Strategies for rapid parametric assessment of microstructure-sensitive fatigue for HCP polycrystals

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1. Introduction

Titanium and its alloys have attractive strength-to-weight ratios and corrosion resistance, both of which are vital for the aerospace, automotive, and biomedical industries. The α-phase of titanium has a hexagonal close packed (HCP) crystal structure while the β-phase has a body centered cubic (BCC) crystal structure. In general, titanium alloys can be categorized as α or near α, α + β, or β alloys [1]. Titanium alloys exhibit an enormous diversity of microstructure arrangements resulting from the combined effect of composition and thermo-mechanical processing routes [2]. Furthermore, these microstructures are characterized by elastic and inelastic anisotropy at multiple length-scales [3–6]. This variation in microstructure and resultant mechanical properties can lead to competing objectives in the material selection or optimization process.

Fatigue resistance is an important performance characteristic for titanium alloys because of their applications of use. Experimental evaluation of the fatigue resistance of materials is costly and labor intensive. In addition, the information extracted is often limited to simple metrics such as the number of cycles to failure. Unfortunately, it can be difficult to relate this data to microstructure features or parameters (FIPs); however, the practical viability of employing CPFEM for microstructure-sensitive design of polycrystalline microstructures...
for improved high cycle fatigue (HCF) performance is rather limited due to the high demands placed on computational resources.

To circumvent the difficulties mentioned above, an alternative approach is proposed in this work that leverages modern machine learning techniques to significantly reduce the computational cost of evaluating the HCF performance of polycrystalline materials. Specifically, this approach takes advantage of a convenient trait of the HCF regime; the magnitudes of the cyclic plastic strains are generally much lower than the magnitudes of the cyclic elastic strains. This feature enables the use of the recently developed Materials Knowledge System (MKS) to efficiently predict the elastic strain fields in the polycrystalline microstructures [6,10–14].

Recent years, Smith et al. [23] calibrated the model to three distinct candidate microstructures. In this work, these novel protocols are demonstrated for the analysis of the HCF resistance of a diverse set of α-titanium microstructures subjected to uniaxial loading conditions. This represents the first use of the MKS framework to accelerate fatigue analyses.

2. Background

2.1. Crystal plasticity framework

The anisotropic deformation response of polycrystalline materials can be simulated using crystal plasticity [9,15,16] to successfully rank-order the HCF resistance of different α-titanium microstructures. Specifically, the crystal plasticity framework considered in this work was initially developed as a CPDEM model for 2D analysis of duplex Ti-6Al-4V [17], was extended to 3-D [18], and then further modified by various authors [19–23]. Most recently, Smith et al. [23] calibrated the model to three distinct titanium alloy microstructures via uniaxial tension and fully-reversed tension-compression experimental data (employing periodic boundary conditions for uniaxial stress in simulation). In the remainder of this section, the features of this crystal plasticity framework relevant to the present modeling of α-titanium are discussed in detail (features relevant to the modeling of α-β titanium colony grains are not discussed).

HCP crystal structures have the following slip systems: (i) basal slip \{0001\}(1120), (ii) prismatic slip \{1010\}(1120), (iii) (a) pyramidal slip \{1011\}(1120), (iv) first-order (c+a) pyramidal slip \{1011\}(1123), and (v) second-order (c+a) pyramidal slip \{1122\}(1123). These slip planes and their associated slip directions are shown in Fig. 1.

In the α-phase of Ti-6Al-4V, prismatic slip has the smallest critical resolved shear stress (CRSS), followed by basal slip, while the pyramidal families exhibit much higher slip-resistance values. Deformation twinning can also be present in titanium alloys, but is severely diminished with an Al content above 6% in Ti-6Al-4V [24]. Accordingly, we will only consider slip and will neglect twinning in this study.

The crystal plasticity model employed in this work is based on the two-term multiplicative decomposition of the deformation gradient into elastic and plastic parts (i.e., \( F = F^e \cdot F^p \)). The plastic velocity gradient is determined in the intermediate configuration [15], which is both isoclinic and lattice invariant. The symmetric second Piola-Kirchhoff stress, \( \sigma^{PK2} \), is obtained by application of linear elasticity in the intermediate isoclinic configuration, i.e.,

\[
\sigma^{PK2} = C_0 : F^e
\]

(1)

where \( C_0 \) is the fourth-rank elasticity tensor in the intermediate configuration. The elastic Green strain is defined by

\[
\varepsilon^e = \frac{1}{2} \left[ (F^e)^T \cdot F^e - I \right].
\]

(2)

The Cauchy stress (\( \sigma \)) can be found by mapping the second Piola-Kirchhoff stress to the current configuration, i.e.,

\[
\sigma = \frac{1}{\det(F)} \left[ F^e \cdot \sigma^{PK2} \cdot (F^e)^T \right].
\]

Finally, the resolved shear stress on slip system (\( \zeta \)) is given by

\[
\tau^{(\zeta)} = \sigma^{PK2} : \left( s^{(\zeta)}_h \otimes n^{(\zeta)}_h \right).
\]

(4)

where \( s^{(\zeta)}_h \) and \( n^{(\zeta)}_h \) are the slip direction and slip plane normal, respectively, in the intermediate (and reference) configuration. The isothermal slip system shearing rate, \( \dot{\gamma}^{(\zeta)} \), is defined according to a power-law flow rule of the form

\[
\dot{\gamma}^{(\zeta)} = \frac{\gamma_0 \left( |\tau^{(\zeta)} - \dot{\tau}^{(\theta)}| - \kappa^{(\zeta)} \right)^M \text{sgn}(\tau^{(\zeta)} - \dot{\tau}^{(\theta)})}{D^{(\theta)}}
\]

(5)

where \( \gamma_0 \) is the reference shearing rate coefficient. The drag stress is the back stress, \( \kappa^{(\zeta)} \) is the threshold stress, \( D^{(\theta)} \) is the drag stress, and \( M \) is the inverse strain-rate sensitivity exponent. The threshold stress is defined as the sum of a Hall-Petch strength term and a softening term due to breakdown of short-range order, i.e.,

\[
k^{(\zeta)} = \frac{K_p}{\sqrt{d}} + \kappa^{(\zeta)}.
\]

(6)

In Eq. (6), \( K_p \) is the Hall-Petch slope, \( d \) is the mean slip distance in the α-phase, and \( \kappa^{(\zeta)} \) is a softening parameter. The evolution of the threshold stress is governed solely by the softening term, which follows a dynamic recovery law and takes the form

\[
k^{(\zeta)} = k^{(\zeta)} - \mu \kappa^{(\zeta)} |\dot{\gamma}^{(\zeta)}|.
\]

(7)

The drag stress does not evolve (i.e., \( D^{(\theta)} = 0 \)), while the back stress is initially set to zero and evolves according to a direct hardening/dynamic recovery relation of the form

\[
\dot{\chi}^{(\zeta)} = h\dot{\gamma}^{(\zeta)} - h_0 \chi^{(\zeta)} |\dot{\gamma}^{(\zeta)}|.
\]

(9)

where \( h \) is the direct hardening coefficient and \( h_0 \) is the dynamic recovery coefficient. The parameter values for the crystal plasticity framework described in this section are included below in Table 1 [23].

2.2. Materials knowledge system

In recent years, a computationally efficient localization framework for hierarchical material microstructure called the Materials Knowledge System (MKS) has been developed [6,10–14,26]. The MKS is an algebraic series capable of predicting response fields on the mesoscale given the corresponding macroscale averaged loading or boundary conditions. The details of the MKS framework relevant to its application in the present study are briefly described next.

The response of hierarchical materials systems has been addressed using generalized composite theories [27–34], wherein a localization tensor relates the material response at the mesoscale to the macroscale averaged values. In the case of linear-elastic
response, the fourth-order localization tensor \( A(\mathbf{x}) \) relates the elastic strain at a location in the microstructure, \( \mathbf{x} \), to the average macroscopic strain imposed on the microstructure:

\[
\varepsilon(\mathbf{x}) = A(\mathbf{x}) : (\varepsilon(h))
\]  

(10a)

\[
A(\mathbf{x}) = I - (\Gamma(\mathbf{x}, \mathbf{x}'): C(\mathbf{x}')) + (\Gamma(\mathbf{x}, \mathbf{x}'): C(\mathbf{x}'): \Gamma(\mathbf{x}', \mathbf{x}'): C(\mathbf{x}'')) - \ldots
\]  

(10b)

In Eq. (10b), \( I \) is the fourth-rank identity tensor, \( C(\mathbf{x}) \) is the deviation in elastic stiffness from some arbitrary reference medium at a location \( \mathbf{x} \). \( \Gamma \) is a symmetrized derivative of the Greens function defined with the elastic properties of the reference medium and \( f \) signifies the ensemble average of a variable \( f \) over all spatial locations in the microstructure.

Eq. (10b) can be transformed to a more convenient form through the introduction of the microstructure function, \( m(\mathbf{x}, h) \) [35], which captures the probability density of finding local state \( h \) at the spatial location \( \mathbf{x} \). The local state descriptors are selected in such a manner that allows one to define the local mesoscale properties at the spatial location \( \mathbf{x} \) (these may include phase identifiers, crystal orientation, etc.). Through the introduction of \( m(\mathbf{x}, h) \), substitution of \( r = \mathbf{x} - \mathbf{x} \) and invocation of the ergodic hypothesis, Eqs. (10a) and (10b) can be rewritten as

\[
\varepsilon(\mathbf{x}) = \left( I - \int_{\mathbf{R}} \int_{\mathbf{H}} \mathbf{a}(\mathbf{r}, h) m(\mathbf{x} + \mathbf{r}, h) d\mathbf{r} d\mathbf{h} \right) \varepsilon(h) + \int_{\mathbf{R}} \int_{\mathbf{H}} \mathbf{a}(\mathbf{r}, \mathbf{r}', h) m(\mathbf{x} + \mathbf{r}, h) m(\mathbf{x} + \mathbf{r} + \mathbf{r}', h') d\mathbf{r} d\mathbf{r}' d\mathbf{h} d\mathbf{h}' - \ldots (\varepsilon(h))
\]  

(11)

where \( \mathbf{a}(\mathbf{r}, h) \) and \( \mathbf{a}(\mathbf{r}, \mathbf{r}', h, h') \) are the first- and second-order influence functions [11], respectively. \( H \) is the set of all possible distinct local states \( h \in H \) and \( \mathbf{R} \) is the set of all vectors \( \mathbf{r} \in \mathbf{R} \). The first-order influence functions \( \mathbf{a}(\mathbf{r}, h) \) quantify the contribution to the local response in the current spatial location due to the presence of local state \( h \) at a vector \( \mathbf{r} \) away. Note that the influence functions are fourth-rank tensors and satisfy the mapping established in Eq. (10). The influence functions are computationally advantageous as they are completely independent of microstructure. Eq. (11) is an infinite series where each successive term captures the influence of the local topology for higher levels of interactions between the local states [14]. It is worth noting that when the variation of local properties (or contrast) throughout the range of \( H \) is low, the series in both Eqs. (10b) and (11) can be truncated to the first-order terms with minimal loss of accuracy [6,10,11,14].

Unfortunately, \( \Gamma(\mathbf{r}) \) has a singularity as \( \mathbf{r} \) approaches zero, and the convergence of the series is highly sensitive to the selection of the reference medium. The MKS avoids these computational issues through a calibration of the influence functions using results from numerical simulations (e.g., based on finite element simulations) that include a variety of microstructures and their local response fields. Once the influence functions are calibrated, the resulting linkages can be used to predict the response field of any new microstructure in the materials system at a far lower computational cost than using existing numerical frameworks.

Next, a generalized MKS framework is presented which extends Eq. (11) to complex microstructures (e.g., polycrystalline microstructures studied in this work). First, \( m(\mathbf{x}, h) \) and \( \mathbf{a}(\mathbf{x}, h) \) are expressed as Fourier series using products of orthonormal basis over both the local state space and the spatial domain of the microstructure [6,14]:

\[
m(\mathbf{x}, h) = \sum_{l} \sum_{\mathbf{s}} M_{ls}^{h} Q_{l}(h) \chi_{s}(\mathbf{x}),
\]  

(12)

\[
\mathbf{a}(\mathbf{x}, h) = \sum_{l} \sum_{\mathbf{s}} A_{ls}^{h} Q_{l}(h) \chi_{s}(\mathbf{x})
\]  

(13)
where $Q_l(h)$ and $X_l(x)$ denote the basis indexed by $L$ and $s$, respectively. $X_l(x)$ is referred as the indicator basis and return one for all values of $x$ within the spatial bin indexed by $s$, and zero elsewhere. This uniform discretization of the spatial domain allows for the application of the FFT algorithm in the evaluation of Eqs. (12) and (13). If the same indicator basis is chosen for $Q_l(h)$, the local state space will be binned discretely (e.g., a two phase composite material). If the desired local state space is crystal lattice orientation, this binning strategy proves computationally inefficient as the number of bins required to accurately represent the orientation space is very large (1,944,000 bins for 1 of bins required to represent the orientation space is very large [43]).

Through the utilization of the orthogonality of the bases, expressions for $M^L_s$ and $A^L_t$ can be derived from Eqs. (12) and (13) [14]. Introducing these definitions, the MKS can be expressed as

\[
\varepsilon_s = \left( \sum_{l} \sum_{r} A^L_t \frac{\Delta^L}{N_l} M^L_{s+t} + \sum_{l} \sum_{r} \frac{\Delta^2}{N_l N_{r}} A^L_t \frac{\Delta^L}{M^L_{s+t} M^L_{s+t+r}} + \ldots \right) : (\varepsilon).
\]

where $\Delta$ is the volume of a spatial bin and $N_l$ is a constant that may depend on $L$.

### 2.3. Fatigue indicator parameters

The driving force for growth of long cracks in metals is adequately described by the stress intensity factor in the context of LEFM [37]. In particular, a variety of stress-, strain-, and energy-based relations have been employed to predict fatigue crack growth at the macroscopic length scale [38]. The driving force for small fatigue crack formation and early growth, however, is strongly dependent on the local driving force, which in turn is directly linked to the microstructure of the material and local cyclic slip conditions [39]. Fatigue indicator parameters (FIPs) have been used in macroscale and mesoscale data analysis to serve as surrogate measures of the driving force for fatigue crack nucleation and early growth [40,41].

The HCF regime typically requires more than 100,000 cycles to failure and is characterized by heterogeneous plastic deformation among grains, with the majority of grains undergoing elastic deformation throughout the specimen. The majority of cycles to failure for HCF involves processes of crack nucleation and early growth through the first few grains. Additionally, the fatigue crack formation process is strongly affected by the spatial variation of microstructure features (e.g., grain size, orientation, disorientation) that give rise to heterogeneous stress and plastic strain states. These local elevated states of cyclic plastic shear strain can lead to localized damage and, ultimately, the formation of a single dominant crack that eventually propagates to failure [42]. For example, for Ti-6Al-4V tested at room temperature with $R = 0.1$, more than 85% of the high-cycle fatigue life (strain amplitude not reported) was spent initiating and propagating small cracks up to 0.5 mm in length [43].

Distinct FIPs were introduced [44] to explicitly account for cyclic (reversed) slip per cycle as well as cumulative directional slip and have since been used in conjunction with macroscopic experimental [45–50] and computational [51] data of titanium alloys. FIPs have also been combined with finite element simulations to make life estimates [52,53] and compare the relative fatigue resistance of multiple microstructures or materials [54]. In these cases, the selection of a specific FIP is important to reflect the deformation mechanisms that contribute to fatigue crack formation and early growth. For example, the Fatemi–Socie [40,55] shear-based FIP has been shown to correlate well in the LCF and HCF regimes for multiaxial fatigue crack initiation [56] and is defined by [54].

\[
FIP_{FS} = \frac{\Delta \gamma_{pl}^s}{2} \left[ 1 + k \frac{\sigma_{max}^s}{\sigma_y} \right],
\]

where $\Delta \gamma_{pl}^s$ is the maximum cyclic plastic shear strain range, $\sigma_{max}^s$ is the maximum stress normal to the maximum cyclic plastic shear strain, $\sigma_y$ is the macroscopic yield strength of the material and $k$ is a constant with typical values between 0.5 and 1. The overbar ($\bar{\Delta \gamma_{pl}^s}, \bar{\sigma_{max}^s}$) indicates that volumetric averaging should be performed [54]. In this work, the volumetric averaging is performed over $2 \times 2 \times 2$ voxel regions to better account for the stress and plastic strain in a region and not values from a single material point. The Fatemi–Socie FIP correlates well with fatigue crack formation and early growth for metals that exhibit planar slip [25]; a graphical representation is shown in Fig. 2. Additionally, FIP values can be extended to assist in the calculation of life estimates [52,53,57], which could in turn be used to make a probabilistic prediction of HCF life and capture the scatter associated with these life measurements. The $FIP_{FS}$ in Eq. (15) serves as an effective grain-level surrogate measure for the cyclic crack tip displacement range of small crystallographic fatigue cracks [52]. More recent work has explored length – scale dependent FIPs [58], but these models differ from the one presented here because of the inclusion of strain gradient effects and geometrically-necessary dislocations in the model formulation.

### 2.4. Extreme value statistics

Microstructure locations with the lowest resistance to fatigue crack formation are associated with the largest FIP values identified through Eq. (15). A single FIP value, however, is not sufficient to evaluate a microstructure’s resistance to HCF. Instead, the distribution of the most extreme FIP values for a sufficient volume of material gives some indication of the relative presence of HCF susceptible locations in the microstructure. In previous work [54,59], a statistical approach was taken where multiple instantiations of each microstructure were simulated using CPFEM and the maximum FIP values in each were used to perform an EVD analysis. The FIP distributions were fit to a Gumbel distribution [60], i.e.,

\[
F_{y_n}(y_n) = \exp \left[ -\exp \left( -y_n - \bar{y}_n \right) \right],
\]

\[y_n = \frac{\sigma^{\bar{y}_n}}{\bar{\sigma}^{\bar{y}_n}}, \quad \bar{y}_n = \frac{\bar{\sigma}^{\bar{y}_n}}{\bar{\sigma}^{\bar{y}_n}}\]
where $F_F(y_j)$ is the probability that $Y_n$ will be equal to or less than $y_n$, $u_n$ is the characteristic largest value of the sampled population, and $x_n$ is an inverse measure of dispersion of the largest values of the population. The Gumbel distribution is unbounded and the shape of the probability density function is the same regardless of the population. The Gumbel distribution is re-formulated as a linear function of $y$ with expressions for slope ($x_n$) and y-intercept ($x_n u_n$), i.e.,

$$\ln \left[\frac{1}{F_F(y_n)}\right] = x_n y_n - x_n u_n.$$  \hspace{1cm} (18)

These resultant distributions are the basis for comparing fatigue resistance among different microstructures in this work.

3. Proposed methodology

The main purpose of this work is to explore a novel, computationally-efficient method for rank-ordering the HCF resistance of polycrystalline microstructures. The conventional approach, shown in the bottom row of Fig. 3, adheres to the following steps: (i) digital microstructures are obtained, (ii) CPFEM is used to determine the local cyclic plastic strain tensors, (iii) FIP fields are computed for each microstructure, and (iv) extreme value distributions of FIPs are constructed to rank-order the microstructures in terms of their HCF resistance. The new approach explored in this study (also displayed in Fig. 3) utilizes the MKS method to determine the local total strain fields and calculate the local plastic strain tensors through a decoupled integration scheme that employs the relevant constitutive relations described in Section 2.1. The remainder of this section describes this new approach in detail.

First, a diverse set of microstructures of interest are identified for a given composition as a function of thermo-mechanical process path. Traditionally, a representative volume element (RVE) is established to capture the microstructure for subsequent computational evaluations. RVEs are intended to approximate the response of the overall material microstructure by encompassing a volume that is large enough to contain a sufficient number of microstructure-specific features for statistical homogeneity [62]. Additionally, RVEs must have measurable properties (e.g., elastic modulus, thermal conductivity) that are in agreement with the properties of an extremely large volume of the true material microstructure. Unfortunately, this typically requires performing simulations on prohibitively large volumes of material, especially to describe extreme value phenomena such as HCF. Instead, the microstructures may be represented by an ensemble of smaller statistical volume elements (SVEs), which are constructed such that their size is sufficient to sample microstructure-specific features (e.g., grains), but whose individual responses might differ from that of an RVE. In this framework, a large enough set of SVEs is selected for each microstructure to demonstrate the convergence of a representative property.

Next, if they have not been previously computed for the specific material system being studied, the MKS influence functions are calibrated with an ensemble of calibration SVEs and their responses as computed using linear-elastic FE simulations. These simulations are performed using appropriate periodic boundary conditions for the applied loading of interest and the elastic model parameters given in Table 1. The use of an MKS calibrated with linear-elastic simulations is justified as the cyclic plastic strains in the HCF regime are expected to be orders of magnitude smaller than the elastic strains; therefore the total strains are approximately equal to the elastic strains. Once the Fourier coefficients of the influence function (herein called influence coefficients) are calibrated for each set of boundary conditions and for all unique components of the strain tensor, Eq. (14) is employed to efficiently predict the elastic strain fields in each SVE at the minimum and maximum applied strains in strain-controlled cyclic loading. The stress tensor is calculated from the strain tensor in each voxel for the local fourth-order elastic stiffness tensor (see Eq. (1)). Assuming a linear relationship between the initial and final stress tensors, each loading segment is discretized into a number of increments. The stress tensor is then used to determine the resolved shear stress in each slip system ($\tau^{(i)}$) for each time increment, according to

$$\tau^{(i)} = \sigma : (s^{(i)} \otimes n^{(i)}),$$  \hspace{1cm} (19)

where $s^{(i)}$ and $n^{(i)}$ are the slip direction and slip plane normal, respectively. The resolved shear stress is then used to solve for the slip system shearing rate (Eq. (5)) and evolution equations.
(Eqs. (7) and (9)) in each time increment. A forward Euler routine, commonly used in explicit CPFEM simulations [63], is employed to obtain the cumulative plastic strains on the slip systems. Finally, the plastic strain tensor at a time indexed by $i$ may be approximated as

$$\varepsilon_i^p = \sum_\xi \tau_i^{(\xi)} (s^{(\xi)} \otimes n^{(\xi)})_{sym},$$

from the associated cumulative plastic shear strains. This method accounts for the spatial variance of the local fatigue response in the digital microstructures due to local crystal orientations. As such, the local stress/strain quantities and derivative quantities account for the geometric imperfections present in the digital microstructure, which are primarily the grain boundaries for this study.

A graphical representation of this procedure is shown in Fig. 4. The back stress and plastic shear strain are initialized at zero for each slip system. The plastic strain quantities are orders of magnitude smaller than the total strain quantities in the HCF regime, and each slip system. The plastic strain quantities are scales orders of magnitude smaller than the total strain quantities in the HCF regime, and therefore their impact on redistribution of the stress and total strain tensors relative to the elastic solution are minimal. Accordingly, phenomena of cyclic stress redistribution and relaxation are neglected in this work, as well as local lattice rotation.

Finally, FIP fields are computed in all SVEs using Eq. (15), and the extreme value distributions are extracted following the procedures of Section 2.4. Through the FIP EVDS, microstructures may be rank-ordered by their resistance to HCF.

4. Case study

To demonstrate the protocols described in Section 3, four different $\alpha$-titanium microstructures in three separate loading directions are rank-ordered by their HCF resistance. Synthetic microstructure volumes are first generated using the open-source DREAM.3D software. The MKS is then calibrated with linear-elastic FE simulations and employed to predict elastic strain fields in the volumes. Stresses are calculated from the elastic strain fields and the integration scheme is used to compute the cyclic plastic strains. These quantities are used to calculate the FIP fields in each SVE. The microstructures and loading directions are rank-ordered by their HCF resistance through a comparison of the FIP EVDS. The details of this case study are provided in the remainder of this section.

4.1. Digital microstructures

Four crystallographic textures are selected for analysis in this work: (a) random, (b) $\beta$-annealed, (c) transverse, and (d) basal/transverse. The $\beta$-annealed texture is taken from previous work [23] while the other textures are extracted from the literature [2,64–66]. All three-dimensional digital microstructures are generated using the open-source DREAM.3D software [67] with inputs of desired grain-size, orientation, and misorientation distributions. The grain-size distribution for all microstructures is modeled as a log-normal distribution with a mean and standard deviation of 30 $\mu$m and 15 $\mu$m, respectively. The instantiated microstructures contain 9,261 hexahedron elements, each with 8 integration points (i.e., C3D8-type in ABAQUS 6.10-1 [68]) and an individual side length of 10 $\mu$m. Each digital SVE has a total side-length of 210 $\mu$m in the x-, y-, and z-directions. A total of 500 SVEs are instantiated for each of the four microstructures and their statistics are compared to the desired statistics. Representative pole figures for each microstructure analyzed in this work are shown in Fig. 5. DREAM.3D is used to generate the fully periodic microstructures employed in this work.

To determine how many SVEs are adequate to approximate an RVE, the mean and standard deviation of a particular value of interest (elastic stiffness in this instance) are compared with tolerance values [69]. The details of these calculations are provided in the Appendix. As shown in Fig. 6, the mean of the elastic stiffness converges extremely quickly (in fewer than 50 simulations) for loading in each direction while the standard deviation requires approximately 250 simulations for each loading direction. Similar results are found for the other textures.

4.2. MKS model calibration

The MKS framework described in Section 2.2 was successfully employed in prior work for the prediction of elastic strain fields in polycrystalline HCP microstructures with a wide range elastic constants, resulting in a variety of contrasts between local constituents [6,14]. In this study, however, the influence coefficients of Eq. (13) are re-calibrated for the set of elastic parameters in Table 1. Truncation to the first term of Eq. (14) is justified as $\alpha$-titanium single crystals exhibit low contrast (e.g., the ratio of the highest modulus to the lowest modulus is approximately 1.40); prior work has shown that this truncation provides excellent results for composite systems with low to moderate contrasts [6,10–12,14]. Consequently, the influence coefficients calibrated in this work are expected to provide high prediction accuracy for the textures under consideration. Furthermore, only fifteen GSH
basis functions are employed in Eqs. (12) and (13), as it has been previously demonstrated that this is sufficient for the prediction of the elastic response of hexagonal polycrystals [6]. The influence coefficients are calibrated for all unique components of the strain tensor for three different loading directions.

The influence coefficients are calibrated using the linear-elastic FE responses (using ABAQUS) of uniform-textured SVEs (generated via DREAM.3D). For each loading direction (x, y and z), periodic, displacement-controlled boundary-conditions are employed such that the macroscopic strain tensor only has only one non-zero component (in the direction of loading). It is noted that the MKS influence coefficients may be calibrated for any desired macroscopic strain tensor; uniaxial strain is selected in this work because it has been successfully employed in many previous studies [6,10–12,14]. The number of SVEs used in calibration of the MKS is determined through examining the mean and maximum error metrics in the strain field predictions for different sets of validation SVEs. From this analysis, it was seen that an ensemble of 400 SVEs is suf-

![Fig. 5. Representative pole figures for (a) β-annealed, (b) basal/transverse, (c) transverse, and (d) random texture inputs to DREAM.3D.](image-url)
sufficient to calibrate the influence coefficients. When elastic strain fields are compared for 100 SVEs not included in the calibration set, the mean voxel-to-voxel difference between MKS and linear-elastic FEM responses is 0.28% and the maximum error per microstructure averages to only 1.50% for the \( \epsilon_{11} \) component. Furthermore, the MKS evaluation requires only 0.7 s on a single processor compared to the 10 min on four processors required for the linear-elastic FE simulation of a single SVE. The local stress fields are also predicted with high accuracy. The mean and average maximum error per microstructure are 1.00% and 2.37%, respectively, for the \( \epsilon_{11} \) fields from 100 instantiations of the \( \beta \)-annealed microstructure simulated with CPFEM (subject to the cyclic loading described in Section 4.3) and the MKS computed fields. These results indicate that stress relaxation or redistribution are minimal in the CPFEM simulations, which is an expected result for the HCF regime. Furthermore, the accuracy of the prediction for the \( \beta \)-annealed microstructure demonstrates the predictive capabilities of the MKS framework for new microstructures.

### 4.3. Auxiliary decoupled estimation of plastic strains

In this study, cyclic plastic strain fields are computed from the stress fields in each SVE using the decoupled numerical integration scheme described in Section 3. Three cycles of fully reversed \( R = -1 \) cyclic loading are performed (see Fig. (7)) to ensure that cyclic plastic strains saturate before FIPs are computed. Furthermore, loading is performed to 0.5% strain amplitude so that \( | \epsilon^p | \ll | \epsilon^e | \) and stress redistribution is minimal. This roughly corresponds to 60–67% of the applied strain to yield, depending on the specific microstructure and loading direction. As a consequence, the stress and elastic strain fields are identical at points A, C, and E for any selected microstructure. However, this is not the case for the corresponding plastic strain fields; their evolution is a result of the plasticity-related fields computed using the crystal plasticity framework presented earlier. In this decoupled numerical integration algorithm, the stress tensor is discretized into 50 increments for each loading segment (e.g., A-B, B-C, etc.).

To check the accuracy of the predicted plastic strain fields, CPFEM simulations are performed for 100 SVEs belonging to the \( \beta \)-annealed microstructure. The crystal plasticity formulation described in Section 2.1 is employed in Abaqus/Standard through a User MATerial subroutine (UMAT). Three cycles of fully reversed loading are applied to the volumes using the same displacement-controlled, uniaxial-strain boundary-conditions described in Section 4.2. Fig. 8 displays the plastic strain fields obtained using the novel protocols and CPFEM for a slice of an example SVE.

Fig. 8 demonstrates that the plastic strain fields computed using the two approaches are indeed very similar. Note that the magnitudes of the plastic strains are several orders smaller than the elastic strain fields (the average \( \epsilon_{11} \) strain is 0.5%). In this example SVE, the mean and maximum relative errors (of the novel approach versus CPFEM) do not exceed 0.39% and 0.84%, respectively, for any component of the plastic strain tensor. This error is defined as the local difference in plastic strains normalized by the maximum plastic strain obtained via CPFEM. This definition ensures that relative error is well characterized for locations in the volume exhibiting high levels of plastic strain. Later results will demonstrate that this level of agreement is sufficient to reliably rank-order the HCF performance of the microstructures studied in this work. The main benefit of the proposed approach continues to be the dramatic savings in computational cost. The CPFEM simulation requires approximately 45 min to complete on four processors (and a total of 8 ABAQUS licenses) per SVE, while the decoupled numerical integration scheme requires 70 s on a single processor.

### 4.4. High cycle fatigue analysis

Given the results of Section 4.3, FIP fields are computed for all SVEs in each loading direction using Eq. (15). FIP EVDs are then calculated by compiling the maximum FIP value in each SVE. At this stage, it would be desirable to compare the FIP EVDs resulting from...
the novel protocols described in this work and the traditional CPFEM approach. Therefore, FIP EVDs are obtained from the CPFEM predicted plastic strain fields computed in the previous section for 100 \( \beta \)-annealed SVEs. In general, the FIP EVDs from the new protocol closely match the CPFEM results, as demonstrated in Fig. 9. The two approaches indicate identical rank-ordering of HCF resistance based on a specified loading direction at a selected high probability of failure. At a low probability of failure, however, the rank-ordering is different between the two methods. This discrepancy can be traced back to the difference in the local plastic strain tensors, and that both methods approximate the local plastic strain tensors via Eq. (20). The plastic strain quantities are an approximation because they are a function of the time step. The time step can vary within CPFEM simulation depending on the integration criteria and the nonlinearity of the simultaneous equations, while the proposed methodology uses an explicit integration method with fixed time increments.

Due to the high computational costs of the conventional approach (which provide the main motivation for this work), comparisons between the two approaches were not performed for all microstructures studied here. Instead, the FIP EVDs were constructed using the novel protocols presented in this work for all four microstructure classes, each with a full ensemble of 500 SVEs (note that comparison presented in Fig. 9 used only 100 SVEs). Fig. 10 compares the resultant FIP EVDs for all four microstructures and three loading directions. As expected, the FIP EVDs of the random textured microstructure are nearly coincident for all loading directions. The basal/transverse and \( \beta \)-annealed textured microstructures exhibit similar FIP EVD responses, with the lowest fatigue resistance for loading in the z-direction.

Finally, the HCF resistance of the transverse textured microstructure is distinctly different from the other microstructures, exhibiting a significant positive correlation with the effective modulus in the direction of loading. This microstructure is distinct as compared to the other three due to a strong c-axis fiber texture component parallel to the sample x-axis. This particular texture feature essentially dominates this microstructure. As a result, when this sample is loaded along the x-axis, we should expect a minimum amount of interactions between neighboring grains, especially in the elastic regime due to the transverse isotropy of the elastic response in each crystal in the plane normal to the c-axis. It is therefore not surprising that x-axis loading produces the best HCF response for this microstructure with most of the FIP values being lower compared to the loading in the other directions. Note that this is the case despite the higher stiffness of the material along the x-axis (i.e., stresses are higher because the same strain amplitude is imposed in all cases) as compared to the other directions. It is also interesting to note that there are a few high FIP values in the x-axis loaded microstructure that are comparable to the values obtained in the other two loading directions on the same microstructure. This is because the high FIP values would correspond to locations of high local plastic strains. In the case of x-axis loading, once plastic deformation initiates, transverse isotropy in the local response of the c-axis grains is completely lost (note that only the elastic response is transversely isotropic in the HCP crystals) and the degree of interactions between neighboring

![Fig. 8](image1.png) **Fig. 8.** A two-dimensional cross-section comparison of the \( e_{11}^p \) values from CPFEM (left) and MKS plus decoupled numerical integration (right).

![Fig. 9](image2.png) **Fig. 9.** Comparison of the \( \beta \)-annealed microstructure extreme value distribution Fatemi-Socie FIP plot with 100 SVEs obtained via (a) MKS plus decoupled numerical integration and (b) CPFEM.
grains dramatically increases. As a result of these strong interactions, the local plastic strains can be high in this microstructure. Overall, it should be noted that this microstructure provides the best HCF response out of all of the microstructures studied. This improved performance is largely attributed to lower levels of interactions between the neighboring grains (in the HCF loading regime dominated by elasticity).

5. Conclusions

A new methodology that employs MKS and a decoupled numerical integration scheme is presented to reliably predict cyclic plastic strain fields in hexagonal, $\alpha$-titanium, polycrystalline aggregates under low-amplitude loading conditions. These quantities inform the computation of FIP distributions which are used to rank-order the HCF resistance of polycrystalline microstructures. This analysis is specifically designed to support rapid microstructure selection and optimization, assuming the proper material and application have been identified. These new protocols are demonstrated on an ensemble comprising over 6000 individual SVEs; the same task would demand major computational resources when using traditional CPFEM-based approaches. In fact, the low computational cost allows for the consideration of such a large ensemble of microstructures in the present work. The approximate speed-up of the new protocols is approximately 40× versus traditional CPFEM. The study also identifies the critical role of grain interactions in the HCF performance through a consideration of twelve different conditions (four microstructures, each loaded in three directions). While this study has established the feasibility of the new protocols, much additional work is needed to extract new insights into the HCF response of polycrystalline microstructures. These will be targeted in future studies where the new protocols developed in this work will be employed on a much larger ensemble of microstructures. Additionally, the computational fatigue response needs to be validated against experimental data, such as damage measurements relevant to HCF.

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Appendix A

In this work, the number of SVEs required to approximate the RVE for a microstructure of interest is selected by examining the convergence of the mean and standard deviation of the effective
elastic modulus in each loading direction. In this section, protocols are set forth to calculate these moduli values for the boundary conditions employed in this work.

HCP crystal structures have a transversely isotropic elastic response, meaning that the elastic properties exhibit rotational symmetry around the HCP crystal c-axis. For z-titanium, the elastic modulus can vary between 104 and 146 GPa, the shear modulus between 40 and 47 GPa, and Poisson’s ratio between 0.265 and 0.337. This degree of anisotropy for the elastic modulus (40%) and the shear modulus (18%) is much higher than that of other HCP metals [5] and can have a pronounced effect on the material deformation response.

Mechanical properties (such as elastic stiffness) can be determined from datasets generated in this study. Since the boundary conditions used in this work result in non-zero normal stress components in all normal directions, additional steps are taken to determine directional effective elastic modulus values. The MKS determines local quantities, therefore the stress and strain components are volume-averaged to obtain the macroscopic quantities (e.g., $\sigma_{ij} = \sum_{k=1}^{N} \sigma_{ij}^{k}/N$ where $N$ is the total number of centroidal averaged values for uniform voxel size). The averaged stress and strain quantities are then used to determine the effective stiffness components. The effective stiffness tensor can then be inverted to recover the effective compliance tensor. Subsequently, the effective elastic modulus values for each loading direction are extracted from the diagonal components of the compliance tensor. The mean and standard deviation of the effective elastic modulus values for each loading direction and microstructure are presented in Table 2.

### References


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