Dislocation density informed eigenstrain based reduced order homogenization modeling: verification and application on a titanium alloy structure subjected to cyclic loading

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Abstract

This manuscript presents a dislocation density informed eigenstrain based reduced order homogenization model (DD-EHM), and its application on a titanium alloy structure subjected to cyclic loading. The eigenstrain based reduced order homogenization (EHM) approach has been extended to account for the presence of HCP (primary α phase) and BCC (β phase) grains, within which the deformation process is modeled using a dislocation density based crystal plasticity formulation. DD-EHM has been thoroughly verified to assess the accuracy of the reduced order model in capturing local and global behavior compared with direct crystal plasticity finite element method (CPFEM) simulations. A structural scale study of titanium alloy Ti-6242S is performed using DD-EHM to quantify and characterize the spatial distribution and evolution of the dislocation pile-ups subjected to cyclic loading. The evolution of pileups at two spatial scales are tracked using a nonlocal parameter based on dislocation density discrepancy across neighboring grains. The effect of non-uniform texture on the response of the structural component has been investigated.

Keywords: Crystal plasticity, Titanium alloys, Dislocation Pile-ups, Multiscale modeling, Reduced order modeling

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1 Introduction

Predicting the response of structural components made of polycrystalline metals using microscopically informed multi-scale models requires efficient and accurate upscaling (homogenization) and downscaling (localization) strategies. In particular, the crystallographic physics that are local at the grain or subgrain scale must be retained during upscaling, and the computational cost must be sufficiently low to allow simulation of large structural components. Concurrent multiscale approaches such as the computational homogenization [1, 2], variational multiscale enrichment [3, 4, 5], heterogeneous multiscale method [6, 7], multiscale finite element method [8], among others provide the appropriate ways for rigorous scale bridging. Unfortunately, the high computational cost of these approaches limit their application to relatively small size problems.

While the high computational cost associated with these approaches can be alleviated by massive parallelization [9], employing reduced order approximations of the microstructure scale response is a more practical alternative and has been pursued by different researchers. A number of reduced order modeling approaches have been proposed and employed to efficiently replace crystal plasticity finite element method (CPFEM) simulations, including the classical Sachs and Taylor models, and more recent and sophisticated approaches such as spectral crystal plasticity method [10], grain cluster method [11], elasto-plastic self-consistent (EPSC) method [12, 13, 14], fast Fourier transform (FFT) method [15] and nonuniform transformation field analysis [16, 17]. Among others, sequential multiscale has been proposed as an alternative approach to devise structural scale models. In this approach, structural analysis is uncoupled from the microstructure scale, but a macro-scale constitutive model is trained based on microscale simulations on representative volume elements (RVEs) or statistical volume elements (SVEs), retaining local information in the form of internal state variables (e.g., [18, 19, 20]).

Recently, the eigenstrain based reduced order homogenization method (EHM) has been proposed to alleviate the computational cost of CPFEM simulations [21]. The EHM approach relies on the pre-computation of a small set of “constitutive tensors” that retain the microstructure morphological information, and employing these tensors to approximate the microstructure scale response fields using a much smaller basis obtained through constrained kinematics. EHM approach was later extended to achieve sparse and scalable formulations that allow efficient analysis of structures in the presence of large representative volumes by selectively eliminating long range interactions at the scale of the RVE [22]. An important advantage of the EHM is that the grain interactions and the intra-granular strain and stress variations with the microstructure could be retained during the up-scaling such that the individual grain information will be kept in the multiscale modeling.

In the aforementioned works, capabilities of the EHM approach was demonstrated in the context of the monotonic response of FCC polycrystals. In this manuscript, we extend the capabilities of the EHM framework to incorporate HCP, BCC and multi-phase microstructures subjected to monotonic and cyclic loading conditions. A reversible dislocation density based
crystal plasticity constitutive model is adopted to capture the dislocation evolution physics under cyclic loading. The generalized crystal plasticity EHM implementation has been thoroughly verified to assess the accuracy of the reduced order model in capturing local and global behavior compared with the direct CPFEM simulations. Structural scale investigations are performed to study the spatial distribution of dislocation pile-ups in a large structure made of titanium alloy, Ti-6Al-2Sn-4Zr-2Mo-0.1Si (Ti-6242S).

The remainder of the manuscript is organized as follows: In Section 2, the basic formulation of the EHM approach and the dislocation density based crystal plasticity model are provided. In Section 3, the dislocation density informed EHM framework is verified for HCP and BCC crystals in direct comparison with CPFEM simulations. Section 4 provides the calibration of model parameters using the experimental data for Ti-6242S; hereinafter, a component-level analysis is conducted for this material to investigate dislocation pile-ups at the grain boundary and the effect of non-uniform texture.

### 2 Eigenstrain based reduced order homogenization for polycrystalline plasticity

The detailed derivation of the EHM approach in the context of computational homogenization is provided in [21, 22]. A similar approach has been developed for variational multiscale enrichment in [23, 24]. In what follows, we summarize the governing equations of the EHM modeling approach and describe the dislocation density based evolution equations used to describe the slip and hardening evolution within the material microstructure.

We consider the domain of a macroscopic structure, denoted as $\Omega$. The structure consists of a periodic construction of a polycrystalline microstructure, denoted as $\Theta$. In what follows, we loosely refer to the polycrystalline microstructure as the RVE indicating that the microstructure is statistically representative in the context of ergodic measure of deformation. In order to ensure the applicability of the EHM approach, we make the following two assumptions on the inelastic behavior within the structure: (1) the size of the macroscopic spatial deformation wave form is large compared to the microstructure domain, i.e., the material response is devoid of weak or strong discontinuities such as shear bands or cracks, and that the classical scale separation assumption is valid; and (2) the strains at the scale of the material microstructure remains small under the applied load cycles, and the material is taken to undergo negligible amount of texture evolution. While texture evolution is an important issue in a number of applications that involve large deformations, total micro- and macroscale strains in fatigue problems often remain small (see, e.g., [25, 26] for near $\alpha$ titanium alloys) and negligible texture evolution is observed.

In the context of the EHM approach, we consider the decomposition of the RVE into $n$ subdomains (or reduced order “parts”) such that $\Theta^{(\alpha)} \cap \Theta^{(\beta)} = \emptyset$ when $\alpha \neq \beta$; $\alpha, \beta = 1, 2, ..., n$, and $\bigcup_{\alpha=1}^{n} \Theta^{(\alpha)} = \Theta$, where $\Theta^{(\alpha)}$ denotes the domain of part $\alpha$. The kinetics and the kinematics
in the reduced order model are constrained such that the stress and the visco-plastic strain fields are taken to spatially vary within the RVE in a piecewise constant fashion, based on the reduced order partitioning of the domain.

The boundary value problem governing the equilibrium at the macroscopic scale is expressed as:

\[ \nabla \cdot \bar{\sigma}(x, t) + \bar{b}(x, t) = 0 \quad x \in \Omega; \quad t \in [0, t_0] \]  

(1)

where, \( \bar{\sigma} \) is the macroscopic Cauchy stress; \( \bar{b} \) is the body force; and \( \nabla \cdot \) denotes the divergence operator. The boundary conditions are given as:

\[ \bar{u}(x, t) = \bar{u}_0(x, t) \quad x \in \Gamma^u \]  

(2)

\[ \mathbf{n} \cdot \bar{\sigma}(x, t) = \bar{t}_0(x, t) \quad x \in \Gamma^t \]  

(3)

in which, \( \bar{u} \) denotes the macroscopic displacement field, \( \bar{u}_0 \) and \( \bar{t}_0 \) are the prescribed displacement and traction on the boundaries \( \Gamma^u \) and \( \Gamma^t \), where \( \Gamma^u \cup \Gamma^t = \partial \Omega \) and \( \Gamma^u \cup \Gamma^t = \emptyset \). \( \mathbf{n} \) is the unit normal to \( \Gamma^t \). The macroscale strain tensor, \( \bar{\varepsilon}(x, t) \) is expressed in terms of macroscale displacement based on small deformation assumption: \( \bar{\varepsilon} = \nabla^s \bar{u}(x, t) \), where \( \nabla^s \) is the symmetric gradient operator.

Considering the kinetic and kinematic approximations of the model reduction strategy and employing influence functions (i.e., discrete Green’s functions) at the scale of the RVE to express the microscopic response fields, the part average stress and inelastic strain tensors for each part, \( \beta \) are related to each other as:

\[ \mathbf{M}^{(\alpha\beta)} \dot{\bar{\sigma}}^{(\beta)}(x, t) - \sum_{\alpha=1}^{n} [\mathbf{P}^{(\beta\alpha)} - \delta^{(\alpha\beta)} \mathbf{I}] \dot{\mu}^{(\alpha)}(x, t) = \mathbf{A}^{(\beta)} \bar{\varepsilon}(x, t); \quad \beta = 1, \ldots, n \]  

(4)

where, \( \sigma^{(\alpha)} \) and \( \mu^{(\alpha)} \) respectively denote the part-averaged Cauchy stress and inelastic strain tensor associated with part \( \alpha \); a superscribed dot over \( f \) indicates time derivative of \( f \); \( \delta^{(\alpha\beta)} \) is Kronecker delta ( \( \delta^{(\alpha\beta)} = 1 \) if \( \alpha = \beta \); \( \delta^{(\alpha\beta)} = 0 \) if \( \alpha \neq \beta \)); and \( \mathbf{I} \) is the fourth order identity tensor. \( \mathbf{M}^{(\alpha\beta)} \), \( \mathbf{P}^{(\beta\alpha)} \) and \( \mathbf{A}^{(\beta)} \) are respectively the part-averaged compliance, interaction and concentration tensors. These tensors are integral functions of the influence functions providing
the morphological information of the RVE. The specific expressions for the coefficient tensors are provided in [21]. The macroscale stress is then computed as the volume average of the part-averaged stress coefficients:

\[ \bar{\sigma} = \frac{1}{|\Theta|} \sum_{\beta=1}^{n} \frac{|\Theta^{(\beta)}|}{|\Theta|} \sigma^{(\beta)} \]  

(5)

in which, \( |\Theta^{(\beta)}| \) denotes the volume of part \( \beta \) and \( |\Theta| \) is the volume of the RVE.

Since the static texture and dislocation slip are the sole sources of plastic deformation, inelastic strain in part \( \alpha \), \( \mu^{(\alpha)} \), results from dislocation slip over all slip systems within the grain that occupy \( \Theta^{(\alpha)} \) through the Schmid law:

\[ \dot{\mu}^{(\alpha)}(x, t) = \sum_{s=1}^{N} \dot{\gamma}_{s}^{(\alpha)}(x, t) Z_{s}^{(\alpha)} \]  

(6)

in which, the superscript \( s \) denotes the \( s^{th} \) slip system in each part. \( Z^{s(\alpha)} \) is the Schmid tensor in part \( \alpha \), uniquely describing the orientation of the \( s^{th} \) slip system as the dyadic product of the slip direction, \( n^{s(\alpha)} \) and the direction normal to the slip plane \( m^{s(\alpha)} \) (i.e., \( Z^{s(\alpha)} = n^{s(\alpha)} \otimes m^{s(\alpha)} \)). \( N \) is the number of slip systems. The accuracy of the slip evolution naturally limits the reduced order discretization of the RVE. In particular, the RVE domain is discretized such that each part coincides with the domain or a subdomain of a single grain. By this approach, no averaging over slip systems within multiple grains forming a single part is necessary in the description of slip and hardening evolution. This constraint implies that the coarsest reduced order discretization corresponds to the case when each part occupies the domain of a single grain, in what follows referred to as the one-part-per-grain model. Under this constraint, the compliance tensor of each part is equal to the compliance tensor of corresponding grain within the RVE. If a grain is divided into multiple separate parts, the resulting reduced model is referred to as a multi-part-per-grain model. The consequences of grain partitioning is investigated in Section 3.2.

The above mentioned reduced-order formulation relies on the assumption of piece-wise constant spatial distribution of the inelastic strain field within the RVE. It is possible to choose other, more complex forms of spatial distribution functions to represent the inelastic strain field, such as non-uniform plastic modes [27, 17]. When the approximate direction of the applied loading (i.e., the history of macroscopic strain field) on the microstructure is known a priori, very accurate plastic modes could be identified through proper orthogonal decomposition and the resulting reduced order model could yield higher accuracy than the piece-wise constant approximation. A critical benefit of employing piece-wise constant approximation is that the construction of the reduced order model is purely geometrical and does not rely on prior knowledge of the direction of loading on the microstructure, which is typically unknown and time-varying in the context of a multiscale simulation. While it is possible to also consider adaptive enrichment of the approximation basis during a multiscale analysis to improve accuracy, this step is typically considerably expensive from the computational point of view.
2.1 Reversible dislocation density based crystal plasticity under cyclic loading

The classical dislocation-mediated plasticity was first introduced by [28, 29] and [30]. Based on these fundamental theories, major progress has been made in the development of dislocation density based crystal plasticity constitutive models in the past few decades (see e.g., [31, 32, 33]). These constitutive models have been shown to reveal the underlying plastic deformation mechanisms in various metallic material microstructures, validated by experimental observations [12, 34, 35]. Langer and co-authors have recently developed an alternative, physics-based plasticity theory consistent with the thermodynamics principles. This theory proposes an advanced dislocation model, which incorporates the energy and entropy in the dislocation flow in the presence of strain rate sensitivity and non-uniform Bauschinger effects [36, 37, 38]. In this manuscript, the classical dislocation theory has been adopted, but the modeling strategy can be extended to incorporate others in a straightforward manner.

In what follows, the part index \( \alpha \) is omitted in the equations for simplicity, but the variables are to be understood as part-averaged quantities. The slip rate at the \( s \)th slip system is derived from the Orowan’s equation and expressed as [39, 35]:

\[
\dot{\gamma}_s = \frac{\rho_s \nu_{id}(b^s)^2}{2} \text{sgn}(\tau_s) \exp \left( -\frac{\Delta F^s}{k\theta} \right) \exp \left( \frac{(\tau_s - s^s)\Delta V^s}{k\theta} \right) 
\]

(7)

where, \( s^s \) is the critical resolved shear strength (CRSS), \( \Delta V^s \) is the thermal activation volume, \( k \) the Boltzmann constant (1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}) and \( \theta \) the temperature in Kelvin. In Eqn. (7), \( \dot{\gamma}_s \) is related with \( \rho_s \), the average mobile dislocation density, \( \nu_{id} \), the vibration frequency of the dislocation segment, \( b^s \), the magnitude of the Burgers vector and \( \Delta F^s \), the activation energy. The resolved shear stress \( \tau_s \) is associated with the Cauchy stress through \( \mathbf{Z}^s \) as:

\[
\tau_s = \sigma : \mathbf{Z}^s
\]

(8)

In addition, it has been widely acknowledged that the stored sessile dislocation would be the main source for fatigue deformation behaviour, such as local strain or stress concentration and strengthening [26, 40, 41], including geometrically necessary dislocation and stored statistical dislocation density. Thus, here the strength hardening evolution in HCP dominated crystals are expressed as [31, 42]:

\[
s^s(\dot{\gamma}_s) = s^s_0 + s^s_{\text{for}} (\dot{\gamma}_s) + s^s_{\text{deb}} (\dot{\gamma}_s),
\]

(9)

in which, \( s^s_0 \) is the temperature-dependent initial slip resistance. \( s^s_{\text{for}} \) and \( s^s_{\text{deb}} \) respectively denote the contributions to strength evolution by the sessile (i.e., forest and debris) dislocations, described as

\[
s^s_{\text{for}} (\dot{\gamma}_s) = \mu b^s \sqrt{\rho_{\text{for}}} \ln \left( \frac{1}{b^s \sqrt{\rho_{\text{deb}}}} \right),
\]

(10)

\[
s^s_{\text{deb}} (\dot{\gamma}_s) = \mu b^s k_{\text{deb}} \sqrt{\rho_{\text{deb}}} \ln \left( \frac{1}{b^s \sqrt{\rho_{\text{deb}}}} \right),
\]

(11)
where, \( \mu \) is the shear modulus, \( \chi \) the dislocation interaction parameter (set to 0.9) satisfying the Taylor relationship [31]. The latent hardening effects have not been incorporated in this study, because dislocation density evolution induced by latent hardening has been found to be small compared with that due to self-hardening in the alloys investigated here [43, 34, 44]. The latent hardening effects could be added by replacing the scalar \( \chi \) with an interaction coefficient matrix as employed in [42]. \( k_{\text{deb}} = 0.086 \) is the material independent factor associated with low substructure dislocation density [32]. \( \rho_{s} \) for \( s \) and \( \rho_{s, \text{deb}} \) are the forest and debris dislocation densities, respectively.

Experimental observations by [45, 33, 46, 47] indicate that the forest and debris dislocations and their evolution significantly impact the mechanical behavior of HCP and BCC polycrystalline materials. Under monotonic loading, the forest dislocation density evolves through the competing mechanisms of generation and annihilation associated with recovery [12]. The evolution is affected by the current dislocation density as well as the extent of plastic slip. Stored forest dislocations annihilate by the effect of shearing along the opposing strain path when the loading is reversed under cyclic loading conditions [48, 14]. The total forest dislocation density is expressed as:

\[
\rho_{\text{for}}^s = \rho_{\text{fwd}}^s + \rho_{\text{rev}}^{s+} + \rho_{\text{rev}}^{s-}
\]  

(12)

where, \( \rho_{\text{fwd}}^s \) is the forward dislocation density and \( \rho_{\text{rev}}^{s+} \) denote the reversible terms corresponding to loading and unloading paths along the \( s \)th slip system as shown in Fig. 2. Superscripts \( s+ \) and \( s- \) denote the particular slip direction in the slip system. The initial forest dislocation density is relatively low in the pure HCP- or BCC-based materials corresponding to the experimental observations [49, 33, 45, 50] and a small value \( \rho_{\text{for},0} = 1.0 \times 10^{12} \text{ m}^{-2} \) is used for materials considered in this study. The evolution of the forward term is expressed as:

\[
\frac{\partial \rho_{\text{fwd}}^s}{\partial \gamma^s} = (1 - p) \frac{\partial \rho_{\text{gen,fwd}}^s}{\partial \gamma^s} - \frac{\partial \rho_{\text{rec,fwd}}^s}{\partial \gamma^s} = (1 - p) k_1^s \sqrt{\rho_{\text{for}}^s} - k_2^s (\dot{\gamma}, \theta) \rho_{\text{for}}^s \chi g^s,
\]  

(13)

where \( \rho_{\text{gen,fwd}}^s \) and \( \rho_{\text{rec,fwd}}^s \) are the athermal storage and temperature dependent recovery of classical Kock-Mecking law [51]. \( p \) is a reversibility parameter determining the fraction of the reversible loosely tangled forest dislocations. Since the shear strain is relatively small in cyclic loading, a greater value of \( p = 0.8 \) is chosen according to [48]. \( k_1^s \) and \( k_2^s \) are the coefficients controlling the generation of forest dislocations and the annihilation due to dynamic recovery, respectively. The recovery coefficient is taken to be proportional to generation rate:

\[
k_2^s (\dot{\gamma}, \theta) = k_1^s \frac{b^s \chi g^s}{D^s} \left[ 1 - \frac{k \theta}{D^s b^s} \ln \left( \frac{\dot{\gamma}}{\dot{\gamma}_0} \right) \right]
\]  

(14)

Equation 14 is similar to the law proposed in [31], but employs the slip rate of the current slip system rather than the total strain rate. \( \dot{\gamma}_0, g^s \) and \( D^s \) are respectively the reference shearing rate defined as \( 10^7 \text{ s}^{-1} \) (satisfying the high cycle and low cycle fatigue loading conditions), effective activation enthalpy and drag stress. The evolutions of the remaining components of
the forest dislocation density are expressed as functions of the loading direction along the slip system [48]:

Case 1: if $\tau^s > 0$

$$\frac{\partial \rho_{\text{rev}}^+}{\partial \gamma^s} = pk_1^s\sqrt{\rho_{\text{for}}^s} - k_2^s(\dot{\gamma}^s, \theta)\rho_{\text{rev}}^+$$

$$\frac{\partial \rho_{\text{rev}}^-}{\partial \gamma^s} = -k_1^s\sqrt{\rho_{\text{for}}^s} \left( \frac{\rho_{\text{rev}}^+}{\rho_0^s} \right) \hat{m}$$

(15)

Case 2: if $\tau^s < 0$

$$\frac{\partial \rho_{\text{rev}}^-}{\partial \gamma^s} = pk_1^s\sqrt{\rho_{\text{for}}^s} - k_2^s(\dot{\gamma}^s, \theta)\rho_{\text{rev}}^-$$

$$\frac{\partial \rho_{\text{rev}}^+}{\partial \gamma^s} = -k_1^s\sqrt{\rho_{\text{for}}^s} \left( \frac{\rho_{\text{rev}}^-}{\rho_0^s} \right) \hat{m}$$

(16)

where, $\rho_0^s$ is the value of the total dislocation density at the point of load reversal and $\hat{m}$ is the dislocation density recombination coefficient taken to be 0.4 for HCP and BCC crystals [14]. The state of $\tau^s = 0$ incurs no plastic flow or dislocation density evolution. It is worthy to note that $\tau^s$ is the part-averaged Cauchy stress $\sigma$ resolved onto the $s^{th}$ slip system. Thus, the change in sign of $\tau^s$ does not necessarily correspond to the load reversals in the macroscopic load cycles.

The recovery process through dislocation climb or cross-slip is naturally related to the debris dislocation formation. Thus, the evolution rate of debris dislocation density is taken to be proportional to the recovery rate. As implied by Eq. 11, hardening at a given slip system, $s$, is taken to be affected by the total debris dislocations on all slip systems. The evolution of
the debris dislocation density is expressed as the sum of contributions from each slip system:

\[ d\rho_{\text{deb}} = \sum_s \frac{\partial \rho_{\text{deb}}^s}{\partial \gamma^s} d\gamma^s \]  \hspace{1cm} (17)

where,

\[ \frac{\partial \rho_{\text{deb}}^s}{\partial \gamma^s} = q b^s \sqrt{\rho_{\text{deb}}} \frac{\partial \rho_{\text{rec,fwd}}^s}{\partial \gamma^s} \rho_{\text{for}}^s \] \hspace{1cm} (18)

where, \( q \) is the recovery rate coefficient. The initial debris dislocation density in all slip systems is defined as the same quantity, \( \rho_{\text{deb},0}^s = 1.0 \times 10^{10} \) m\(^{-2} \) [52, 53].

The dislocation density based crystal plasticity model defined in Eqs. 7-18 has been implemented within the EHM framework (Eqs. 1-6). In contrast to the classical crystal plasticity finite element approach, the evolution equations and the state variables are associated with each reduced model part rather than a material point. The implementation has been performed by employing the commercial finite element package, ABAQUS. The reduced order model is incorporated using the user supplied material subroutine capabilities. A two-level semi-implicit stress integration algorithm is applied to obtain the convergence of Cauchy stress and CRSS. In the first level, Newton-Raphson algorithm is used to calculate the stress update with full-implicit integration. Then the dislocation densities and CRSS are explicitly updated. The two steps of the integration process is repeated until convergence.

### 3 DD-EHM model verification

The accuracy characteristics of the reduced order model (referred to as DD-EHM in what follows) introduced in the previous section are verified against classical CPFEM simulations at the microstructure scale [54, 55, 56]. The model is not restricted to specific evolution laws. We therefore employ a bottom-up verification approach where, the proposed model is verified using a pure HCP (Magnesium) and a pure BCC (Niobium) microstructures first. The capability of the model is then demonstrated in a more complex alloy (Section 4). In the current section, the effect of the model order in capturing the local stress distribution within the RVE is also investigated. In the next section, the verified model has been further demonstrated using a more complex two-phase alloy. Verification of the EHM approach for multi-phase materials (in FCC polycrystals) has been performed in [5]. Twinning, an important deformation mechanism, could also be incorporated in the EHM formulation. For simplicity of the verification studies, twinning is not included in the description of plastic deformation.
3.1 Single phase HCP or BCC polycrystal verification

The model verifications have been performed for material behavior that does not exhibit severe strain softening (e.g. shear bands) where deformation localizes at a length scale below the size of the RVE [57]. The verifications are performed by comparing the results of the proposed DD-EHM approach with those of the CPFEM simulations (i.e., the reference model) performed on a representative volume. Figure 4 illustrates a sample microstructure employed in the verification analyses. The grain orientations are sampled from the uniform orientation distribution function which contains 145 grains and is generated by the previous workflow [21, 35]. The DD-EHM model employs a part-per-grain model reduction approach (i.e., \( n = 145 \)). Identical constitutive models (Section 2.1) and constitutive parameters (Table 1) have been employed in the DD-EHM and CPFEM simulations. The full field CPFEM simulation contains 82,561 four-noded tetrahedra elements.

Table 1 summarizes the model parameters of the HCP and BCC grains, respectively, used in the model verification studies. The slip systems considered for the HCP and BCC lattices are shown in Fig. 3. The HCP model includes 30 slip systems including the basal, pyramidal and prismatic systems. The parameters are obtained based on the stress-strain behavior of magnesium polycrystals provided by [58]. The BCC model includes 48 slip systems, and the model parameters are obtained based on the curves provided in [34] for niobium polycrystals. The mobile dislocation density within a grain is likely to be different for different slip systems and evolves with deformation, however it remains difficult to experimentally quantifying the magnitude and evolution of mobile dislocations. In this study, its value is taken to be constant and set to the same in all slip systems following Ref. [40].

Figure 5 shows the comparison of the RVE-averaged (i.e., overall) stress strain behavior for the proposed and the reference models for a pure HCP polycrystal subjected to strain controlled uniaxial tension, fatigue cycle, dwell fatigue cycle and a more complex biaxial load path. The overall stress reported for CPFEM simulations are calculated by volume-averaging
Figure 4: Sample microstructure used in verification. (a) Discretization used in the CPFEM simulations; (b) Selected grains used in the verification of the DD-EHM simulations.

Figure 5: Overall stress-strain curves for the HCP polycrystal subjected to: (a) uniaxial tension; (b) pure fatigue cycle; (c) dwell fatigue cycle; (d) biaxial loading.
Table 1: Model parameters for the HCP and BCC crystals used in the verification studies.

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Figure 6: Overall stress-strain curves for the BCC polycrystal subjected to: (a) uniaxial tension; (b) pure fatigue cycle.

of element-wise stresses in the RVE. In the uniaxial tension case (Fig. 5a), a 2 % strain is applied along the X-direction with a constant strain rate of 0.05 s^{-1}. In the fatigue cycle case (Fig. 5b), a maximum strain amplitude of 2 % is applied along the X-direction at strain rate of 0.04 s^{-1}. The R-ratio is set to $R = -1$. In the dwell fatigue cycle case (Fig. 5c), the same maximum strain, strain rate and R-ratio are applied along the X-direction. Upon reaching maximum strain in tension and compression, the strain is held for 0.5s before the loading is reversed. In the biaxial loading case (Fig. 5d), a 6 % tensile strain is applied at the X-direction with constant strain rate of 0.04 s^{-1} and the strain is held until the end of the test. Concurrently, the RVE is subjected to a cyclic load with a peak strain of 4 % along the Y-direction at 0.04 s^{-1} strain rate and with $R = -1$. The total duration of the cyclic biaxial tension and the fatigue cycle tests are 2.5 s, whereas the total time of the dwell fatigue cycle testing is 3.5 s. In Figure 6, the comparison between the proposed and the CPFEM model is shown for the BCC polycrystal subjected to strain controlled uniaxial tension and fatigue cycle. The same loading rate, total strain and R-ratio are applied in the BCC case.

Figures 5 and 6 illustrate that the overall stress-strain behavior predicted by the proposed approach matches well with the reference CPFEM simulations. DD-EHM shows slightly stiffer
Figure 7: Local Mises stress, principal strain and dislocation density distributions at the peak load for the HCP polycrystal subjected to: (a) uniaxial tension; (b) pure fatigue cycle; (c) dwell fatigue cycle; and (d) biaxial loading.
Figure 8: Local Mises stress contours for the HCP microstructure using: (a) DD-EHM model; (b) CPFEM model. Local maximum principal strain contours using: (c) DD-EHM model; (d) CPFEM model.

Figure 9: Stress-strain curves comparison of 5 random grains chosen in the (a) HCP and (b) BCC polycrystals under uniaxial tension.
responses compared with the reference case due to constrained kinematics associated with the reduced basis. In order to ensure the consistency of the accuracy, 50 separate uniaxial tension simulations were performed with random grain orientations sampled from uniform orientation distribution. The error in the overall stress-strain curves as defined by the discrete L2 norm were bounded by approximately 10% for all cases considered. As a reference for accuracy of model predictions, experiments on Ti-6242S exhibited about 5% variation in flow stress predictions at low temperature and about 12% variation at high temperatures [59].

In addition to the overall stress responses, we tested the ability of the DD-EHM model in capturing the local stress variations within the microstructure. Figure 7 shows the comparison of the local stress, strain and dislocation density distributions between the proposed approach and the CPFEM simulations at the peak load state of all four loading conditions applied to the HCP polycrystal. Using the form of a histogram plot, the volume fraction of grains within the microstructure are plotted as a function of the stress and strain levels experienced by the grains. The bin plots represent the CPFEM model whereas the stars at the mid-point of each bin refer to the proposed model. The magnitudes of the local stresses match well with those of the reference simulations under the four loading conditions. The magnitudes of the local strains deviate slightly more than the respective stress distributions under the four loading conditions with peak strain amplitudes underestimated by the proposed approach. Dislocation density distribution patterns are similar to that of strain distributions. Figure 8 illustrates the variation of equivalent stress and maximum principal strain within the RVE as predicted by the DD-EHM and CPFEM approaches. The contour plots are from the biaxial loading at the end of the loading period. The CPFEM simulation captures the spatial variation of the stresses and strains within each grain, whereas the part-per-grain DD-EHM model tracks a grain-averaged fields only.

Figure 9 compares the stress-strain curves at a number of grains within the microstructure shown in Figure 4. The results indicate that the accuracy of the DD-EHM in capturing the local stresses are bounded by approximately 13.4% error. Implemented with the dislocation density based constitutive law, the EHM has the similar accuracy of the local grain-scale responses in keeping with CPFEM results, compared with the previous EHM numerical results [21].

### 3.2 Hierarchical model improvement: sub-grain responses prediction

In polycrystalline microstructures with high anisotropy or in the presence of multiple phases with high property contrast, stress and deformations could vary significantly within each grain and concentrate near the grain/phase boundaries and triple junctions. In the proposed reduced order modeling approach, the variability of the response fields within each grain could be better approximated by considering larger number of reduced order parts per each grain (denoted as multi-part-per-grain approximation). The multi-part-per-grain approximation therefore considers a non-uniform variation of the inelastic response field within each grain.
In this section, the effect of using a multi-part-per-grain scheme and improvement of accuracy with increasing model order are investigated. The investigations are performed on an idealized microstructural configuration that contains 13 grains as shown in Fig. 10a. The idealized microstructure is subjected to uniaxial tension along the $X$ direction up to 5% total strain with $0.05 \, s^{-1}$ strain rate. Five different reduced order models with hierarchically increasing orders are considered starting from part-per-grain (i.e., 13 parts as shown in Fig. 10a) up to 136 parts (Fig. 10e). The grains are taken to be HCP with random orientations sampled from uniform orientation distribution. The material parameters summarized in Table 1 are used. For each DD-EHM model as well as the reference CPFEM approach, 50 simulations are performed using randomly sampled orientations for each grain. The full field CPFEM discretization contains 62,513 four-noded tetrahedra elements.

In comparison with the CPFEM model, the overall stress-strain curves and local stress distributions are presented in Fig. 11. The figure is from one out of 50 sets of simulations. All 50 sets exhibit relatively similar error distributions with the plots showing close to average
errors. The figure shows that as the partition number increases, the overall response of the DD-EHM model improves by a small amount. In contrast, the distribution of local stresses (Fig. 11b) significantly improves as a function of model order. This result indicates that model refinement would lead to further improvement in capturing the local response fields within the microstructure.

Figure 11: DD-EHM model refinement study: (a) Overall stress vs. strain curves; (b) Local stress distributions

Figure 12 shows the stress distributions predicted by the reduced order models at the peak strain amplitude and compared to that of the reference simulation. The figure indicates that not only that the local stress distributions improve as a function of the increased model order, but that the stress concentrations within the microstructures are predicted in reasonable accuracy. The high stress regions that occur near the triple points and grain boundaries are captured in a progressively more accurate manner as a function of the model hierarchy.

The assessment of model error as a function of model order across all 50 sets of simulations are shown in Fig. 13. The error is defined as:

\[
\text{error} = \int_0^\varepsilon \left| \frac{\sigma_{\text{DD-EHM}} - \sigma_{\text{CPFEM}}}{\sigma_{\text{CPFEM}}} \right| d\varepsilon
\]  

(19)

Figure 13a indicates that the error magnitude is stable and approximately range between 2 % and 10 % across 50 simulations regardless of the model order. While the mean error does not appear to be significantly reduced, confirming the above mentioned results, the variance in the predictions are smaller with higher model order as shown in Fig. 13b.

The speedup \( Q \) of the DD-EHM model compared with CPFEM calculation,

\[
Q = \frac{t_{\text{CPFEM}}}{t_{\text{DD-EHM}}}
\]  

(20)
Figure 12: Local stress contours from: (a) DD-EHM grain partition; (b) DD-EHM triangular prism partition; (c) DD-EHM surface grain interaction pattern; (d) DD-EHM triple junction partition; (e) DD-EHM triangular partition with double precision; (f) CPFEM fully resolved mesh.

Figure 13: Statistical error analysis of overall stress prediction using all 50 sets of grain orientations: (a) error scattering pattern; (b) the stress error as a function of the DD-EHM model order.
is a function of the partition scheme, the sparsity of the matrix calculation and the grain number, which were investigated in [22]. The computational speedup $Q$ is 43 and 47 for BCC and HCP cases, respectively, using the 145-grain RVE. The slight variation is due to differences in number of iterations needed to convergence the equilibrium equations.

This study demonstrates that the hierarchical model improvement capability allows more accurate model prediction with increasing model order, especially in better capturing the local (e.g., sub-grain) fields. Assessment of this feature is important for characterization of convergence of the reduced model to full CPFE simulations when sufficiently large number of parts are used. However, the cost of simulations naturally increases with refinement of the reduced order models. Efficiently employing hierarchical model improvement in structural simulations also require adaptive model refinement algorithms, which will be investigated and developed in the future.

4 DD-EHM simulation for near-α Ti-6242S

Ti-6242S, is a near-α titanium alloy that has been used in a variety of applications such as aircraft structure and turbine engine compressor. This material exhibits high resistance to failure associated with creep, fatigue and environmental degradation. Its hierarchical microstructure exhibits characteristic features, such as the primary α grains, matrix of lamellar α+β and microtextured regions of α particles with similar orientations, that contribute to the observed mechanical and physical properties [60, 61, 62]. Alloying elements Al, Sn and Zr primarily serve to stabilize the α phase, whereas Mo acts as a β phase stabilizer. Si is utilized to improve the creep resistance at high temperature.

The experimental data of Ti-6242S in [59] is used as the input to generate the microstructure and to calibrate the proposed EHM model. The chemical composition of the Ti-6242S material is shown in Table 2. Here, the primary α occupies most of the material with the remainder occupied by the β phase. The duplex annealing process is applied to obtain this microstructure. The α phase has the crystal structure of HCP and the β phase is BCC. Above approximately 990 °C, the fully transformed beta phase could be obtained. Its melting temperature is about 1700 °C. Burgers orientation relationship (BOR) is usually observed in colony, Widmanstatten or Basketwave structure inside the ($α + β$) microstructure [63]. EBSD scans do not indicate that equiaxed alpha/beta phase forms BOR inside this type of Ti-6242S.

Under service performance of cyclic loading, the inner dislocation behavior of plastic deformation in Ti-6242S is quite different from that during the forming process. Under experimental microscopy, a net dislocation accumulation is observed in each loading cycle of high cycle fatigue and very high cycle fatigue loading, and generation and annihilation of dislocations describes the nonlinear behavior and contributes to the onset of fatigue crack nucleation [64]. In addition, low angle boundaries are observed in the titanium alloys during the α to β phase transformation, which means that the sub-grain or dislocation substructure exists.
inside individual grains [65]. In the micro-textured α/β colonies of titanium alloys, the sessile dislocation storage or pile-ups is promoted by the crystallographic and morphological features on both basal and prismatic slip, and mobile dislocation usually passes through the α/β interface [66, 67]. Under cyclic loading conditions at room temperature, plastic deformations are taken to be dominated by dislocation glide [68, 69]. Thus, the sub-grain sessile dislocation storage inside individual crystal [35] and the reversal dislocation under cyclic loading [48] introduced in Section 2.1 are applied here for better describing the dislocation mechanism inside Ti-6242S. This alloy does not exhibit significant deformation twinning at the relatively small strain levels [25].

4.1 DD-EHM calibration

The material used in this study follows ref. [59], which has 94 % stabilized primary α grains with no micro-texture zones or α/β colonies. Thus, the influence of the β phase on the mechanical response is relatively low [70]. In fact, the choice for the parameters for the beta phase is relatively insensitive to stress-strain data employed in model calibration. Since the volume fraction of β phase is low, the β-phase model is simplified by considering the same parameters for all the BCC slip systems shown in Fig. 3. The model parameters for β grains are chosen consistent with previous studies [71, 72].

The 3D polycrystalline RVEs are generated from 2D SEM images assuming identical features in the orthogonal directions to the image. Experimentally characterized grain size distribution, grain orientation and misorientation distribution functions are employed in the construction of the RVE to provide an accurate description of the crystallographic features. The beta phase volume fraction is much lower than that of the alpha phase. Only 8 small grains are identified as beta phase in the 145-grain RVE. Grain size distributions are fitted by two continuous probability distribution functions, i.e., lognormal distribution \((\sigma, \mu) = (10.21, 0.16)\) for the β phase and normal distribution with cutoff \((\sigma, \mu) = (0.43, 1.74)\) for the α phase. The chosen distribution functions are best fits to the experimental data provided in [59] as shown in Figs. 14(c)-(d). Misorientation distribution and the pole figures from [59] are shown in Fig. 14. The misorientation angle are the ones for each HCP grain boundaries. The misorientation angles are divided into 36 bins with the bin size of 2.5 degrees. The volume fraction of each bin is added up and collected into each bin. The misorientation distribution in the RVE are enforced by using the misorientation probability assignment method (MPAM) introduced by [71]. Consistent with the previous literatures [25, 73, 50], the evolution of sessile dislocation densities in basal, prismatic and pyramidal slip systems of HCP and three types of BCC slip systems are considered.

The cyclic response of the polycrystalline Ti-6242S is described using the aforementioned dislocation density based crystal plasticity model. Two sets of information have been employed to calibrate the model parameters of crystal plasticity model. The first set consists of the existing experimental datasets and corresponding calibrated models of Ti-6242S provided
Figure 14: (a) Orientation distribution in pole figure; (b) Misorientation distribution for Ti-6242S data from [59]; (c) grain size distribution of \( \alpha \) phase; and (d) grain size distribution of \( \beta \) phase.
The experiments and model predictions of these studies have been fitted with the proposed dislocation density based model. The model parameters were then further tuned to accurately capture the stress-strain curves performed at two strain rates at room temperature [59]. A single set of material parameters are obtained by matching experimental datasets for quasi-static uniaxial tension experiments under two constant strain rates (QS: $8.33 \times 10^{-5}$ s$^{-1}$; HS: 0.01 s$^{-1}$) at room temperature, summarized in Table 3. Figure 15 (a) shows the comparison of the stress-strain curves from the experiments and the calibrated model.

Table 2: Chemical composition in weight % of Ti-6242S [59].

<table>
<thead>
<tr>
<th>Component</th>
<th>Al</th>
<th>Sn</th>
<th>Zr</th>
<th>Mo</th>
<th>Si</th>
<th>C</th>
<th>N</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured</td>
<td>5.96</td>
<td>1.98</td>
<td>3.92</td>
<td>1.99</td>
<td>0.09</td>
<td>0.02</td>
<td>&lt;0.01</td>
<td>0.10</td>
</tr>
</tbody>
</table>

Table 3: Calibrated model parameters for Ti-6242S.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Basal $(a)$</th>
<th>Prismatic $(a)$</th>
<th>Pyramidal $(a)$</th>
<th>Pyramidal $(c + a)$</th>
<th>BCC Slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta F$</td>
<td>J</td>
<td>$3.95 \times 10^{-20}$</td>
<td>$3.81 \times 10^{-20}$</td>
<td>$4.27 \times 10^{-20}$</td>
<td>$4.73 \times 10^{-20}$</td>
<td>$3.74 \times 10^{-20}$</td>
</tr>
<tr>
<td>$\Delta V$</td>
<td>m$^3$</td>
<td>$5.91 \times 10^{-29}$</td>
<td>$8.20 \times 10^{-29}$</td>
<td>$7.40 \times 10^{-29}$</td>
<td>$8.85 \times 10^{-29}$</td>
<td>$6.30 \times 10^{-29}$</td>
</tr>
<tr>
<td>$k$</td>
<td>J - K$^{-1}$</td>
<td>$1.381 \times 10^{-23}$</td>
<td>$1.381 \times 10^{-23}$</td>
<td>$1.381 \times 10^{-23}$</td>
<td>$1.381 \times 10^{-23}$</td>
<td>$1.381 \times 10^{-23}$</td>
</tr>
<tr>
<td>$\rho_m$</td>
<td>m$^{-2}$</td>
<td>$5.00 \times 10^{12}$</td>
<td>$5.00 \times 10^{12}$</td>
<td>$5.00 \times 10^{12}$</td>
<td>$5.00 \times 10^{12}$</td>
<td>$5.00 \times 10^{12}$</td>
</tr>
<tr>
<td>$\nu_id$</td>
<td>Hz</td>
<td>$1.00 \times 10^{12}$</td>
<td>$1.00 \times 10^{12}$</td>
<td>$1.00 \times 10^{12}$</td>
<td>$1.00 \times 10^{12}$</td>
<td>$1.00 \times 10^{12}$</td>
</tr>
<tr>
<td>$b^s$</td>
<td>$\mu$m</td>
<td>$2.94 \times 10^{-4}$</td>
<td>$2.95 \times 10^{-4}$</td>
<td>$2.95 \times 10^{-4}$</td>
<td>$4.68 \times 10^{-4}$</td>
<td>$2.86 \times 10^{-4}$</td>
</tr>
<tr>
<td>$k_1^s$</td>
<td>m$^{-1}$</td>
<td>$1.80 \times 10^{7}$</td>
<td>$1.68 \times 10^{7}$</td>
<td>$1.67 \times 10^{7}$</td>
<td>$2.40 \times 10^{7}$</td>
<td>$1.03 \times 10^{7}$</td>
</tr>
<tr>
<td>$D^s$</td>
<td>MPa</td>
<td>300</td>
<td>330</td>
<td>100</td>
<td>90</td>
<td>230</td>
</tr>
</tbody>
</table>

RVE size convergence is investigated using both CPFEM and DD-EHM models to identify the proper size of the RVE that adequately resolves the local response fields under cyclic
Figure 16: Local stress distribution as a function of RVE size: (a) DD-EHM model; (b) CPFEM model for RVEs with (c) 56 grains; (d) 97 grains; (e) 145 grains; (f) 245 grains; (g) 302 grains; and (h) 335 grains.

loading. Figure 16 shows the distribution of local stresses within the RVE as a function of RVE size (ranging from 56 to 335 grains). Figure 15 (b) shows that the stress-strain loops stabilize quickly under a pure fatigue load cycle by approximately the eighth cycle. The variation of the response fields is slight from cycle to cycle. Figure 16(a,b) captures the stress distributions at the peak of the first load cycle. Using both models, the local response of the microstructure converges when the edge length of RVE is larger than 19.58 µm (i.e., 145 grains). Thus, the 145-grain microstructure is deemed representative for the overall mechanical response. Since CPFEM resolves the microstructure response, the stress distribution is smoother than that of the DD-EHM.

4.2 Structural-scale simulation of near-α titanium during cyclic loading

The capabilities of the proposed reduced order modeling approach in capturing crystal-scale characteristics is further assessed using structural simulation. The structural domain is an L-shaped bracket made of Ti-6242S. The geometry, discretization and the boundary conditions used for the structural scale problem are shown in Fig. 17. Displacement-controlled cyclic loading is applied at the anchors of the bottom edge. The applied displacement rate and maximum displacement amplitude are 12 mm/s and 3 mm, respectively. The geometry is discretized used 3,940 tri-linear eight-node hexahedral elements. Reduced order integration is
Figure 17: A L-shape plate of Ti-6242S under strain controlled cyclic loading: (a) geometry and loading condition of the plate; (b) finite element mesh; (c) strain-controlled loading history.

employed with hourglass control to alleviate zero energy modes. Each quadrature point of the macroscale mesh is associated with a microstructure that consists of 145 grains with the edge length of 19.58 µm as shown in Fig. 16e. Identical microstructures have been used at each quadrature point. The simulation therefore tracks the response of a total of 571,300 grains. Simulations have been performed using the one-part-per-grain model reduction strategy. The simulation of the structure using the classical computational homogenization approach or the direct resolution (i.e., CPFEM) of the microstructure is computationally prohibitive, therefore not included in this study.

4.2.1 Dislocation pile-ups at two spatial scales

Transmission electron microscopy of Ti-6242S specimen indicate intense dislocation pile-ups at the grain boundaries slightly beneath the crack nucleation surface [68, 69]. Using scanning electron microscopy on the same material, the dislocation pile-ups are revealed as the zigzag boundary between hard and soft grain pairs [76]. Prior numerical investigations using CPFEM identified that the dislocation pile-up length is a critical parameter indicating fatigue crack nucleation [75, 20]. Accumulated dislocation pile-ups could induce crack nucleation through multiple mechanisms, including slip band localization [77, 78], stress concentrations at the alpha/alpha grain boundaries or at the alpha/beta phase boundaries [79] and basal stress concentration in the neighboring hard grain due to load shedding phenomenon inside hard-soft grain pairs [80, 81, 82].

The experimental observations of Ti-6242S show that the dislocations prefer to directly transfer through the alpha/beta phase boundary [68]. Strong slip bands do not occur during the low-cycle fatigue loading [69]. Thus, we assume that the dislocation pile-ups at the alpha/alpha grain boundary has the main effect on crack nucleation. The amount of pile-ups is quantified
by the relative dislocation density discrepancy $\Delta \rho_{\text{tot}}$ between neighboring grain pairs (Fig. 18).

Since the plastic anisotropy of HCP crystal is involved and the slip system activation is mainly dominant by a single type of slip system [83, 43, 31], hence, the maximum dislocation pile-ups is obtained in the slip system with the highest sessile dislocation density regardless of the slip system type and the order of slip system.

The maximum relative dislocation density discrepancy in an RVE is obtained using the following steps:

1. At the beginning of the simulation: For each grain in the microstructure, identify all the neighboring grains that share surface facets with the grain to form the grain pairs.

2. During the simulation at a given load increment:
   
   (a) For each grain, $i$, within the RVE, the maximum dislocation density is obtained by looping over all the slip systems ($s = 1, \ldots, n$) inside the grain.

   $$(\rho_{\text{tot}})^i = \max_{s \in \{1, \ldots, N\}} \left\{ (\rho_{\text{tot}})^s \right\}$$

   (21)

   (b) For each grain, $i$, maximum dislocation discrepancy is set to the largest difference between the maximum dislocation density in grain $i$ and that of all its neighboring grains ($j = 1, \ldots, m_i$), where $m_i$ is the total number of neighbors of grain $i$.

   $$(\Delta \rho_{\text{tot}})^i = \max_{j \in \{1, \ldots, m_i\}} \left\{ \left| (\rho_{\text{tot}})^i - (\rho_{\text{tot}})^{k(j)} \right| \right\}$$

   (22)

   where, $k(j)$ is the grain ID for the $j^{th}$ neighbor of grain $i$.

   (c) Maximum dislocation discrepancy in the entire RVE is chosen as the highest value of the maximum dislocation discrepancies of all grains $i$ within the RVE:

   $$\Delta \rho_{\text{tot}} = \max_{i \in \{1, \ldots, n\}} \{(\Delta \rho_{\text{tot}})^i\}$$

   (23)

The time evolution of relative dislocation density distributions are reported from three different spatial positions within the structure as illustrated in Fig. 17a. Figure 19 shows the microstructure-maximum relative dislocation density distributions at six time instances at the three spatial positions (the time instances are identified in the inset figure). Two key observations are that the relative dislocation densities exhibit significant spatiotemporal variations and that the peak relative dislocation densities do not necessarily coincide with the peak loads (i.e., $t = 0.25$ s and $t = 0.75$ s). The spatial variations shown in Fig. 18a are naturally due to geometrically induced non-uniform stresses within the structure, but the spatial distributions also significantly change as a function of applied displacement amplitude and time due to load redistributions induced by viscoplasticity. At peak applied displacement amplitude (at $t = 0.25$ s), very small amount of plastic deformation and dislocation generation are observed at positions 2 and 3, whereas many of the grains undergo plastic deformation and
Figure 18: Schematic illustration of capturing dislocation pile-ups at grain boundary: (a) extract $\Delta \rho_{\text{tot}}$ of a microstructure at a given macroscopic integration point; (b) identify neighboring grains according to adjacent nodes; (c) potential crack interface.

Figure 19: $\Delta \rho_{\text{tot}}$ distribution at different time steps in: (a) position 1; (b) position 2; (c) position 3. The insert shows the loading profile and the red dots in the black curves represent the displacement history at $t = 0.25, 0.4, 0.55, 0.7, 0.85, 1.0$ sec.
dislocation generation at position 1. The unloading and reloading (in the opposite direction) processes demonstrate a non-monotonic growth of relative dislocation density indicating a non-monotonic increase in dislocation pile-up. At the end of the loading process, (at $t = 1.0 \text{ s}$), a much wider range of relative dislocation density levels are observed in position 1 compared with the positions 2 and 3. It is important to note that the tail ends of the distributions are likely to be more indicative of failure nucleation process than the distribution means, since failure is likely to nucleate near a few grains with high degree of dislocation pile-up.

### 4.2.2 Effect of non-uniform texture

Strain partitioning due to non-uniform texture is widely observed in the experimental studies of titanium alloys [84, 85, 86]. The strong anisotropic HCP crystals enhance strain localization due to hard or soft crystallographic orientations [87]. Recent studies suggested small clusters of similar crystal orientations, called micro-textured regions (MTR) or macrozones, can have a significant effect on the fatigue and dwell fatigue sensitivities in titanium alloys, even though no severe texture is observed in the experiments [88, 89]. However, the non-uniform texture could have the potential benefit of reducing the strain localization in specific locations, which might be a critical region during the service of the structural component. Through a selection of non-uniform texture, it might be possible to alleviate or defer crack nucleation in critical spots of the components.

In this section, three different texture orientations are selected and assigned to different parts of the L-shape component in Fig. 20a to form a non-uniform textured structure. In part 1, the $\alpha$ grain orientation selection in the RVE remains the same as the experiments by [59], and the dominant direction of crystal c-axis is along the Y axis. The orientations in part 2 and 3 are such that the dominant c-axis directions are along Z and X axises, respectively. Same strain-controlled load is applied as shown in Fig. 17b. The L-shape geometry and the loading location at the edge result in a inhomogeneous stress distribution within the component. However, Fig. 20b shows compression- or tension-like behaviors (along X axis) at the top and bottom of the adjacent area between part 1 and part 2. The high stress levels at these spots contribute to local plastic slip and the corresponding strain concentration shown in Fig. 21a and b. Due to the geometry of the fillet, higher stress localization is observed and leads to more severe plastic deformation at the top area. While the texture of the component considered in this example is artificial, this study allows us to investigate the effect of microtexture, and demonstrate the capability of DD-EHM in quantifying the effect of microtextured regions at the scale of a structural component.

The high spot zone of strain distribution occurs in part 1 and it diminishes in part 2 in Fig. 21(b), whereas high strains are observed in both part 1 and part 2 in the original case. This is due to different dominant crystallographic orientations. Part 1 and 2 form a stress-state at the macro-scale similar to that near the hard-soft grain boundary observed at micro-scale. The crystal c-axis of part 1 is mainly perpendicular to the direction of maximum
Figure 20: (a) Non-uniform texture selections in three separate parts of L-shape component; (b) the directions of maximum principal stress at the middle of the cycle; (c) the directions of maximum principal stress at the end of the cycle. $\sigma_{\text{abs,principal}}$ refers to the maximum principal value compared using absolute value.

Figure 21: Maximum principal strain $\varepsilon_{\text{max,principal}}$ and $\Delta \rho_{\text{tot}}$ distributions in L-shape panel: uniform-texture case from experiments (a and c); non-uniform-texture case (b and d). The hexagonal prism indicate the dominant grain orientation.
principal stress which favors the prismatic dislocation activation to trigger the plastic slip near boundary of part 1 and 2, but only localized at part 1. In contrast, the c-axis of part 2 is nearly parallel to the local load. Prismatic and basal dislocations are hard to activate at this crystal configuration and it needs much higher stresses to overcome the energy barrier of pyramidal slip. Thus, much less plastic deformation is observed in part 2 compared with part 1. This strain partitioning phenomenon is analogous to the observations in the micro-textured regions of titanium [84, 62]. Individual hard or soft grains in the microstructure could not form the macro-scale strain partitioning. As the plastic slip is blocked in part 2, it could not be transferred to part 3 and no plastic deformation is observed in part 3.

The maximum dislocation pile-ups inside hard-soft grain pairs are also investigated for the non-uniform-texture case in Fig. 21d. It is observed that the high dislocation pile-up is only observed in part 1. The bottom area of the panel contributes more dislocation pile-ups in the macro-scale hard-soft texture pairs than that in the uniform-texture case, which is consistent with the strain distribution. The reduction in strain and dislocation pile-up in part 2 indicate that non-uniform texture selections could be used to alleviate the local strain concentration and crack nucleation.

5 Conclusions

This manuscript presented an extension of the EHM approach to gain the ability to perform multiscale simulations of titanium alloy structures coupling the scale of representative volumes that resolve polycrystalline microstructure to the structural scale. The proposed approach was verified for accuracy in modeling the behavior of HCP and BCC polycrystals. This manuscript also investigated the evolution of dislocation pile-ups at grain boundaries, which serves as an important factor for fatigue crack nucleation in titanium alloys. The following main conclusions are drawn from our investigations:

- The DD-EHM approach is extended to the HCP and BCC based polycrystal plasticity. A reversible dislocation density based model is utilized to capture physics beneath the crystal anisotropy and plastic slip during cyclic loading. RVE-level investigations on HCP and BCC polycrystal verify the macro- and micro-scale accuracy of the method.

- The DD-EHM approach demonstrates high accuracy when compared with the CPFEM approach, but with significantly lower computational cost, allowing for relatively large structural scale simulations and accounting for grain interactions. The accuracy in capturing the localized behavior at sub-grain-scale is improved by proper selection of the reduced basis through appropriate microstructure partitioning.

- Structural simulations on an L-shape panel shows that texture orientation has an important influence on the strain distribution, and could be leveraged at the structural scale to reduce strain concentrations and dislocation pile-ups thereby improving fatigue life.
The reduced order modeling approach, as well as the multi-scale fatigue nucleation modeling will be advanced in a number of fronts in the near future. Firstly, this manuscript focused on the verification of the EHM approach in the context of material behavior that does not exhibit severe strain softening. The presence of strain softening results in the formation of localization bands with length scales that may be lower than the size of the RVE. The EHM methodology will be extended to address problems that exhibit this phenomenon. Next, the proposed dislocation pile-up parameter is not the only factor in fatigue crack nucleation. It is reasonable to demonstrate a criterion of the combination of the dislocation pile-up and basal stress to predict the I-type crack nucleation observed in titanium under fatigue or dwell fatigue loading condition. The multi-scale fatigue nucleation site prediction approach will also be extended for life predictions and validated against experimental observations.

6 Acknowledgments

Part of the research has been performed with research funding from Air Force Office of Scientific Research (Grant No: FA9550-13-1-0140. Program Manager: Jamie Tiley), which is gratefully acknowledged. The authors thank Dr. Brian T. Gockel for sharing the experimental data originally published in [59]. The authors also acknowledge the discussions with Dr. Adam Pilchak that contributed to the analyses presented in this manuscript. The lead author has conducted this research at Vanderbilt University through the financial support of the China Scholarship Council (No. 201606060105), which is gratefully acknowledged.

References


30
[26] Zhang Z and Dunne F P 2018 *Int. J. Fatigue* 113 324 – 334 ISSN 0142-1123
[37] Le K, Tran T and Langer J 2018 Scr. Mater. 149 62–65
[38] Le K and Tran T 2018 Phys. Rev. E 97 043002


[64] Castelluccio G M, Musinski W D and McDowell D L 2016 Int. J. Fatigue 93 387 – 396


[68] Joseph S, Bantounas I, Lindley T C and Dye D 2018 Int. J. Plast. 100 90 – 103

[69] Joseph S, Lindley T C and Dye D 2018 Int. J. Plast. 110 38–56 ISSN 07496419


33


[81] Evans W and Bache M 1994 Int. J. Fatigue 16 443–452

[82] Benjamin B T and Wilkinson A J 2012 Acta Mater. 60 5773–5782 ISSN 13596454


