formation is still expected to occur on basal planes within primary $\alpha$ grains, and the colony EV FIP grains become more common at these higher strains. There are also small variations in grain locations according to the volume fraction of each phase with approximately the same grain size effects.

For the positive strain ratio ($R_\varepsilon = 0.1$) EV FIPs, Table 4.5b, primary $\alpha$ grains remain the majority locations for FIP$_{FS}$, with T1 having the largest shift towards colony grains, followed by T2, and the least with T3. The texture T1 is clearly the most sensitive to loading conditions with respect to fatigue crack formation. Volume fraction of the primary $\alpha$-phase seems to have a similar effect as EV FIP$_{FS}$ locations, with only a small difference made by grain size. For the EV FIP$_{GBl}$, all three textures remain majority primary $\alpha$ grain locations,
with the neighboring grain defined by the larger volume fraction of each microstructure. Compared with the work underway at 0.4% peak strain, the percentage of EV FIP\(_{\text{FS}}\) values in colony grains increases at different rates as the peak strain increases.

Table 4.5: a) Percentage of EV FIP\(_{\text{FS}}\) grain location types at a maximum strain of 0.8% over selected thresholds for R\(_e\) = -1, and b) percentage of EV FIP\(_{\text{FS}}\) and FIP\(_{\text{GBI}}\) grain location types at a maximum strain of 0.8% over selected thresholds for R\(_e\) = 0.1.

<table>
<thead>
<tr>
<th>a. EV FIP(_{\text{FS}})</th>
<th>b. EV FIP(_{\text{FS}})</th>
<th>EV FIP(_{\text{GBI}})</th>
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<td>(\alpha-\alpha) col-(\alpha) col-(\alpha) col-col</td>
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<tr>
<td>T1 2x 30 30% 70%</td>
<td>T1 2x 30 71% 29% 20% 41% 14% 25%</td>
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<tr>
<td>T1 2x 60 57% 43%</td>
<td>T1 2x 60 86% 14% 50% 33% 10% 8%</td>
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<tr>
<td>T1 3x 30 33% 67%</td>
<td>T1 3x 30 69% 31% 16% 40% 14% 30%</td>
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<tr>
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<td>T1 3x 60 85% 15% 50% 35% 10% 4%</td>
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<td>T2 2x 30 52% 48%</td>
<td>T2 2x 30 76% 24% 20% 55% 8% 17%</td>
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<tr>
<td>T2 2x 60 84% 16%</td>
<td>T2 2x 60 95% 5% 53% 40% 4% 3%</td>
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<td>T2 3x 30 56% 44%</td>
<td>T2 3x 30 79% 21% 26% 56% 5% 13%</td>
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<td>T2 3x 60 83% 17%</td>
<td>T2 3x 60 95% 5% 56% 37% 3% 4%</td>
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<tr>
<td>T3 2x 30 8% 92%</td>
<td>T3 2x 30 86% 14% 22% 62% 6% 10%</td>
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<tr>
<td>T3 3x 60 17% 83%</td>
<td>T3 2x 60 97% 3% 51% 47% 2% 1%</td>
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</table>

4.7.3 Low Cycle Fatigue regime

In the LCF regime, with nominal peak strain of 1.2%, the trend towards increased colony locations continues for all microstructures for both strain ratios, as shown in Table 4.6. The fully reversed EV FIP\(_{\text{FS}}\) continue to shift towards colony grain occurrence, with T1 now showing colony grains over all microstructures, with smaller increases corresponding to higher volume fraction primary \(\alpha\) grains. T2 shifts more slowly, with the volume fraction of each phase corresponding to which phase will result in a higher percentage of EV FIP\(_{\text{FS}}\) grain locations. The EV FIP\(_{\text{FS}}\) of T3 occur almost entirely in colony grains at this peak applied strain.

The increase in colony EV FIP grains is shown under positive strain ratio loading as well. T1 and T2 now depend on volume fraction to define which phase will be have a higher
percentage of locations, and T3 shows a marked increase in the number of EV FIP\textsubscript{FS} colony grains while still remaining primarily located in $\alpha$ grains. The same trend is exhibited for EV FIP\textsubscript{GBI}, where T1 fluctuates between $\alpha$-colony or colony-colony grain boundaries depending on the microstructure’s phase volume fraction. T2 similarly fluctuates between $\alpha$-$\alpha$ or colony-colony grain boundaries. T3 continues to have a highest percentage of $\alpha$ grain locations, though less so than at peak strain of 0.8%.

Table 4.6: a) Percentage of EV FIP\textsubscript{FS} grain location types at a maximum strain of 1.2% over selected thresholds for $R_\varepsilon$ = -1, and b) percentage of EV FIP\textsubscript{FS} and FIP\textsubscript{GBI} grain location types at a maximum strain of 1.2% over selected thresholds for $R_\varepsilon$ = 0.1.

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By characterizing each EV FIP according to the phase or grain boundary phases, it has been shown for the first time that fatigue crack formation is primarily occurs in $\alpha$ grains in the HCF regime and transition fatigue regimes, with an increase in EV FIP colony grains more or less rapidly depending on the texture and strain ratio, as the loading increases through the transition fatigue regime into LCF, though again, the highest EV FIP magnitudes are still associated with large primary $\alpha$ grains.
4.8 Single microstructure attribute descriptors of EV FIP grains

4.8.1 High Cycle Fatigue regime

For grains over the respective threshold as found from POT analysis, the grain size, orientation, phase, and normalized FIP values are plotted to provide insight regarding which microstructure attributes have a higher likelihood to be associated with an EV FIP. All figures are available in Appendix B, but a few examples are discussed here. In Figure 4.11, under fully-reversed loading, most EV FIP$_{FS}$ are located in primary $\alpha$ grains within a range of $\Phi$, the declination angle between the c-axis and applied uniaxial loading direction, from $35^\circ$ to $60^\circ$: this is expected as these orientations correspond to ‘easy’-oriented grains for slip. Clustering within that range is exhibited for all microstructures in this work, and both EV FIP$_{FS}$ banded along basal and prismatic planes are present in this cluster. Note that for this specific microstructure, the maximum grain size is 32.7 $\mu$m, and 54% of the grains containing EV FIP$_{FS}$ are greater than 22.8 $\mu$m in diameter. The EV FIP$_{FS}$ single descriptors

![Figure 4.11: Single descriptors of EV FIP$_{FS}$ grains for microstructure T1 3x 60% loaded to 0.4% strain range for R$_{e}$ = -1. Colors on the left refer to phase, on the right refer to normalized FIP value, with size corresponding to grain diameter.](image)

for positive strain ratio loading of the same SVE ensemble are shown in Figure 4.12. The same clustering attributed to grains oriented for easy basal slip is present, with two secondary clusters at $80^\circ \leq \Phi \leq 90^\circ$ and $\phi_2 \approx 15^\circ$ or $45^\circ$. These correspond to the c-axis range.
where prismatic slip has been experimentally shown to be prevalent [95]. By comparing Figure 4.11 with Figure 4.12, many of the grains that have an EV FIP$_{FS}$ for fully-reversed loading will also have the same for a positive strain ratio for a given nominal peak strain (192 out of 245 EV FIP grains for this microstructure). This can be attributed to the relatively low value of the nominal peak strain in this work, which corresponds to the very high cycle fatigue regime of Ti-6Al-4V, where plastic deformation is highly heterogeneous, and is likely to be occur in only a select number of favorably oriented grains.

Figure 4.12: Single descriptors of EV FIP$_{FS}$ grains for microstructure T1 3x 60% loaded to 0.4% nominal peak strain for $R_e = 0.1$.

Similar clusters are observed for the positive strain ratio EV FIP$_{GBI}$ that occur in primary $\alpha$ grains as the positive strain ratio EV FIP$_{FS}$, Figure 4.13. Given that, the clustering in primary $\alpha$ grain for EV FIP$_{GBI}$ grains still corresponds mainly to grains which are favorably oriented for basal slip.
Figure 4.13: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T3 2x 60\% loaded to 0.4\% nominal peak strain for $R_\varepsilon = 0.1$.

4.8.2 Transition Fatigue Regime

Several microstructure attributes of EV FIP grains are of interest with respect to fatigue crack formation of duplex bimodal Ti-6Al-4V. For each grain/phase associated with an EV FIP in the distributions shown previously, the grain size, orientation, and self-normalized EV FIP value are plotted in Figure 4.14. The Bunge-Euler angles $\Phi$ and $\phi_2$ are considered here specifically to compare with the experimental work done by Lavogiez et al. [160, 161].

Figure 4.14: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 3x 30\% loaded to 0.8\% strain range for $R_\varepsilon = -1$.

There is a clear trend exhibited between the two phases, as shown at the left of Figure
4.14. The EV FIP\textsubscript{FS} that occur in primary $\alpha$ grains generally fall within the relatively soft band of 30-60$^\circ$ of $\Phi$ values, and between 10-50$^\circ$ of $\phi_2$ values. In contrast, the EV FIP\textsubscript{FS} that occur in colony grains fall in the band of 10-40$^\circ$ of $\Phi$ values, and over the entire range of $\phi_2$ values, with more clustering towards 0$^\circ$ and 60$^\circ$. Overall, colony EV FIP\textsubscript{FS} are more likely to occur in smaller grains, with primary $\alpha$ EV FIP\textsubscript{FS} more likely to occur in larger grains. However, the normalized EV FIP\textsubscript{FS} values indicate that both phases are likely to have high FIP\textsubscript{FS}, including some of the very small colony grains of less than 10 $\mu$m in diameter. This indicates that there is a clear increase in the homogeneity of plastic deformation in the transition fatigue regime as opposed to the HCF regime of Ti-6Al-4V.

The role of grain size becomes more distinct when analyzing the results for the same microstructure under positive strain ratio loading, as shown in Figure 4.15. Here, the same phase trends are evident, but now with additional primary $\alpha$ clusters for $\Phi$ values greater than 75$^\circ$ and around $\phi_2$ values of 5-25$^\circ$ and 35-55$^\circ$. These clusters correlated to activation of prismatic slip systems of primary $\alpha$ grains and seem to occur more often in larger grains than the other EV FIP\textsubscript{FS}, including many of the highest FIP\textsubscript{FS} values for this microstructure. However, from experimental results [95, 160, 161] fatigue cracks do not tend to form in grains oriented for prismatic slip and they are most likely not candidate grains for fatigue crack formation.

Figure 4.15: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 3x 30% loaded to 0.8% nominal peak strain for $R_\varepsilon = 0.1$. 

99
Considering only the Bunge-Euler angles $\Phi$ and $\phi_2$ of the EV FIP$_{GBI}$ grains show similar trends to the EV FIP$_{FS}$ for the same microstructures at a nominal peak strain of 0.8%, as shown in Figure 4.16. With the normalized FIP$_{GBI}$ values to the right, despite some clustering within the fundamental zone, there is less correlation with specific Euler angles. Texture 2 and its microstructures display much of the same trends for single descriptors of EV FIP grains. Clearly, additional spatial descriptors are essential to understand correlations with the microstructure neighborhoods at the sites of EV FIPs.

Figure 4.16: Single descriptors of EV FIP$_{GBI}$ grains for microstructure T1 3x 30% loaded to 0.8% nominal peak strain for $R_e = 0.1$.

The microstructures with texture 3 (T3) exhibit a shift in orientation trends compared with the other two textures. In Figure 4.17, there are very few grains oriented in the basal-oriented $\Phi$ range that is optimal for easy basal slip linked to fatigue crack formation, and the majority of the EV FIP$_{FS}$ grains occur in the prismatic activated orientations. Only a few extreme values are found in colony grains for this microstructure, which is also the case for EV FIP$_{GBI}$ grains, as shown in Figure 4.18.
Figure 4.17: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T3 3x 60% loaded to 0.8% nominal peak strain for R\textsubscript{e} = 0.1.

Figure 4.18: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T3 3x 60% loaded to 0.8% nominal peak strain for R\textsubscript{e} = 0.1.
4.8.3 Low Cycle Fatigue Regime

For a nominal peak strain of 1.2\%, the material deformation response falls well within the LCF regime of Ti-6Al-4V fatigue response. Again, the fully-reversed 1.2\% result are presented here for completion. The Bunge-Euler angle descriptors of T2 2x 30\% are shown in Figure 4.19 for the $R_e = -1$ case; similar trends are observed as for the transition fatigue results. There is a distinct clustering of primary $\alpha$ EV FIP$_{FS}$ in the 30-60\$^\circ$ $\Phi$ range. The colony grains also show similar clustering as observed for the case of 0.8\% nominal peak strain, but with much wider variability over both Euler angles plotted here. Similarly, the higher normalized EV FIP$_{FS}$ values are also more spread over the fundamental zone.

Figure 4.19: Single descriptors of EV FIP$_{FS}$ grains for microstructure T2 2x 30\% loaded to 1.2\% nominal peak strain for $R_e = -1$.

A major difference between the two strain ratios can be found comparing Figure 4.19 with Figure 4.20, which show FIP$_{FS}$ for the same microstructure subjected at 1.2\% peak applied strain at different $R_e$ ratios. The clustering that previously has been a feature of all microstructures, loading conditions, and FIP types is substantially less evident by comparison. Though primary $\alpha$ grains still tend to be somewhat larger than most colony grains/phases containing EV FIP$_{FS}$, there is large scatter over the entire fundamental zone, indicating near-homogeneous deformation throughout the SVE ensemble.

The EV FIP$_{GBI}$ grains also exhibit much wider orientation variability in the LCF regime.
than in the transition regime, as shown in Figure 4.21. Some of the previously observed clustering tendencies are evident, but both primary $\alpha$ and colony grains have a larger spread, and grain size is more comparable between both phases, unlike the EV FIP$_{FS}$ grains of this microstructure.

Figure 4.21: Single descriptors of EV FIP$_{GBI}$ grains for microstructure T2 2x 30% loaded to 1.2% nominal peak strain for $R_e = 0.1$.

Again, T3 displays very different characteristics for these single grain EV FIP descriptors in terms of the EV FIP$_{FS}$. The clustering of grains remains for the positive strain ratio case as well, Figure 4.22, but shifts in both orientation and phase to $\Phi$ range of greater than 75° and from colony grain occurrence to primary $\alpha$ grain occurrence. This is likely related to the reversal of fatigue resistance of T3 microstructures with different stress ratios.
4.9 Summary and conclusions

In this chapter, a range of microstructure and loading conditions were simulated to explore and compare the HCF behavior of Ti-6Al-4V for various textures from a computational perspective, apart from considering any physical thresholds for crack formation in this regime. The microstructure variables included phase volume fraction, max-to-mean grain size ratio, and texture. Extreme value distributions of the computed FIPs above a selected threshold (peaks over threshold) were fit to the generalized Pareto distribution. POT extreme value theory showed an improved fit to EV FIP data and includes multiple EV FIP locations within the same SVE instantiation, providing a better approach for ranking microstructures for fatigue resistance based on the SVE approach. Texture 3 (T3), with strong transverse $\alpha$ and few easy basal slip systems, had the highest fatigue resistance as compared to the other textures regardless of grain size ratio, volume fraction, strain ratio, or FIP type. However, the relative effect of each of these microstructure attributes on fatigue resistance was different for each set of loading conditions, and even with this large set of microstructures, it is not possible to predict the ranking of fatigue performance in the HCF regime beyond general trends. Larger grains tend to dominate the EV FIPs, and this points to the importance of detailed characterization and quantification of rarely occurring alpha particle sizes (up-
per tail of the distribution) instead of the average grain sizes, when assessing the effect of microstructure on fatigue behavior. Further work would need to be done filling out the design of experiments for other Ti-6Al-4V microstructures to provide predictive capabilities as well as comparison of FIPs with experimental characterization of fatigue crack initiation sites.

By using peaks-over-threshold extreme value theory based on the GPD, EV FIPs for each ensemble of Ti-6Al-4V SVE instantiations per microstructure were determined above respective thresholds. For a nominal peak strain of 0.8%, these extreme value distributions were plotted and used to rank-order microstructures in terms of fatigue resistance. In this transition regime, there were more frequent crossovers and overlap between fatigue resistance, and clear trends in fatigue behavior were not found. At the highest nominal peak strain studied, 1.2%, T3 displayed higher fatigue resistance than the other two textures for the $R_e = -1$ case for EV FIP$_{FS}$ but displayed the lowest fatigue resistance for the $R_e = 0.1$ case in terms of both FIP$_{FS}$ and FIP$_{GBI}$. Overall, the T2 2x 30% microstructure displayed high fatigue resistance for all loading conditions/microstructures investigated here, predominantly having the highest (or nearly so) fatigue resistance for the transition fatigue and LCF regimes.

The constituent phase or grain boundary type of the grains coincident with EV FIPs were then characterized. In the HCF regime of Ti-6Al-4V, it had previously been shown that grains with sufficient local plastic deformation to result in EV FIP$_{FS}$ values were primary $\alpha$ grains, and also for most EV FIP$_{GBI}$ grains. In this work at higher applied strain ranges in the transition fatigue and LCF regimes, EV FIP locations switched to varying degrees to a greater percentage occurring in colony grains. Texture served as the primary microstructure attribute observed to trigger this switch of EV FIP occurrence from primary $\alpha$ grains to colony grains, followed by volume fraction of primary $\alpha$, with little effect of grain size.

Finally, discrete microstructure descriptors of phase, grain size, and orientation of EV FIP grains were plotted to identify trends regarding the effects on normalized FIP values.
Compared with previous HCF results, the plots for nominal peak strain of 0.8% (transition fatigue regime) show increased EV FIPs correlate with the $\alpha$ range that is associated with prismatic slip. In the LCF regime, less clustering was evident in terms of grain orientation, and much wider variability was observed over the fundamental zone of HCP structure; this is likely due to the decrease of heterogeneity of cyclic plastic deformation in the microstructure at higher applied loading conditions. Texture T3 manifests the largest change between $R_\varepsilon = -1$ and $R_\varepsilon = 0.1$ loading conditions, with almost entirely different parts of the $\alpha$ range being activated. For T3, this informs which $\alpha$ grain values result in a relative decrease of resistance to fatigue crack formation in the nucleant grain/phase.
CHAPTER 5
NEIGHBORHOOD SPATIAL CORRELATIONS OF CANDIDATE FATIGUE
HOT-SPOTS FOR TI-6AL-4V

5.1 Introduction

Crystal plasticity finite element models (CPFEM) coupled with extreme value statistics of FIP distributions have been successfully employed to rank-order different microstructures under specified loading conditions. By using a statistical volume element approach to approximate the fatigue response, the range of microstructures and mechanical loading conditions can be more rapidly explored while also taking advantage of the increased computational power offered by high-performance computing. This coupling has been advanced in recent years by the development of programmatic workflows to increase computational speed and parallelization, and to handle the batch generation and post-processing of such a number of SVE instantiations and the datasets generated by such an approach. Rank-ordering of microstructures for fatigue resistance using EV FIP distributions is useful for decision support in engineering applications, but does not explicitly identify the locations where a life-limiting fatigue crack will both form and grow through the first grain/phase boundary. Most computational approaches for modeling crack growth assume fatigue crack formation at notches or other pre-identified locations and focus on studying physically short crack growth through the first few neighboring grains. The ability to computationally identify these fatigue crack formation ‘hot-spots’ is critical to develop to improve study of crack growth through lifetime prediction.

This order-of-magnitude increase in the number of simulations and computations for computational fatigue research shifts the traditional set of computational analysis methodologies closer to data science and materials informatics approaches. The material informat-
ics based MKS approach previously introduced by Kalidindi and co-workers [4, 102, 128, 131, 133, 134, 136, 137, 139, 144, 170, 171] incorporates data-science methodologies and high throughput assays to investigate process-microstructure and microstructure-property relationships. For the discretized simulated microstructures of previous fatigue research, 2-point correlations are applied over SVE instantiations to predict both bulk and localized responses after reducing the dimensionality via principal component analysis [102, 128, 134]. Much of this materials informatics work has focused on predicting bulk material properties, but the statistically rare nature of fatigue crack formation poses unique challenges to applying these data science methodologies.

Previous work loaded ensembles of SVE instantiations using CPFEM in ABAQUS for both fully reversed and positive strain ratio loading, and FIPs were computed from the crystal plasticity stress-strain results. EV FIPs were defined using the peaks-over-threshold (POT) approach. In this section, all candidate experimentally informed fatigue hot-spots are identified (termed ‘candidate grains’) out of roughly 2 million simulated grains of the generated SVE ensembles of duplex bimodal Ti-6Al-4V. Candidate grains that contain EV FIPs are compared against candidate grains that did not undergo sufficient localized strain to result in an extreme value FIP, along a grain neighborhood defined as their first nearest neighbor (NN) grains. Spatial statistics of the grain neighborhoods are then convoluted to ensure each 2-point vector has its tail in the EV FIP grain or candidate grain, resulting in what is termed neighborhood spatial correlations. Principal component analysis (PCA) is applied to these neighborhood spatial correlations to reduce the dimensionality of the data.

5.2 Background

5.2.1 Fatigue crack formation in duplex Ti-6Al-4V

Bimodal Ti-6Al-4V consists of primary \(\alpha\) grains with colony grains of secondary \(\alpha\) in a lamellar structure with residual \(\beta\)-phase. The bimodal morphology offers a promising combination of fatigue crack resistance of both short and long crack growth [172]. Previous
computational efforts attempted to link single descriptors of EV FIP grains with fatigue life [164] or higher likelihood of extreme FIP values but have proved insufficient to explain why these specific grains result in such highly localized driving forces for crack formation. These fatigue hot-spots are a result of a combination of microstructure attributes in the surrounding neighborhood, including both immediate 1st- and 2nd-nearest neighbors as well as longer range effects.

Although duplex $\alpha + \beta$ titanium alloys have been extensively studied for decades, there are still ongoing experimental efforts to investigate the fatigue crack initiation locations using various techniques. Experiments performed by McBagonluri et al. [173] on Ti-6242 for dwell and cyclic fatigue for three microstructure morphologies all showed crack initiation due to a Stroh-type like mechanism of dislocation pileup at a grain boundary [64]. Kirane and Ghosh [174] found that crack initiation occurred on facets formed on the basal plane of primary $\alpha$ grains for dwell fatigue, with the surrounding region showing a high Schmid factor ($\sim 0.5$), though the initiation grain itself had a moderate Schmid factor for the basal plane ($\sim 0.45$). Uta et al. [175] studied dwell fatigue of IMI 834, and found crack initiation by pure cleavage on basal planes in a grain oriented 10-30° from the loading direction, with more grains along the crack propagation path with similar orientations. For near-$\alpha$ Ti-6Al, Bache et al. [65] observed crack formation under cyclic fatigue loading at a triple point of three grains with the highest basal stresses in the sample. Similarly, for Ti-6246, under a range of applied stress levels, and regardless of surface or subsurface initiation, fatigue cracks initiated in primary $\alpha$ grains [176]. A more recent novel alloy, $\alpha + \beta$ TIMETAL 407 (Ti-407) exhibited fractures along basal plane facets of primary $\alpha$ grains under HCF, LCF and dwell fatigue loadings [177].

Nalla et al. [27] investigated fatigue of bimodal and fully lamellar Ti-6Al-4V and found for bimodal, subsurface cracks initiated at primary $\alpha$ grains suitably oriented for planar slip in the basal plane perpendicular to the stress axis under positive load ratios. These cracks initiated in $\alpha$ grains that were surrounded by similarly oriented $\alpha$ grains, most likely a
microtexture effect arising from the material processing steps. Another study of bimodal Ti-6Al-4V under fully reversed load ratio loading at an applied stress in the transition between high cycle fatigue (HCF) and low cycle fatigue (LCF) found that cracks coincided with either basal or prismatic slip of primary $\alpha$ grains [178]. Bridier et al. [62] identified cracking along basal planes in primary $\alpha$ grains as the most critical damage mode of Ti-6Al-4V under a stress load ratio of 0 in the HCF regime. Pilchak and coworkers [158] later found using direct-method tilt fractography that the initiation facets in primary $\alpha$ grains were inclined 40-45° to the loading axis. Further, a study comparing crack initiation in the cases of both life-limiting and long-lifetime failure of Ti-6Al-4V had similar results, with facet formation occurring in primary $\alpha$ grains for both failure types [179]. For Ti-6Al-4V, it is clear from experiments that fatigue crack initiation occurs in primary $\alpha$ grains with a specific orientation to the loading axis to induce basal slip.

More recently, Lavogiez and coworkers [160, 161] further found that crack initiation occurs at primary $\alpha$ grain pairs well oriented for basal slip, between 10-60° to the loading axis, regardless of subsurface vs. surface initiation, or cyclic vs. dwell fatigue. The primary $\alpha$ grain pairs were found high normal stress on their basal planes and to have a (0001) twist boundary of 10-20°. They also found that basal slip was activated before prismatic slip, and that high Schmid factors were not associated with slip traces.

5.2.2 Current theoretical framework of PyMKS

Given the importance of grain orientation on both fatigue crack formation locations and crack growth paths, it is critical that such a discretization of microstructure can include crystal symmetry information for understanding structure-property relationships. Given a set the crystal lattice orientations, $g$, the corresponding local state space is the orientation space. The fundamental zone of orientation space for the HCP structure of Ti-6Al-4V for the primary $\alpha$ phase and $\alpha + \beta$ lamellar colony grains (homogenized following Ref. [33]),
is expressed as

\[ FZ_h = \{ g = (\phi_1, \Phi, \phi_2) \mid 0 \leq \phi_1 \leq 2\pi, 0 \leq \Phi \leq \pi/2, 0 \leq \phi_2 \leq \pi/3 \} \quad (5.1) \]

This orientation space is prohibitively large when considering binning approaches, so a modification to the microstructure function above (cf. Equation 2.30) using generalized spherical harmonics (GSH) [133, 135, 180] for hexagonal crystal structures was made to account for discretization and then extended by Paulson et al. [102, 128, 134] to account for single phase \( \alpha \)-titanium. This approach changes the basis for the orientation space but retains the primitive binning of spatial variables required for discretization. Using GSH and a phase indicator for the two phases of bimodal Ti-6Al-4V, \( \chi_\alpha \), we now express the microstructure function as

\[
m(\alpha, g, x) \, dg \approx \sum_{l,m,\nu} \sum_{s=1}^{S} \sum_{\alpha=1}^{2} M_{ls}^{m\nu} T_{l}^{m\nu}(g) \chi_s(x) \chi_\alpha \quad (5.2)
\]

where \( x \) is the spatial bin step size, \( M_{ls}^{m\nu} \) are the GSH Fourier coefficients, and \( T_{l}^{m\nu} \) are the symmetrized GSH functions. Mapping every distinct combination of \( l, m, \nu \) to a single index \( L \), the implicit convolution in Eq. 5.2 becomes

\[
F_{LK}^L = \frac{1}{|S_t|} \sum_{s=1}^{S_t} M_{ls}^L M_{s+t}^K \quad (5.3)
\]

and allows the same exploitation of rapidly computing the spatial correlations using FFT algorithms.

Jha and coworkers [143] recently proved the viability of this approach by applying PCA to slip and grain neighborhood metrics of near \( \alpha \)-Ti and showed strong correlation between higher \( \text{FIP}_{FS} \) values and principal components. 2-point statistics may not be sufficient to capture possible longer-range effects of microstructure but represent improvement on 1-point statistical attempts to predict fatigue behavior, such as volume fraction or average
5.2.3 Reduced order models

A review by Geers and Yvonnet [181] lays out the need for reduced order models (ROMs) of microstructures within multiscale modeling, due to the high computational cost that comes with finite element methods, even with high-performance computing improvements leading to massive parallelization of such computations. Nonlinear materials, such as Ti-6Al-4V are strongly path and history dependent. This dependency is stored in internal state variables (ISVs) [46] of constitutive equations in FEM, which take up a major amount of computational memory, so it is desirable to develop reduced order models capable of projecting a high dimensional, fully discretized multi-scale problem into a lower dimensional space. Ganapathysubramanian and Zabaras [182] attempted to find an alternative to ODF to represent crystallographic texture for finite element simulations. Oliver et al. [183] studied feasibility of reduced order model to studying multiscale fracture of a hypothetical three phase material. Chang et al. [184] reduced modeling cost by considering slip systems to be inactive and modeling only the active slip systems of HCP Mg for stress-strain response, yield surface evolution, and texture, which reduced computational time by a quarter. Fritzen and Kunc [185] lay out a methodology for informing reduced order models from FE, then a second step of interpolating ROM data to find the effective response, linking reduced order models with data science methodologies.

In the context of ICME, Kalidindi and coworkers [4] argue for the need of a standardized, multiscale representation of microstructure, built on a framework of rigorous mathematical formalism of lower length scale microstructures described by conditional probability densities at higher length scales. de Oca Zapiain et al. [186] demonstrated the tremendous promise of reduced order models which capture complex material microstruc-
ture for systematic study of damage models, when combined with materials data science and informatics methodologies. There is great potential for expanding the MKS framework to a diverse set of microstructures as well as customizing for other damage criterion. Paulson and coworkers [127, 128, 134] demonstrated significant computational advantage of the mathematically rigorous framework of the Materials Knowledge System approach of using reduced order representation of microstructures and forming structure-property linkages over traditional CPFEM brute force approach.

5.3 Methodology

5.3.1 Simulated microstructure ensembles

In previous works [164], 12 different microstructures were generated to statistically match the distributions of duplex $\alpha + \beta$ Ti-6Al-4V, spanning three different textures, Figure 5.1, two maximum grain size to average grain size ratios, and two different phase volume fractions. Due to the length scale difference between the transformed secondary $\alpha$ and $\beta$-phase lathes and the grain size, a homogenization scheme is used to model such grains, referred to hereafter as colony grains. The average grain size was kept consistent at 10.9 µm, with a maximum grain size of either 21.8 µm or 32.7 µm. The two phase volume fractions were selected to represent the outer bounds of the bimodal microstructure, 30% $\alpha$/70% colony and 60% $\alpha$/40% colony. Dream3D was utilized to reconstruct the ensemble of microstructure SVE instantiations, see Table 5.1 below. Each ensemble consists of 200 SVE instantiations, with a volume of 421,875 $(75^3) \mu m^3$ and 33 ABAQUS C3D8R voxel elements and were generated for the 12 microstructures and resulting a dataset of 7,200 instantiations. Each instantiation was loaded with both a fully reversed cyclic strain ratio ($R_e = \frac{\epsilon_{\min}}{\epsilon_{\max}}$) of $R_e = -1$ and positive strain ratio of $R_e = 0.1$ loaded to a three different nominal peak loading strains of 0.4%, 0.8% and 1.2%. The strain ranges are 0.8%, 1.6%, and 2.4% for $R_e = -1$, respectively, and 0.36%, 0.72%, and 1.08% for $R_e = 0.1$. Full details regarding the crystal plasticity model and microstructures can be found in Section 2.4. From
the CPFEM stress-strain results, Fatemi-Socie FIPs (FIP\textsubscript{FS}) and grain boundary impingement FIPs (FIP\textsubscript{GBI}) were computed for the positive strain ratio case, with only the FIP\textsubscript{FS} computed for the fully-reversed case, as FIP\textsubscript{GBI} was formulated specifically to take into account mean stress effects which result in dislocation pileup on a grain boundary. The extreme value distributions of each FIP were determined using the second extreme value theorem, peaks-over-threshold (POT), and fit to the cumulative distribution function of the Generalized Pareto Distribution (GPD) [166].

Table 5.1: Simulated microstructures for bimodal Ti-6Al-4V.

<table>
<thead>
<tr>
<th>Microstructure</th>
<th>Grain size (μm)</th>
<th>α-phase vol. frac.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Avg.</td>
<td>Max.</td>
</tr>
<tr>
<td>T1 2x 3070</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T1 2x 6040</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T1 3x 3070</td>
<td>10.9</td>
<td>32.7</td>
</tr>
<tr>
<td>T1 3x 6040</td>
<td>10.9</td>
<td>32.7</td>
</tr>
<tr>
<td>T2 2x 3070</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T2 2x 6040</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T2 3x 3070</td>
<td>10.9</td>
<td>32.7</td>
</tr>
<tr>
<td>T2 3x 6040</td>
<td>10.9</td>
<td>32.7</td>
</tr>
<tr>
<td>T3 2x 3070</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T3 2x 6040</td>
<td>10.9</td>
<td>21.8</td>
</tr>
<tr>
<td>T3 3x 3070</td>
<td>10.9</td>
<td>32.7</td>
</tr>
<tr>
<td>T3 3x 6040</td>
<td>10.9</td>
<td>32.7</td>
</tr>
</tbody>
</table>

To first validate the MKS approach as outlined above, the 2-point spatial correlations are computed over the entire SVE ensemble of 200 instantiations as discretized in Equations 5.1 and 5.2, and reduced using PCA. The first three PC scores are plotted in Figure 5.2. Clustering between the instantiations of each ensemble is visually evident, validating that this discretized microstructure representation using MKS approach captures the differences between the microstructures.

Further, the Euclidean distance between the average of each cluster in PC space is also shown in Figure 5.3 in a dendrogram. The primary clustering follows the α phase volume fraction, and then the orientations by texture, with the grain size ratio showing the least
Figure 5.1: Inverse pole figures of simulated microstructure textures with from Dream.3D, units in multiple of random distribution: a) texture 1 (referred to as T1 in Table 1), b) texture 2 (T2), and c) texture 3 (T3).

Figure 5.2: PC1, PC2, and PC3 scores of the 12 microstructures reduced from 2-point correlations of entire SVE instantiations for each microstructure ensemble.
effect on the spatial correlations of these microstructures.

Figure 5.3: Dendrogram of comparing the Euclidean distance in PC space of the 12 microstructures.

Following the results from Lavogiez et al. [160, 161], we identify candidate grains as fulfilling the following criteria: a pair of primary $\alpha$ grain neighbors, both with declination angle of 10-60° to the loading axis, with a twist boundary of 10-20° between their basal planes. Based on these experiments, we make the assumption that such grain pairs result in forming a fatigue crack with sufficiently high slip to propagate the crack through the grain boundary between the two grains, rather than trying to predict from the statistical approach of our computational modeling efforts.
The full set of instantiations models ~2.3 million grains of Ti-6Al-4V. Out of this set of grains, roughly 45.4% are primary $\alpha$ grains, and in total, only 17,557 (or 0.77%) of the full dataset fulfill the experimentally informed candidate fatigue crack formation grain criteria. Furthermore, when selecting for candidate fatigue crack formation grains from the computational extreme value statistical analysis, the number of grains fulfilling both criteria reduces even further, shown in Tables 5.2 and 5.3 below. It should be noted that since each SVE instantiation was loaded under both strain ratios, some grains can be candidate grains for both FIPs and/or loading conditions. There was no single grain that was an EV FIP grain for all three combinations of FIPs and strain ratios out of the entire dataset.

The statistically rare event nature of fatigue crack formation and early growth is reflected in these statistics. However, as there is a relatively large number of candidate grains in the dataset, but only a few grains that are undergoing sufficiently large enough local plastic deformation to be defined as an EV FIP candidate grain, there must be other local neighborhood effects contributing to these fatigue hot-spots.
Table 5.2: Comparison number of total grains in SVE ensemble, number of primary-\(\alpha\) grains, number of experimentally informed candidate \(\alpha\) grain pairs, and number of grains that fulfill both experimental and computational criteria.

<table>
<thead>
<tr>
<th>Micro.</th>
<th>Peak applied strain</th>
<th>Grains in SVE ensemble</th>
<th>(\alpha) grains</th>
<th>(\alpha) grain pairs</th>
<th>(\text{FIP}_{FS}, R_e = -1)</th>
<th>(\text{FIP}_{FS}, R_e = 0.1)</th>
<th>(\text{FIP}_{GBI}, R_e = 0.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1 2x 3070</td>
<td>0.4%</td>
<td>68,239</td>
<td>20,799</td>
<td>360</td>
<td>5</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>T1 2x 3070</td>
<td>0.8%</td>
<td>67,652</td>
<td>20,896</td>
<td>357</td>
<td>13</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>T1 2x 3070</td>
<td>1.2%</td>
<td>68,220</td>
<td>20,949</td>
<td>365</td>
<td>22</td>
<td>16</td>
<td>3</td>
</tr>
<tr>
<td>T1 2x 6040</td>
<td>0.4%</td>
<td>67,548</td>
<td>40,649</td>
<td>737</td>
<td>28</td>
<td>39</td>
<td>0</td>
</tr>
<tr>
<td>T1 2x 6040</td>
<td>0.8%</td>
<td>67,595</td>
<td>40,674</td>
<td>689</td>
<td>12</td>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>T1 2x 6040</td>
<td>1.2%</td>
<td>67,197</td>
<td>40,424</td>
<td>681</td>
<td>12</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>T1 3x 3070</td>
<td>0.4%</td>
<td>59,461</td>
<td>18,210</td>
<td>335</td>
<td>1</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>T1 3x 3070</td>
<td>0.8%</td>
<td>59,027</td>
<td>18,093</td>
<td>301</td>
<td>18</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>T1 3x 3070</td>
<td>1.2%</td>
<td>59,623</td>
<td>18,104</td>
<td>305</td>
<td>11</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>T1 3x 6040</td>
<td>0.4%</td>
<td>59,277</td>
<td>35,578</td>
<td>634</td>
<td>7</td>
<td>7</td>
<td>0</td>
</tr>
<tr>
<td>T1 3x 6040</td>
<td>0.8%</td>
<td>59,651</td>
<td>36,068</td>
<td>613</td>
<td>21</td>
<td>14</td>
<td>11</td>
</tr>
<tr>
<td>T1 3x 6040</td>
<td>1.2%</td>
<td>59,478</td>
<td>35,825</td>
<td>615</td>
<td>8</td>
<td>9</td>
<td>0</td>
</tr>
<tr>
<td>T2 2x 3070</td>
<td>0.4%</td>
<td>67,780</td>
<td>20,876</td>
<td>343</td>
<td>2</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>T2 2x 3070</td>
<td>0.8%</td>
<td>67,958</td>
<td>20,585</td>
<td>381</td>
<td>32</td>
<td>17</td>
<td>4</td>
</tr>
<tr>
<td>T2 2x 3070</td>
<td>1.2%</td>
<td>67,904</td>
<td>20,785</td>
<td>355</td>
<td>13</td>
<td>29</td>
<td>5</td>
</tr>
<tr>
<td>T2 2x 6040</td>
<td>0.4%</td>
<td>67,517</td>
<td>40,617</td>
<td>634</td>
<td>4</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>T2 2x 6040</td>
<td>0.8%</td>
<td>67,589</td>
<td>40,617</td>
<td>712</td>
<td>8</td>
<td>14</td>
<td>7</td>
</tr>
<tr>
<td>T2 2x 6040</td>
<td>1.2%</td>
<td>67,398</td>
<td>40,465</td>
<td>632</td>
<td>13</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>T2 3x 3070</td>
<td>0.4%</td>
<td>59,588</td>
<td>18,083</td>
<td>280</td>
<td>5</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>T2 3x 3070</td>
<td>0.8%</td>
<td>59,258</td>
<td>17,984</td>
<td>314</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>T2 3x 3070</td>
<td>1.2%</td>
<td>59,162</td>
<td>18,226</td>
<td>280</td>
<td>10</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>T2 3x 6040</td>
<td>0.4%</td>
<td>59,260</td>
<td>35,779</td>
<td>585</td>
<td>0</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>T2 3x 6040</td>
<td>0.8%</td>
<td>59,186</td>
<td>35,703</td>
<td>635</td>
<td>7</td>
<td>7</td>
<td>5</td>
</tr>
<tr>
<td>T2 3x 6040</td>
<td>1.2%</td>
<td>59,240</td>
<td>35,978</td>
<td>651</td>
<td>10</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>T3 2x 3070</td>
<td>0.4%</td>
<td>67,831</td>
<td>20,607</td>
<td>350</td>
<td>4</td>
<td>7</td>
<td>4</td>
</tr>
<tr>
<td>T3 2x 3070</td>
<td>0.8%</td>
<td>67,954</td>
<td>20,793</td>
<td>315</td>
<td>6</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>T3 2x 3070</td>
<td>1.2%</td>
<td>68,148</td>
<td>20,825</td>
<td>371</td>
<td>8</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>T3 2x 6040</td>
<td>0.4%</td>
<td>67,315</td>
<td>40,534</td>
<td>714</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>T3 2x 6040</td>
<td>0.8%</td>
<td>67,471</td>
<td>40,678</td>
<td>716</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>T3 2x 6040</td>
<td>1.2%</td>
<td>67,462</td>
<td>40,754</td>
<td>640</td>
<td>22</td>
<td>9</td>
<td>2</td>
</tr>
<tr>
<td>T3 3x 3070</td>
<td>0.4%</td>
<td>59,224</td>
<td>18,083</td>
<td>315</td>
<td>2</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>T3 3x 3070</td>
<td>0.8%</td>
<td>59,337</td>
<td>18,150</td>
<td>296</td>
<td>4</td>
<td>14</td>
<td>5</td>
</tr>
<tr>
<td>T3 3x 3070</td>
<td>1.2%</td>
<td>59,925</td>
<td>18,301</td>
<td>305</td>
<td>2</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>T3 3x 6040</td>
<td>0.4%</td>
<td>59,396</td>
<td>35,969</td>
<td>578</td>
<td>2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>T3 3x 6040</td>
<td>0.8%</td>
<td>59,124</td>
<td>35,692</td>
<td>586</td>
<td>4</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>T3 3x 6040</td>
<td>1.2%</td>
<td>59,324</td>
<td>35,755</td>
<td>577</td>
<td>5</td>
<td>5</td>
<td>2</td>
</tr>
</tbody>
</table>
Table 5.3: Comparison of number of EV FIP types that fulfill criteria for experimentally informed candidate grains.

<table>
<thead>
<tr>
<th>EV FIP types</th>
<th>No. of candidate grains</th>
<th>% of total grains</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = -1</td>
<td>194</td>
<td>0.00848%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = -1</td>
<td>194</td>
<td>0.00848%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1</td>
<td>149</td>
<td>0.00651%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1</td>
<td>90</td>
<td>0.00393%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = -1 + FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1</td>
<td>110</td>
<td>0.00481%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = -1 + FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1</td>
<td>17</td>
<td>0.00074%</td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1 + FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;ε&lt;/sub&gt; = 0.1</td>
<td>19</td>
<td>0.00083%</td>
</tr>
</tbody>
</table>

5.3.2 Extensions to MKS framework for computing neighborhood spatial correlations

Adapting the above PyMKS approach to non-periodic microstructures requires an additional step of applying ‘padding’ to the discretized microstructure representation to ensure that vectors larger than the spatial vectors of the microstructure can wrap around any edge of the volume. In a non-periodic microstructure, S<sub>t</sub> can no longer be reduced to S. For a three-dimensional SVE of volume S<sup>3</sup>, by adding pads of width T so that the SVE side is now (S + T). Very high values of T can result in meaningless answers, so for this work, T < \frac{S}{2}. Let this padded microstructure be denoted by M<sup>n</sup> u<sub>ε</sub>. This allows use of DFTs to compute \( \tilde{m}_k^u = \mathcal{F}(M_u^m) \) where the padding is essentially an additional phase where all of the microstructure values are 0. By padding the microstructure, non-periodic boundary conditions can be accounted for while meeting the requirements to calculate the spatial correlations in DFT space [144]. The concept of padding a microstructure can be further extended to ‘masking’ the microstructure by any set of criteria a researcher could design. A masked region can be defined within the existing region, with the areas of interest masked in the same way that padding is applied, given that the spatial correlations of the unmasked volume are properly normalized. Padding still must be applied to masked microstructure to enforce periodic boundary conditions for DFT calculations.

The neighborhood statistics presented here have been developed to apply spatial correlations and PCA to these probable fatigue crack formation grain neighborhoods. A
schematic of the masking and padding operations is shown below in Figure 5.3. The FIPs are computed from the CPFEM stress-strain results, and the EV FIP locations are determined (Fig. 5.3.2). It is critical to note that the EV FIPs are only used to locate the grains of interest for fatigue crack formation, but then grain phase and orientation information are the only microstructure data included in the computed spatial correlations, marked at fatigue hot-spots. One mask is applied to the SVE instantiation and excludes the voxels of all grains that are not coincident with an EV FIP location (Fig. 5.3.3a). The other is applied to mask a user-defined ‘grain neighborhood’ surrounding the EV FIP grain; in this case, a grain neighborhood is defined as the 1st NN grains surrounding an EV FIP grain (Fig. 5.3.3b). Both masks are padded by 16 voxels (less than half the number of voxels per side) in all 3 dimensions to enforce periodic boundary conditions (Fig. 5.3.4a-b).

Figure 5.4: Two-dimensional schematic of masking and padding of grain neighborhoods at the location of an EV FIP grain. Grain colors refer to grain ID number in Dream.3D generation.

Neighborhood spatial correlations are applied to both masked and padded microstructures, which are then are convoluted together to ensure that either the heads or tails of every 2-point vector are located in the EV FIP grain. An example schematic of such a convolution
is shown in Figure 5.5 for a simple two-phase microstructure.

Figure 5.5: Schematic of neighborhood spatial correlation convolution. a) is the example two phase microstructure, b) shows all correlations between all ‘gray’ phase voxels, c) identifying two voxels of interest, d) is the result of the convolution of the two voxels with respect to all other gray phase voxels.

Once these neighborhood correlations are convoluted, principal component analysis is utilized to reduce the dimensionality of this data. It was determined that using $L = 90$ GSH bases and 29 principal components was sufficient to capture over 99% of the spatial correlations.

5.4 Grain neighborhood correlations of candidate grains

Following the above approach, spatial correlations were computed for each candidate grain neighborhood and reduced using PCA. For brevity, only a select few plots are shown here, with the remainder in Appendix C. The clustering of EV FIP candidate grains can be seen in Figure 5.6 from the first two PC dimensions, which are the dimensions with the largest variance and second-largest variance, respectively for T1 2x 30 candidate grain neighborhoods loaded to a peak strain of 0.4%. For this microstructure, which compares 9 EV FIP
grain neighborhoods with all possible candidate grain neighborhoods, a clear clustering is shown for the EV FIP cases, along a front-like feature. There bulk of the non-EV grain neighborhoods cluster away from the EV FIP locations, though there is some overlap.

Figure 5.6: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of T1 2x 30 microstructure loaded to a nominal peak strain of 0.4%.

The PC plots are shown for same microstructure at higher nominal peak strain of 0.8% strain in Figure 5.7 and 1.2% strain in Figure 5.8. Clustering is still fairly clear at 0.8% strain, with most EV FIP grain neighborhoods along a front of similar PC2 values. There are some outlier EV FIPGBI grain neighborhoods outside of the cluster, but the bulk remain inside the cluster. When the applied strain is increased to 1.2% nominal peak strain, the EV FIP grains become more scattered away from the primary front.

For the remaining microstructures and strains, similar clustering is seen in each plot of the PC scores of the reduced order models of the candidate grain neighborhoods.
Figure 5.7: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores T1 2x 30 microstructure loaded to a nominal peak strain of 0.8%.

Figure 5.8: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores T1 2x 30 microstructure loaded to a nominal peak strain of 1.2%.
5.5 Feedforward neural network classification of grain neighborhoods

Two versatile approaches for building ROMs currently in use are feedforward neural networks (FFNNs) [187, 188] and Bayesian inference [189, 190]. FFNNs utilize successive linear transformations and nonlinear activations to connect input features to output features by producing new features. This nonparametric approach allows FFNNs to successfully model input and outputs with a highly nonlinear relationship. On the other hand, Bayesian inference offers an assessment of uncertainty in creating predictive ROMs [190]. Machine learning techniques in recent years have combined these two tools by utilizing variational Bayesian inference (VBI) [189, 191, 192] to first estimate the uncertainty of the transformation layers of a FFNN, which is then propagated forward to provide an estimate of the uncertainty for the output predictions. Here, a VBI-FFNN-ROM (Variational Bayesian Inference incorporated Feed Forward Neural Network Reduced Order Model) is trained on the dataset of the reduced spatial correlations of candidate grain neighborhoods, to classify the EV FIP candidate grain neighborhoods from the experimental criteria-only candidate grain neighborhoods. Since most machine learning algorithms assume that the dataset has equal number of samples in each class, discriminating between classes efficiently in imbalanced datasets is a very challenging task. Here, experimental-only candidate grain neighborhoods outnumber the EV FIP candidate grain neighborhoods by two orders of magnitude. Several methods have been proposed to address this problem which typically involve restructuring the dataset to reduce the imbalance between the minority and majority samples. Examples of these methods include upsampling, downsampling, and Synthetic Minority Oversampling Technique. The statistically rare-event nature of fatigue crack formation causes this dataset to be heavily populated with 'safe' (non-EV) candidate grain neighborhoods. The upsampling technique is advantageous in this case, wherein the positively classified neighborhoods are repeated in the training dataset in order to reduce the imbalance to zero. The training dataset is then reshuffled to ensure that the gradient descent
process encounters the same number of EV and non-EV neighborhoods in each cycle of training. Nine models are trained with three hidden layers for varying numbers of parameters for a train/test split of 80%/20%. Each of the 12 Ti-6Al-4V microstructures’ candidate grain neighborhoods are included for each case, which separates the dataset by FIP type, strain ratio, and nominal peak strain. The results are shown in Table 5.4.

Table 5.4: Results from training VBI-FFNN-ROM to classify EV FIP grain candidate neighborhoods.

<table>
<thead>
<tr>
<th>Case</th>
<th>NN layers</th>
<th>Activation</th>
<th>Batch norm</th>
<th>Results</th>
<th>Train</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = -1, 0.4%</td>
<td>60, 40, 10</td>
<td>ReLU6, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>41/44</td>
<td>10/11</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = -1, 0.8%</td>
<td>50, 40, 20</td>
<td>ReLU6, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>83/86</td>
<td>21/22</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = -1, 1.2%</td>
<td>60, 20, 10</td>
<td>ReLU, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>59/68</td>
<td>16/18</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 0.4%</td>
<td>50, 30, 20</td>
<td>ReLU6, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>26/28</td>
<td>8/9</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 0.8%</td>
<td>60, 30, 10</td>
<td>ReLU, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>49/52</td>
<td>12/13</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;FS&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 1.2%</td>
<td>60, 40, 20</td>
<td>ReLU6, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>56/60</td>
<td>13/15</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 0.4%</td>
<td>60, 30, 20</td>
<td>ReLU6, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>15/16</td>
<td>5/5</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 0.8%</td>
<td>50, 40, 10</td>
<td>ReLU, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>33/36</td>
<td>8/10</td>
<td></td>
</tr>
<tr>
<td>FIP&lt;sub&gt;GBI&lt;/sub&gt;, R&lt;sub&gt;e&lt;/sub&gt; = 0.1, 1.2%</td>
<td>50, 30, 20</td>
<td>ReLU, ReLU, ReLU</td>
<td>Y, Y, Y</td>
<td>29/30</td>
<td>7/8</td>
<td></td>
</tr>
</tbody>
</table>

For the EV FIP<sub>FS</sub> candidate grains identified for the SVE ensembles loaded to a nominal peak strain of 0.4% under fully-reversed (R<sub>e</sub> = -1) conditions, the trained NN used 60 weights in the first hidden layer, and 40 and 10 in the second and third hidden layers, respectively. There are a total of 55 EV FIP candidate grain neighborhoods used for training the NN, and it was split into a training dataset of 44 EV FIP candidate grains and a test dataset of 11 EV FIP candidate grains. Once the model was trained, it had 41 positive classifications of EV FIP candidate grains out of the 44 total for the training dataset. For each layer, after the inputs are multiplied by the weights in a node and summed together, the resulting sum is transformed by an activation function. In this case, each layer was transformed using a rectified linear unit (ReLU) activation function which returns the value if the value is greater than 0 and returns 0 if the value is less than zero, \( g(x) = \max\{0, x\} \). For weights that oscillate too greatly in the initial iterations, a modified ReLU is used,
ReLU6, which is more stable. The ReLU6 activation function compares the returned value of a ReLU to a value of 6, and returns the minimum, \( g(x) = \min(\max\{0, x\}, 6) \). Each layer is batch normalized to minimize variation between layers. When the trained model was then applied to the test dataset of 11 EV FIP candidate grain neighborhoods, and the model correctly classified 10, for a success rate of 90%. The remaining cases all show a high percentage of classifying the EV FIP candidate grains for each of their respective cases.

These results show that the trained VBI-FFNN-ROM is highly accurate in predicting an EV FIP candidate grain neighborhood from an experimental-only candidate grain neighborhood. This suggests that capturing the 1st nearest-neighbor grains of an EV FIP grain is highly accurate at predicting where a fatigue crack would form and grow, by including those grains in the neighborhood spatial correlations and subsequent PCA dimensionality reduction.

### 5.6 Summary and conclusions

In this chapter, candidate grains for fatigue crack formation and early growth were defined using two sets of criteria, one from experimental literature, the other following computational methodology laid out here to identify EV FIP grains. From the 12 simulated microstructures of Ti-6Al-4V presented here, candidate grains were identified from the \( \sim 2.4 \) million grains for the experimental criteria, of which 0.77% of grains meet. Only 579 grains total meet both the experimental and computational criteria to qualify as an EV FIP candidate grain. To compare the candidate grains with EV FIP candidate grains, each SVE instantiation where one is located was masked and padded twice. First, only the voxels of the candidate grain were included, and the second includes the voxels of the candidate grain and the surrounding grain neighborhood, here defined as 1st nearest-neighbors grains. The microstructures are padded in all 3 dimensions to enforce periodic boundary conditions. 2-point correlations were first applied across all SVE instantiations of each of the
12 microstructures to check that the discretized microstructure from the MKS approach captures the relevant differences in the microstructure statistics of grain phase and orientation. Then, neighborhood spatial correlations are applied to both masked and padded microstructure instantiations, and subsequently reduced using PCA. Visualizations of the first two PC scores, which capture the largest and second-largest variance of the reduced statistics were plotted for each microstructure at each nominal peak strain. Clustering of the EV FIP candidate grains is evident from the plots, confirming the contributions of grain neighborhoods on a fatigue hot-spot likely to form and grow a fatigue crack. Lastly, nine VBI-FFNN-ROMs were trained on the candidate grain dataset, using three hidden layers, with a train/test split of 80%/20%. The results showed that EV FIP candidate grain neighborhoods were classified by the trained VBI-FFNN-ROMs from the experimental-only candidate grain neighborhoods. Thus, the approach outlined in this chapter shows great promise for predicting grains most likely to both form and grow a fatigue crack.
CHAPTER 6
SUMMARY AND FUTURE WORK

6.1 Overview

6.1.1 General workflows for large scale computational studies of structure-property responses

A workflow was developed to facilitate large-scale studies of structure-property relationships using high-performance computing resources. First, the microstructure of interest (here, bimodal Ti-6Al-4V) must be simulated and discretized, using an available microstructure generator and programmatic workflows for creating large ensembles of SVE instantiations as needed. The relevant statistics of the microstructure must be sufficiently captured in the generated ensemble. The mechanical loading conditions of the material were selected and the ensembles are then loaded using a crystal plasticity software, here ABAQUS. The property response of interest, FIPs, are then computed from the CPFEM results, using a subgrain volume averaging scheme that approximates the damage zone of fatigue crack initiation. Lastly, mesh convergence studies are performed for each scale of the microstructure to mitigate mesh effects and ensure convergence. The significant conclusions of this research include:

(i) By leveraging programmatic workflows and batch processing, large scale design of experiments are feasible with current computing resources, including open-source programs. Such studies create many new possibilities for investigating structure-property responses for a wide range of both materials and loading conditions.

(ii) Given a sufficient understanding of the primary deformation mechanisms and a response marker for the property of interest, this approach is entirely material agnostic,
only using Ti-6Al-4V as an example material system, and can easily be expanded to consider other metal alloy systems.

(iii) These large scale computational studies are critical for furthering the development of combined Integrated Computational Materials Engineering and Materials Data Science and Informatics research, and speeding up materials development in the spirit of the Materials Genome Initiative.

6.1.2 Microstructure ranking for fatigue response

A design of experiments simulation assay was created for bimodal Ti-6Al-4V, including variations on texture, maximum grain size to average grain size ratio, phase volume fraction, strain ratio, and maximum applied strain to investigate the fatigue response over a broad range of applications. From CPFEM results, FIPs were computed that capture the two transgranular mechanisms of fatigue crack formation. Thresholds to determine extreme value FIPs were identified using the peaks-over-threshold approach to extreme value theory, and then the EV FIP distributions were fit to the Generalized Pareto Distributions (GPD). The cumulative distribution functions of the GPDs were plotted to facilitate comparison of fatigue response of the different loading conditions, spanning from high cycle fatigue to low cycle fatigue. Then, the grains that contain extreme FIP values were investigated, to determine whether a singular microstructure attribute sufficiently explains the drive for fatigue crack formation.

(i) In the HCF regime, texture 3, with strong transverse $\alpha$, showed the highest fatigue resistance compared with the other textures regardless of grain size ratio, volume fraction, strain ratio, or FIP type. At this lower strain, all EV FIP grains were primary $\alpha$ grains, which is expected from experimental results that show only ’soft’ primary $\alpha$ grains favorably oriented for basal slip undergo sufficient plastic deformation to form fatigue cracks. The computational methodology used here therefore captures this well.
(ii) In the LCF regime, texture 3 again showed increased fatigue resistance compared with other textures for fully reversed loading, but decreased fatigue resistance for the positive strain ratio case. Texture 2 with a 2x grain size ratio and 30\% volume fraction $\alpha$ grains showed the best resistance of all microstructures for nearly all loading conditions in transition fatigue and LCF.

(iii) By investigating single descriptors of EV FIP grains, it was shown that our methodology is capturing the homogenization of localized plastic deformation as applied strain increases from the HCF through transition regimes.

6.1.3 Neighborhood spatial correlations of experimentally informed fatigue hot-spots of Ti-6Al-4V

From the experimental literature, a set of criteria for candidate primary $\alpha$ grain pairs with a specific orientation to the applied loading and misorientation between the basal planes of each grain were identified as the locations of forming and growing fatigue cracks. Combining that set of criteria with the EV FIP criteria as determined with the POT EV method, candidate primary $\alpha$ grain pairs that meet both sets of criteria were compared against grains that met only the experimental criteria. To investigate the neighborhood effects on fatigue hot-spots, 1$^{st}$ NN grains were included. Then, each candidate hot-spot was masked twice, first only including the primary $\alpha$ grain, secondly including the 1$^{st}$ NN grains. The microstructure was then padded, and neighborhood spatial correlations were applied to both masked and padded neighborhoods, with the correlations convoluted to ensure the tail of each 2-point vector lies in the primary $\alpha$ grain of interest. PCA was then applied to these correlations to reduce the dimensionality and produce a ROM. A VBI-FFNN was trained on this dataset, and was able to classify EV FIP hot-spots from the non-EV FIP candidate grain neighborhoods.

(i) The development of grain neighborhood correlations marked at locations of EV FIP candidate grains following the Materials Knowledge System (MKS) approach is first
presented here.

(ii) It was found that 29 Principal Components (PCs) was sufficient for retaining 99% of the relevant microstructure statistics, and the resulting PC plots show clear clustering of the EV FIP candidate grains in PC space, suggesting that the inclusion of 1st nearest-neighbor grains includes substantial contributions from the coupled microstructure attributes leading to fatigue crack formation.

(iii) Further, by using these reduced PC scores as inputs to the variational Bayesian inference feedforward neural network, the trained model was highly accurate at classifying the EV FIP candidate grains from experimental criteria only candidate grains.

6.2 Recommendations for future work

The intersection of large-scale computational studies of structure-property relationships and materials informatics in this dissertation assist in road-mapping for future work. In this dissertation, some answers are found for specific questions regarding the microstructure effects on Ti-6Al-4V fatigue crack formation but additional questions remain. A brief (but by no means exhaustive) list of possible future research directions are as follows:

(i) The large-scale study of fatigue response of Ti-6Al-4V showed that the FIPs considered here, the Fatemi-Socie and the grain boundary impingement, are well-suited for the HCF regime, but may need to be adjusted for the transition and LCF regimes to better fit the experimental literature data showing the prevalence of crack formation in primary $\alpha$ grain pairs of specific orientation. A suggestion is to add a higher order term in the FIP computation that addresses the character of slip, including the spacing of the dislocations along the slip band, and/or a term that captures the ability/ inability of the other slip systems within the grain to relax the stress concentration from the dislocation pileup within the grain or at the grain/phase boundary.
Additionally, the efforts here have ignored the problem of uncertainty quantification of computing EV FIPs, as it is outside of the current scope of work. Combined with the work done by Whelan and McDowell [193], which showed that including the top 400 EV FIPs is most effective at reducing noise uncertainty, a much larger computational study can be considered. In the current work, the number of EV FIPs that met the POT criteria averaged about 330 EV FIPs for each microstructure/loading condition, for ~35,000 EV FIP grains identified from our computational efforts. As shown in Chapter 5, out of the 6.5 million grains simulated, only 17,500 fulfilled the experimental criteria. Only 773 grains fulfilled both the computational FIP criteria and the experimental criteria. Given the uncertainty is reduced with 400 EV FIPs per microstructure/loading condition, this suggest the current study is far too small to adequately reduce its uncertainty. A solution would be to generate a much larger initial dataset, where the microstructures can be investigated initially from the reconstructed DREAM.3D microstructures to determine first which grains fulfill the experimental criteria, as this can be determined from the microstructure alone. Once an appropriate number of SVE instantiations with experimentally informed candidate grain pairs are identified, only those SVE instantiations would require CPFEM loading. The SVE instantiations that do not contain a candidate grain can be safely ignored. This would greatly reduce the computational effort as the CPFEM step requires the longest computational time. Then, the EV FIP distributions of these experimentally informed candidate grains can be computed from the FIPs and subsequent thresholds to define the extreme values. Such an approach should better correspond to the experimental data and, critically, reduce uncertainty within our computational approach for more accurate rank ordering of fatigue response of a material.

Recently, researchers at University of Michigan have developed an open-source CPFEM software alternative, PRedictive Integrated Structural Materials Science (PRISMS) and implemented the McDowell group fatigue pipeline in PRISMS-
Fatigue [194, 195]. PRISMS-Plasticity shows promising reductions in computational time for CPFEM simulations while leveraging high-performance computing resources, which greatly increases the size of volume element that can be investigated in a structure-property study. For fatigue, this would mean a larger SVE instantiation size that better or fully captures the longer wavelength spatial correlations that are a caveat which was neglected for this current work. By being able to run CPFEM simulations on a larger SVE volume, key microstructure features beyond the 1st nearest-neighbor grains can be captured to compare their effects on fatigue crack formation and early growth.

(iv) Next, the large scale computational study design laid out in Chapter 3 needs to be validated by expanding to investigate the structure-property response of fatigue of another metal alloy material system. This validation would require expertise in the new material, to properly account for the physics of mechanisms operating at each length scale of the multiscale modeling approach. The statistical distributions of microstructure attributes, localized plastic deformation on each active slip system as incorporated into the CPFEM UMAT model, fatigue damage response parameter of interest would all need be changed to reflect the new material system and the primary deformation mechanisms that drive the response of interest. This requires scientific expertise of the material at several length scales to appropriately modify the large scale computational approach at each step as defined in this work. The reconstructed simulated microstructures must incorporate the statistical distributions of attributes of interest of the primary phase(s) as well as secondary or tertiary phase(s) or attributes, e.g., voids, inclusions, precipitates. An appropriate number of SVE instantiations in each SVE ensemble would need to be determined, as well as the size of each instantiation to capture the length scale of the higher-order effects of the fatigue response. The crystal plasticity model would require proper selection of the constitutive equations to reflect the localized deformation processes on the order of the slip systems of
each grain, for each phase/attribute under consideration. The CPFEM model would also require calibration to experimental macroscale stress-strain response. Validation of this approach would come from microstructure rank ordering that matches the experimental literature data of the new material.

(v) On a much longer scale, the neighborhood spatial correlations developed in Chapter 5 will be potentially beneficial to a program providing decisions support for additive manufacturing (AM), especially with the ability to record the microstructure development in situ as it is printed. First, additively manufactured components must be fatigue tested under the relevant loading conditions, which identify the fatigue hot-spots of the material. The relevant neighborhood surrounding these hot-spots would need to be properly identified to encompass the training set for a neural network. Once such a neural network has been trained, it can be coupled with the in situ data of the additive process to identify potential failure sites, rather than explicitly having to individually reconstruct and apply loading to each component. Development of concurrent spatial correlations from actual parts during the additive process would allow for rapid analysis of a component for failure criteria or other design concern, and inform component design to minimize failure likelihood to under a desired factor of safety. Such an approach could help provide quality control assessments for AM printed parts, which is a major current challenge in the field, given that the details of the processing conditions lead to wide variations of the microstructures for the same component.
Appendices
APPENDIX A

GENERALIZED PARETO DISTRIBUTION PEAKS-OVER-THRESHOLD PARAMETERS
<table>
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<th>Micro.</th>
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Table A.1: GPD threshold parameters estimates for EV FIP data (0.4% peak strain).
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Table A.2: GPD threshold parameters fit to EV FIP data (0.4% peak strain).
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Table A.3: GPD threshold parameters estimates for EV FIP data (0.8% peak strain).
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Table A.4: GPD threshold parameters fit to EV FIP data (0.8% peak strain).
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Table A.5: GPD threshold parameters estimates for EV FIP data (1.2% peak strain).
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Table A.6: GPD threshold parameters fit to EV FIP data (1.2\% peak strain).
APPENDIX B

SINGLE DESCRIPTORS OF EXTREME VALUE FIP GRAINS

Figure B.1: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 2x 30\% loaded to 0.4\% strain amplitude for $R_\varepsilon = -1$. Colors on the left refer to phase, on the right refer to normalized FIP value, with size corresponding to grain diameter.

Figure B.2: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 2x 30\% loaded to 0.4\% nominal peak strain for $R_\varepsilon = 0.1$. 

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Figure B.3: Single descriptors of EV FIP_{GBI} grains for microstructure T1 2x 30% loaded to 0.4% nominal peak strain for R_{\varepsilon} = 0.1.

Figure B.4: Single descriptors of EV FIP_{FS} grains for microstructure T1 2x 60% loaded to 0.4% strain amplitude for R_{\varepsilon} = -1.

Figure B.5: Single descriptors of EV FIP_{FS} grains for microstructure T1 2x 60% loaded to 0.4% nominal peak strain for R_{\varepsilon} = 0.1.
Figure B.6: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T1 2x 60% loaded to 0.4% nominal peak strain for $R_\varepsilon = 0.1$.

Figure B.7: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 3x 30% loaded to 0.4% strain amplitude for $R_\varepsilon = -1$.

Figure B.8: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T1 3x 30% loaded to 0.4% nominal peak strain for $R_\varepsilon = 0.1$. 

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Figure B.9: Single descriptors of EV FIP\(_{\text{GBI}}\) grains for microstructure T1 \(3x\) 30\% loaded to 0.4\% nominal peak strain for \(R_\varepsilon = 0.1\).

Figure B.10: Single descriptors of EV FIP\(_{\text{FS}}\) grains for microstructure T1 \(3x\) 60\% loaded to 0.4\% strain amplitude for \(R_\varepsilon = -1\).

Figure B.11: Single descriptors of EV FIP\(_{\text{FS}}\) grains for microstructure T1 \(3x\) 60\% loaded to 0.4\% nominal peak strain for \(R_\varepsilon = 0.1\).
Figure B.12: Single descriptors of EV FIP_{GBI} grains for microstructure T1 3x 60% loaded to 0.4% nominal peak strain for R_e = 0.1.

Figure B.13: Single descriptors of EV FIP_{FS} grains for microstructure T2 2x 30% loaded to 0.4% strain amplitude for R_e = -1.

Figure B.14: Single descriptors of EV FIP_{FS} grains for microstructure T2 2x 30% loaded to 0.4% nominal peak strain for R_e = 0.1.
Figure B.15: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T2 2x 30% loaded to 0.4% nominal peak strain for $R_e = 0.1$.

Figure B.16: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T2 2x 60% loaded to 0.4% strain amplitude for $R_e = -1$.

Figure B.17: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T2 2x 60% loaded to 0.4% nominal peak strain for $R_e = 0.1$. 

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Figure B.18: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T2 2x 60\% loaded to 0.4\% nominal peak strain for $R_e = 0.1$.

Figure B.19: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T2 3x 30\% loaded to 0.4\% strain amplitude for $R_e = -1$.

Figure B.20: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T2 3x 30\% loaded to 0.4\% nominal peak strain for $R_e = 0.1$. 

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Figure B.21: Single descriptors of EV FIP_{GBI} grains for microstructure T2 3x 30% loaded to 0.4% nominal peak strain for R_\varepsilon = 0.1.

Figure B.22: Single descriptors of EV FIP_{FS} grains for microstructure T2 3x 60% loaded to 0.4% strain amplitude for R_\varepsilon = -1.

Figure B.23: Single descriptors of EV FIP_{FS} grains for microstructure T2 3x 60% loaded to 0.4% nominal peak strain for R_\varepsilon = 0.1.
Figure B.24: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T2 3x 60% loaded to 0.4% nominal peak strain for R\textsubscript{e} = 0.1.

Figure B.25: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T3 2x 30% loaded to 0.4% strain amplitude for R\textsubscript{e} = -1.

Figure B.26: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T3 2x 30% loaded to 0.4% nominal peak strain for R\textsubscript{e} = 0.1.
Figure B.27: Single descriptors of EV FIP_{GBI} grains for microstructure T3 2x 30% loaded to 0.4% nominal peak strain for R_e = 0.1.

Figure B.28: Single descriptors of EV FIP_{FS} grains for microstructure T3 2x 60% loaded to 0.4% strain amplitude for R_e = -1.

Figure B.29: Single descriptors of EV FIP_{FS} grains for microstructure T3 2x 60% loaded to 0.4% nominal peak strain for R_e = 0.1.
Figure B.30: Single descriptors of EV FIP_{GBI} grains for microstructure T3 2x 60% loaded to 0.4% nominal peak strain for R_ε = 0.1.

Figure B.31: Single descriptors of EV FIP_{FS} grains for microstructure T3 3x 30% loaded to 0.4% strain amplitude for R_ε = -1.

Figure B.32: Single descriptors of EV FIP_{FS} grains for microstructure T3 3x 30% loaded to 0.4% nominal peak strain for R_ε = 0.1.
Figure B.33: Single descriptors of EV FIP\textsubscript{GBI} grains for microstructure T3 3x 30\% loaded to 0.4\% nominal peak strain for $R_e = 0.1$.

Figure B.34: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T3 3x 60\% loaded to 0.4\% strain amplitude for $R_e = -1$.

Figure B.35: Single descriptors of EV FIP\textsubscript{FS} grains for microstructure T3 3x 60\% loaded to 0.4\% nominal peak strain for $R_e = 0.1$. 

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Figure B.36: Single descriptors of EV FIP_{GBI} grains for microstructure T3 3x 60% loaded to 0.4% nominal peak strain for R_e = 0.1.
APPENDIX C

SPATIAL NEIGHBORHOOD CORRELATIONS OF CANDIDATE GRAINS FOR FATIGUE CRACK INITIATION

Figure C.1: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 30% loaded to peak strain of 0.4%.
Figure C.2: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 30% loaded to peak strain of 0.8%.

Figure C.3: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 30% loaded to peak strain of 1.2%.
Figure C.4: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 60% loaded to peak strain of 0.4%.

Figure C.5: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 60% loaded to peak strain of 0.8%.
Figure C.6: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 2x 60% loaded to peak strain of 1.2%.

Figure C.7: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 30% loaded to peak strain of 0.4%.
Figure C.8: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 30% loaded to peak strain of 0.8%.

Figure C.9: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 30% loaded to peak strain of 1.2%.
Figure C.10: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 60% loaded to peak strain of 0.4%.

Figure C.11: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 60% loaded to peak strain of 0.8%.
Figure C.12: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T1 3x 60% loaded to peak strain of 1.2%.

Figure C.13: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 2x 30% loaded to peak strain of 0.4%.
Figure C.14: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 2x 30% loaded to peak strain of 0.8%.

Figure C.15: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 2x 30% loaded to peak strain of 1.2%.
Figure C.16: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 3x 30% loaded to peak strain of 0.4%.

Figure C.17: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 3x 30% loaded to peak strain of 0.8%.
Figure C.18: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T2 3x 30% loaded to peak strain of 1.2%.

Figure C.19: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 2x 30% loaded to peak strain of 0.4%.
Figure C.20: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 2x 30% loaded to peak strain of 0.8%.

Figure C.21: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 2x 30% loaded to peak strain of 1.2%.
Figure C.22: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 3x 30% loaded to peak strain of 0.4%.

Figure C.23: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 3x 30% loaded to peak strain of 0.8%.
Figure C.24: Visualization of fatigue hot-spot neighborhoods from PCA showing the first two PC scores of microstructure T3 3x 30% loaded to peak strain of 1.2%.
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