Effect of Realistic 3D Microstructure in Crystal Plasticity Finite Element Analysis of Polycrystalline Ti-5Al-2.5Sn

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Abstract

The effect of constitutive parameters and microstructure on the kinematic and constitutive responses within grains in a crystal plasticity finite element (CPFE) simulation of a polycrystalline titanium alloy are compared with experimental results. The simulation of a Ti-5Al-2.5Sn sample deformed in uniaxial tension at room temperature used a phenomenological power-law based CPFE model, which includes four families of slip systems commonly observed in structural metals with hexagonal lattice structure. The experimentally characterized microstructure patch was approximated by a quasi-3D columnar grain structure and by a more realistic 3D representation. The quasi-3D microstructure was generated by extending the EBSD characterized surface microstructure in the depth direction, while the 3D microstructure was built based on subsurface orientation information acquired using differential-aperture X-ray microscopy (DAXM). The effect of grain morphology and constitutive parameters on simulation results are compared in terms of stress-strain responses and lattice reorientation.

Keywords: Ti-5Al-2.5Sn, Crystal Plasticity Finite Element Method (CPFEM), subsurface grain structure, Differential-aperture X-ray Microscopy (DAXM), heterogeneous deformation, orientation gradients

1. Introduction

The need to expedite commercial product design with limited resources has led to the development of computational models because traditional material development methodologies are too expensive and time consuming. There are currently two major approaches being actively developed to understand the role of microstructure on plasticity (Bieler et al., 2009): models based on the Taylor (1938) theory and models based on the constitutive framework of crystal plasticity (Asaro and Needleman, 1985) (see also Roters et al., 2010 for a recent review). The Taylor theory based models generally use a statistical representation of the microstructure, *i.e.* several internal variables are used to statistically represent the spatial and angular distribution of the grains within the area of interest. As demonstrated by several studies (Delaire et al., 2000; Guo et al., 2001; Hwang et al., 2004; Jung et al., 2013; Wang et al., 2007; Wu et al., 2007), models based on the Taylor theory are effective at predicting macroscopic responses such as macroscopic stress/strain history and texture evolution. But due to the nature of their statistical representations of microstructure, the Taylor theory based models generally do not keep track of the local deformation history, which makes them less suitable for studies that require site-specific deformation history. Crystal plasticity theory based models on the other hand, spatially discretize (representative) volumes of microstructure and, thus, can directly apply realistic boundary conditions to realistic microstructures (Roters et al., 2010). Because of this more physically based structure, models based on crystal plasticity generally provide a more accurate prediction of local deformation history, as demonstrated by many studies (*e.g.*, Busso et al., 2000; Cheong and Busso, 2004, 2006; Gao et al., 1999; Fleck et al., 1994; Kuhlmann-Wilsdorf, 1999; Rehrl et al., 2012; Li et al., 2014; Liu and Wei, 2014).

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Nevertheless, correct prediction of grain-scale deformation histories from crystal plasticity based models depends on validated constitutive models for crystal plasticity. This validation is generally done via micromechanical measurements of local strains and the evolving grain shape of the selected region in samples.

One common technique for micromechanical measurements is digital image correlation (DIC) (Efstathiou et al., 2010; Pouillier et al., 2012; Huh et al., 2013; Kammers and Daly, 2011; Lebensohn et al., 2011; Viguié et al., 2011; Welsch et al., 2007) that tracks the relative displacement of sampling points on the surface during the deformation. The strain tensor acquired through surface DIC resolves only components within the surface plane and lacks information on the deformation in the out-of-plane direction. To address this information limitation, Yang et al. (2011a) used surface slip trace analysis to identify active slip planes and Burgers vectors, then measured the height of the slip traces by atomic force microscopy (AFM) to derive shear contributions per slip system from which the full three-dimensional strain tensor can be calculated.

The most widely used technique for measuring grain shapes and orientations is electron backscatter diffraction (EBSD) and associated orientation imaging microscopy (OIMTM) (Seward et al., 2004; Niederberger et al., 2010; Mao et al., 2008; Gee et al., 2009). However, without destructive serial sectioning, this technique can only provide the grain orientations and shapes on a sample surface while the subsurface microstructure is not directly accessible. Computational models based solely on EBSD surface measurements have to approximate the true grain structure, either by extending the surface microstructure in the depth direction (resulting in columnar grains) or by introduction of artificial subsurface grains. One strategy for narrowing the resulting disconnect between simulations and reality is to use specially prepared samples with columnar grains (Delaire et al., 2000; Lim et al., 2014; Delannay and Barnett, 2012; Klusemann et al., 2013; Raabe et al., 2001; McDowell and Dunne, 2010; Raabe et al., 2003). These oligocrystalline samples (containing a small number of grains with their grain boundaries perpendicular to the surface, *i.e.* columnar grains running through the sample) can be easily meshed by finite elements.

As surface-only approaches do not allow assessment of general 3D microstructures, true 3D characterization is required to measure the geometry of non-special microstructures. Consequently, a number of different techniques have been developed to characterize and subsequently simulate the full three-dimensional nature of microstructures. Serial sectioning combined with EBSD, also known as 3D-EBSD, is one of the few techniques developed to address the need for 3D characterization (Raabe et al., 2007; Sharma et al., 2010; Zaafarani et al., 2008, 2006). One major drawback of using 3D-EBSD is its destructive nature, which makes it impossible to perform further investigation on the sample. The same is true for other the serial sectioning techniques, which may be further complicated by introducing additional straining or strain relaxation that may render the newly exposed surface different from the bulk state.

To address the difficulties of the destructive 3D characterization techniques, several non-destructive 3D options that use a synchrotron X-ray beam have been developed in the past decade. Differential-aperture X-ray microscopy (DAXM) at Beamline 34-ID-E of the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) is one of the techniques, providing sufficient spatial (1 μm) and angular (0.01°) resolution for microstructure reconstruction purposes (Larson et al., 2002; Yang et al., 2011b; Zhou et al., 2013). However, the data acquisition speed of DAXM is generally slow and the subsurface penetration of DAXM is limited, for example $\approx 200 \mu\text{m}$ for Ti due to the limited X-ray beam energies ($< 30 \text{ keV}$). Consequently, DAXM is suitable for characterizing a small set of near-surface grains with high spatial and angular resolution. Three-dimensional X-ray diffraction (3DXRD) is another 3D characterization technique, initially developed at Beamline ID11 of the European Synchrotron Radiation Facility (ESRF) (Poulsen et al., 1997, 2001) and now also available at Beamline 1-ID-E at APS. Unlike DAXM, which is based on Laue diffraction, 3DXRD uses a monochromatic X-ray beam with high energy ($> 60 \text{ keV}$) that penetrates through a rotating target sample. With the detector far from the sample, sufficient resolution is available to provide averages of orientation and complete stress tensor per illuminated grain (Bernier et al., 2011; Margulies, 2001). With recently developed near-field detector methods, improved spatial resolution is possible, but this requires computationally intensive post processing (Li et al., 2012b; Suter et al., 2006). These methods provide an increasingly available means to assess the ability of crystal plasticity models to accurately predict heterogeneous deformation in polycrystalline samples.

As it is difficult to measure the local stress state in a three dimensional polycrystal, the ability to simulate the deformation accurately also provides stress gradient information that is needed to more effectively analyze and interpret experimental observations. Thus, the objective of this study was to evaluate the effect of using a realistic 3D microstructure as compared to a columnar estimate in the CPFE analysis of a polycrystalline sample of Ti-5Al-2.5Sn. Two microstructure representations were developed from an experimentally characterized microstructure patch. The

first of these was a columnar oligocrystalline microstructure that was constructed based on surface OIM data only. The second model was a full 3D microstructure, constructed using additional DAXM data. Both of the model microstructures were computationally deformed assuming phenomenological power-law kinetics with latent hardening effects. The influence of the realistic 3D microstructure on the evolution of local stress and strain patterns as well as intragranular orientation gradients arising from plastic deformation was assessed using CPFE simulations and compared to the experimental results.

In this paper, the experimental methods used to characterize the mechanical and microstructural properties of the Ti-5Al-2.5Sn sample are described in Section 2, followed by the procedure for microstructure construction, description of the crystal plasticity model, and model calibration in Section 3. The simulation results are given in Section 4, with concluding remarks in Section 5. The following notation will be used: scalars (zero-rank tensors) are denoted by lowercase italic, vectors (first-rank tensor) by lowercase bold, second-rank tensors by uppercase bold, and forth-rank tensors by blackboard bold letters. Examples would be a , $\mathbf{v}$, $\mathbf{S}$, and $\mathbb{C}$, respectively.

2. Experimental Characterization

A tensile specimen with a gauge section of $1.5 \text{ mm} \times 3 \text{ mm} \times 10 \text{ mm}$ was cut from a commercial Ti-5Al-2.5Sn plate with an average grain size of $45 \mu\text{m}$. The chemical composition of the bulk material was (in weight percent) 92.4 % Ti, 4.7 % Al, 2.7 % Sn, 0.2 % Fe, 0.1 % Zn and 0.03 % Cl as measured by inductively coupled plasma mass spectroscopy (ICP-MS). The near- α microstructure of the as-received bulk material is shown in Fig. 1a and contains a small amount (1 % volume fraction) of body-centered cubic (bcc) β -phase dispersed at boundaries between the hexagonal α -phase.¹ One surface of the tensile sample was mechanically polished to a finish of $0.06 \mu\text{m}$ colloidal silica to facilitate EBSD measurements (Fig. 1b) in a Camscan 44FE scanning electron microscope (SEM). EBSD data acquired on the undeformed sample revealed an almost random texture (Fig. 2). After EBSD characterization, the sample was deformed inside a Carl Zeiss EVO LS25 SEM using a screw-driven tensile stage (MTII/Fullam, Albany, NY) operating at constant displacement rate of 0.04 mm s^{-1} and ambient temperature. The load and displacement data were recorded by MTESTW data acquisition and control software (Admet Inc., Norwood, MA, USA). The in-situ test was paused at two strain levels to collect secondary electron images, which resulted in the stress relaxations obvious in Fig. 3. After deformation, OIM and secondary electron imaging of the sample surface in Fig. 1a revealed slip traces on basal and prism slip systems analyzed in depth in (Li et al., 2012a), and the local strain in the region of interest imaged in Fig. 1a was estimated as 3.5 % through a coarse digital image correlation (DIC) approach, where distinctive topographic features were used to evaluate the strain along the tensile direction. Several irregular ledges arising from slip transfer from the underlying grain are visible in the central grain are discussed in (Bieler et al., 2014).

In order to characterize the subsurface microstructure of the region shown in Fig. 1, DAXM was performed on the deformed sample at Beamline 34-ID-E. The experimental configuration of DAXM is illustrated in Fig. 4a. A Pt wire of $50 \mu\text{m}$ diameter was used as the differential aperture, scanning above the sample surface using a $2 \mu\text{m}$ step size to provide a resolution of $1 \mu\text{m}^3$ for crystallographic orientation mapping down to a depth of about $100 \mu\text{m}$. The detailed procedure of DAXM is described by Larson et al. (2002). The crystallographic orientation maps were generated using the LaueGo software packages developed by beamline scientists at APS.²

3. Simulation Setup

3.1. Quasi-3D microstructure construction

As crystal plasticity simulations are frequently based on surface orientation data only, a quasi-3D microstructure was constructed by extending the surface grain morphology (Fig. 5a) into the third dimension, yielding 18 columnar grains in a volume of $134.5 \times 145 \times 60 \mu\text{m}^3$ that was meshed by about 40 000 tetrahedral elements (Fig. 5c).

¹Preliminary CPFE simulations based on extruding the oligocrystalline surface structure into columnar grains showed that the scattered β -phase had negligible effect on the deformation history of the dominating α -phase and was therefore ignored.

²Software available at: http://www.aps.anl.gov/Sectors/33_34/microdiff/downloads/

(a) Secondary electron contrast image at approximately 3.5% deformation. Linear features are slip lines and surface ledges (particularly within the central grain). β -phase (bright) is present along few grain boundaries. (b) Inverse pole figure map of initial grain structure. Hexagonal unit cells represent crystallite orientations at dotted locations.

Figure 1: Microstructure patch of interest selected on the Ti-5Al-2.5Sn sample.

Figure 2: EBSD measured pole figures indicate a relatively weak texture.

3.2. 3D microstructure construction

To develop a more realistic microstructure, an approximation³ of the initial subsurface morphology was constructed based on four DAXM line scans (three H-scans and one X-scan, Fig. 4b). By combining the surface OIM (Fig. 1b) and the four subsurface crystallographic orientation maps generated by LaueGo, a “paper model” (Fig. 5b) was built to visualize the 3D microstructure of the volume of interest. Based on this, a $134.5 \times 145 \times 60 \mu\text{m}^3$ volume containing the roughly realistic microstructure was manually constructed (Fig. 5d) using the commercial software Mentat 2012 (MSC Software Corporation, Newport Beach, CA 92660, USA). The reconstruction resulted in some grains having irregular shapes not expected for an annealed microstructure. Due to limited data available from the DAXM characterization, only the central part of the volume was fully constructed with DAXM data, while the grain boundaries of surrounding grains were assumed to be perpendicular to the surface. The resulting patch of 29 grains, 11 of which were subsurface grains, was discretized with about 50 000 tetrahedral elements.

³Since no subsurface orientation data of the initial grain structure is available, the undeformed grain morphology is assumed to differ only minimally in terms of grain orientation and grain boundary locations from the state measured after 3.5% strain.

Figure 3: In situ (dotted) and approximated (solid) stress–strain response of the Ti-5Al-2.5Sn sample. Stress relaxation during SEM image acquisition caused the two intermittent drops in the dotted curve.

(a) Schematic drawing of the DAXM experimental setup (Zhou et al., 2013).

(b) Four line scans (H1, H2, H3, X1) were performed in the central region of the selected area.

Figure 4: Characterization of selected volume of interest by differential aperture X-ray microscopy (DAXM).

(a) Surface EBSD map used to generate quasi-3D microstructure.

(b) Surface EBSD map plus four DAXM maps arranged according to their 3D relationship.

(c) Exploded grain structure and corresponding quasi-3D microstructure of columnar grains based on (a).

(d) Exploded grain structure and corresponding 3D microstructure developed from (b).

(e) Fractional extent of the surface grain orientation into the depth. White shade indicates constant orientation through thickness (*i.e.*, a columnar grain). The darker the shade, the closer a differing grain orientation is to the surface.

Figure 5: Grain construction based solely on surface EBSD data of the undeformed sample (a and c) compared to reconstruction using additional subsurface DAXM scans (b and d). Note the central grain on the surface (purple) in the 3D microstructure is much thicker on one side (positive y) than the other due to the existence of a subsurface grain (green) right beneath it (see also e).

3.3. Geometry approximation error

To quantify the similarity between the 3D microstructure and its approximation by the quasi-3D microstructure, we introduce the fraction over which the surface orientation at position x, y extends into the depth

$$\kappa(x, y) = \frac{d(x, y)}{h},$$

where $d(x, y)$ is the depth at which the surface orientation changes due to the presence of a subsurface grain and h is the overall depth of the modeled volume. The resulting map of the structure approximation error is shown in Fig. 5e. Each white-shaded grain is columnar in both geometries (compare Fig. 5c and d). The darker the shade, the earlier the surface grain orientation is replaced by a subsurface grain along the depth (z) direction. It turns out that within a volume fraction of about 0.6 the same lattice orientations (*i.e.*, identical grain structure) are found in the 3D microstructure and its quasi-3D approximation.

3.4. Initial conditions

Although various studies have shown that the initial intragranular misorientation can affect the crystal reorientation during plastic deformation (Cheong and Busso, 2004, 2006), here we assume a single initial lattice orientation in each grain. This is consistent with the fact that the bulk material is known to be recrystallized (Li et al., 2012a) and with the EBSD analysis of the undeformed material that shows that about 85 % of the grains have a maximum grain orientation spread below 0.5° , which is close to the precision of standard Hough transformation-based EBSD measurements (Schwartz et al., 2009).

3.5. Boundary conditions

In order to approximate the loading experienced by the modeled microstructure volume during the uniaxial tensile test, two different boundary conditions corresponding to two extreme cases (Fig. 6) were used. For the “soft” boundary condition (Fig. 6a), the constraint of the neighboring grains was assumed to be negligible such that all faces except the two loading faces were unconstrained during the deformation. The “hard” boundary condition (Fig. 6b), on the other hand, assumed that the influence of the neighboring grains was strong enough to force all faces except the top free surface, to remain planar during the deformation. The realistic loading environment of the microstructure volume should fall in between these soft and hard boundary conditions. For both boundary conditions, the displacement of the node at $(0, 0, 0)$ was partially constrained in the transverse (x -axis) and vertical directions (z -axis) to provide numerical stability.

Figure 6: Schematic representation of two boundary conditions representing the extreme cases of the loading environment of the microstructure volume. In the soft boundary condition, all faces except the two normal to y are unconstrained. In the hard boundary condition, all faces except the top (surface) are forced to remain planar during deformation. For both boundary conditions, all nodes on the two y faces have prescribed displacement to approximate the tensile loading, and one node in the corner was constrained in the transverse (x -axis) and vertical directions (z -axis) to provide numerical stability.

3.6. Constitutive model

The kinematics of the constitutive model used in this paper follows the established continuum mechanical framework of elastoplasticity at finite strain, as summarized by, for instance, [Roters et al. \(2010\)](#), with a multiplicative decomposition of the total deformation gradient into elastic and plastic parts

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \quad (1)$$

where $\mathbf{F}_e$ represents the elastic stretching and rotation of the crystal lattice and $\mathbf{F}_p$ denotes the deformation gradient associated with dislocation slip. The elastic Green–Lagrangian strain tensor can be calculated from the elastic stretching of the crystal lattice, *i.e.*

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \mathbf{F}_e - \mathbf{I}), \quad (2)$$

where $\mathbf{I}$ is the second rank identity tensor. The second Piola–Kirchhoff stress tensor, as the work-conjugate to the Green–Lagrangian strain tensor, is defined through

$$\mathbf{S} = \mathbb{C} \mathbf{E}_e = \mathbf{F}_e^{-1} (\det \mathbf{F}_e) \boldsymbol{\sigma} \mathbf{F}_e^{-T}, \quad (3)$$

where $\mathbb{C}$ is the elastic stiffness tensor and $\boldsymbol{\sigma}$ is the Cauchy stress tensor. The evolution of the plastic deformation gradient can be defined as

$$\dot{\mathbf{F}}_p = \mathbf{L}_p \mathbf{F}_p. \quad (4)$$

The plastic velocity gradient $\mathbf{L}_p$ is caused by dislocation slip and twinning activity and is described by

$$\mathbf{L}_p = \dot{\gamma}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha. \quad (5)$$

In the formula above, $\dot{\gamma}^\alpha$ is the shear rate of slip system α with slip direction $\mathbf{m}^\alpha$ and slip plane normal $\mathbf{n}^\alpha$; summation is taken over the slip systems $\alpha = 1, \dots, N_{\text{slip}}$. The shear rate due to dislocation flow, $\dot{\gamma}^\alpha$, is defined as

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{s^\alpha} \right|^n \text{sgn}(\tau^\alpha) \quad (6)$$

with a reference shear rate $\dot{\gamma}_0 = 10^{-3} \text{ s}^{-1}$, resolved shear stress $\tau^\alpha = \mathbf{S} \cdot (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)$ of slip system α , and corresponding critical resolved shear stress s^α . The exponent $n = 50$ represents the stress sensitivity (inverse rate sensitivity) of dislocation slip. The evolution of the saturation stress for dislocation slip, *i.e.* work hardening, is central to the material model. The hardening rule implemented in this study is defined as

$$\dot{s}^\alpha = h_0 \left(1 - \frac{s^\alpha}{s_s} \right)^a q_{\alpha\beta} |\dot{\gamma}^\beta|, \quad (7)$$

where h_0 is the reference hardening parameter for dislocation slip interaction, s_s is the saturation stress that is taken as constant for each slip system family, parameters $a = 1/3$, $q_{\alpha\alpha} = 1$, $q_{\alpha\beta} = 1.4$ control the latent hardening, and summation is taken over $\beta = 1, \dots, N_{\text{slip}}$.

A phenomenological power-law module from the Düsseldorf Advanced Material Simulation Kit (DAMASK, [Roters et al., 2012](#)) was used as a user subroutine implemented into the commercial Finite Element Method (FEM) solver Marc 2012 (MSC Software Corporation, Newport Beach, CA 92660, USA). Four slip system families were used, basal, prism, and first order pyramidal $\langle a \rangle$ and $\langle c + a \rangle$ slip. As very little twinning was observed in the sample, and none in the modeled volume, no twinning deformation systems were used in the model.

3.7. Calibration of constitutive model

The parameters of the constitutive model were determined by fitting to the measured stress–strain behavior the response of a spectral method simulation (?) for uniaxial tension of a periodic geometry that is discretized by a regular $10 \times 10 \times 10$ grid. The texture measured by EBSD⁴ was discretized using 8000 distinct orientations following the

⁴We note that this (weak $\langle 10\bar{1}1 \rangle$ fiber) texture differs markedly from the texture reported in ([Li et al., 2012a](#)) for the same material but measured by X-ray diffraction.

method of Eisenlohr and Roters (2008). This orientation population was distributed in groups of 8 orientations per grid point and homogenized by assuming isostrain conditions (*i.e.*, Taylor assumption) at each grid point.

The calibration procedure minimizes the cumulative difference between the measured and simulated uniaxial von Mises stress–strain curve up to a strain of 4 %. The minimization strategy is based on the simplex algorithm of Nelder and Mead (1965) and implemented as a Python script that adjusts the constitutive parameters and reruns the simulation until the stress deviation integrated along the strain falls below the tolerance of 1 MPa.

This calibration procedure was performed eight times starting with different initial sets (simplexes) of constitutive parameters resulting in the shaded band of Fig. 7. No unique (global) optimum was observed, but each of the eight starting populations converged to a different set of optimized constitutive parameters that all produce a good approximation of the stress–strain response of the tensile test. Among the eight outcomes, one set of constitutive parameters, denoted as PS₁ (parameter set 1), was selected based on previous statistical analysis of the critical resolved shear stresses (CRSS) on the same sample by Li et al. (2013), where prism slip is slightly more easily activated than basal slip. In order to study the influence of constitutive parameters on the outcome of CPFEE simulations, a second set, termed PS₂, of constitutive parameters that has the largest Euclidean distance from PS₁ in the parameter space was selected as an exemplary comparison group. Figure 7 presents the von Mises stress–strain curves of both PS₁ and PS₂ in comparison to the experimental measurement. The CRSS range and hardening slope of PS₁ and PS₂ are shown in Fig. 8. The parameters of set 2 reverse the relative ease of prism and basal slip, and thus provide an interesting computational experiment that assesses the significance of the CRSS ratios between the two most easily activated slip systems.

Figure 7: Experimental stress–strain curve (dashed) compared to simulation (solid) resulting from optimized values of variable constitutive parameters listed in Fig. 8. The initial population of constitutive parameter sets results in stress–strain responses within the shaded range. After Nelder–Mead (simplex) optimization, each population member produces a stress–strain response very similar to the exemplary cases PS₁ and PS₂. The observed effective hardening range results from the (nonlinear) superposition of hardening ranges per individual slip family illustrated in Fig. 8.

4. Results and Discussion

To evaluate the influence of the grain morphology, boundary conditions, and constitutive model on the kinematic and constitutive response of the CPFEE model, the quasi-3D and 3D microstructure (see Sections 3.1 and 3.2) were deformed under two alternative boundary conditions (soft and hard, see Section 3.5) and using two alternative sets of constitutive parameters (PS₁ and PS₂, see Section 3.7). Deformation to 4 % tensile strain was simulated for all eight cases (two grain morphologies under two different boundary conditions with two sets of constitutive parameters). The simulation results were analyzed in terms of lattice reorientation and stress response. The simulated lattice reorientation data was used to identify the best combination of the aforementioned three factors by comparing with the EBSD measurement. The simulated stress data were analyzed at both macro (volume-average) and micro scale.

Figure 8: Visualization of the initial (s_0 , ▲) and saturated (s_s , ▼) critical resolved shear stresses (CRSS; vertical range is between ▲ and ▼ as $s_0 \rightarrow s_s$) and hardening slope (h_0) for constitutive parameter sets PS₁ and PS₂. Both PS₁ and PS₂ are an outcome of the calibration process and have volume-averaged stress–strain behavior that fits well with most of the experimental reference as shown in Fig. 7.

4.1. Lattice reorientation

The crystal orientation of a given material point changes with plastic deformation from its initial orientation $\mathbf{O}_0 \in SO(3)$ to $\mathbf{O}$. The resulting change in orientation (reorientation) is $\Delta\mathbf{O} = \mathbf{O}\mathbf{O}_0^T$, which can be conveniently transformed into a Rodrigues vector or quaternion to extract the lattice reorientation angle θ . Surface maps of the lattice reorientation angle at 4 % simulated tensile strain are shown in Fig. 9 for the two different grain morphologies using both constitutive parameter sets and the hard and soft boundary conditions. To facilitate comparison of the kinematic responses of the eight different simulation conditions with experiment, the EBSD-based measurement at 4 % tensile strain is also included at the bottom of Fig. 9.

The eight simulated lattice reorientation maps (upper two rows in Fig. 9) show magnitudes of rotation similar to those in the EBSD-based map (*i.e.*, comparing maximum and minimum brightness levels).⁵ However, there are significant differences in the details of the in-grain rotation between the eight simulations and the EBSD lattice reorientation map. A distinct feature observable in all four quasi-3D simulations is a band of larger reorientation that runs across multiple grains from about the lower left to the upper right corner. This feature is not present in the EBSD measurement. The EBSD map shows a distinct band of larger reorientation running almost vertically across the central grain. This feature also appears in the simulations when using the 3D microstructure (left two columns in upper two rows of Fig. 9), but is completely missing in the quasi-3D microstructure simulations (right two columns in upper two rows of Fig. 9). This relationship between the lattice reorientation band and the grain morphology indicates that the simulated crystal reorientation is notably affected by the morphology of the grains. A similar outcome was obtained in a strictly computational model where the shapes of grains but not the neighbor orientations was changed (Wong et al., 2013). The fact that the reorientation band is present with two different boundary conditions and two different parameter sets suggests that using microstructures with realistic grain morphology may be as important as having a good constitutive model.

Furthermore, a closer inspection of the first two columns of Fig. 9 reveals that the simulation with the hard boundary condition and constitutive parameter set PS₁ produces the closest match to the EBSD map. The fact that simulation with the hard boundary condition produced better prediction of the lattice reorientation is expected since the selected volume is in the middle of the sample where only its surface (top face) is truly free. In other words, the more constrained boundary condition used in this study is more realistic than a simple uniaxial tension boundary condition. Similarly, the relationship between the choice of the constitutive parameters and the quality of the simulated lattice reorientation can be explained by the fact that PS₁ is selected based on additional statistical analysis of the same sample, such that the CRSS values for each slip system are closer to reality than with PS₂.

⁵The maximum measurement error is less than 2°, based upon prior experience in obtaining the same orientation in the same location on the same specimen mounted in the same microscope stage by the same person a few days apart.

Figure 9: Simulated lattice reorientation maps for patches with different boundary condition, grain morphology, and constitutive parameters compared to the experimental reference.

It is clear from this qualitative analysis that grain morphology, boundary conditions, and the constitutive parameters affect the kinematic response of the CPFE simulation. To quantify the influence of these factors on the kinematic response of the simulation, point-wise differences $\Delta\theta(\mathbf{x})$ of the lattice reorientation were calculated between corresponding members of groups of four shown in Fig. 9. For example, to quantify the correlation between the choice of boundary condition and the simulated lattice reorientation, each of the four maps in the first row is subtracted from the map below it such that boundary condition is the only variable. Then the frequency of absolute lattice reorientation $|\Delta\theta|$ is binned every 2° and normalized by the total number of data points. The resulting histograms for these four comparisons are shown in the leftmost diagram in Fig. 10, where the blue curves with different line styles represent the reorientation change due to switching the boundary conditions with other conditions fixed as labeled. Similarly, the middle two histograms in Fig. 10 present the effect of changing between the two grain morphologies and the two constitutive parameter sets (black and red curves, respectively).

It is seen from the four histograms of $\Delta\theta_{\text{hard-soft}}$, that the majority of the lattice reorientation changes are less than 4° . Nevertheless, high lattice reorientation changes (larger than 4°) do exist in various cases with different constitutive parameters and grain morphology. The general trend of the four curves of $\Delta\theta_{\text{boundary condition}}$ shows that changes in the boundary condition do not lead to large lattice reorientation changes in most area of the sample surface. A similar conclusion can also be drawn for the grain morphology (black) and constitutive parameters (red) curves. However, in the blue curves with “3D” labels and in the black curves with the “hard” boundary condition, there are significant fractions of the populations with higher $|\Delta\theta|$ values that extend to the right side of the histogram plots, indicating that there are larger differences in the lattice reorientation than in the quasi-3D simulations. This implies that the 3D microstructure is more sensitive to the boundary condition change than the quasi-3D microstructure. Also, the hard boundary condition is more sensitive to the effect of changing the morphology. In contrast, the change in the constitutive parameters has a mild effect on the simulated lattice reorientation, as all the curves are in the left half of the graph. Furthermore, there is no clear correlation between the different morpholo-

Figure 10: Histograms of point-by-point difference in lattice orientation at the surface when altering the boundary condition (column 1), microstructure (column 2), or constitutive model parameters (column 3). The averaged influence of each factor on simulated lattice reorientation is compared in the last histogram (column 4), which shows that a change in the boundary condition or grain morphology would more likely lead to large change in the simulated lattice reorientation than changing the constitutive parameters. The change of lattice reorientation $\Delta\theta$ shown here is in degrees.

gies or boundary conditions for the different constitutive parameters, suggesting that lattice reorientation is largely insensitive to the constitutive parameter values. This point can be emphasized by averaging the curves in each of the three difference plots, where the overall effect of each factor on the simulated lattice reorientation is compared in the rightmost plot in Fig. 10. Altering the boundary condition or grain morphology causes a similar and greater change in the lattice reorientation than the constitutive parameters.

4.2. Average stress response

The previous section discussed the effect of boundary condition, grain morphology, and constitutive parameters on the lattice reorientation, a kinematic response. In this section, the influence of these factors on the volume-averaged stress-strain response is examined.

Figure 11 presents the volume-averaged von Mises stress-strain curves for the columnar and three-dimensional grain morphologies simulated using both constitutive parameter sets and both boundary conditions. Recalling that the two constitutive parameter sets are calibrated against the same stress-strain curve by homogenizing 8000 orientations, it is expected that the differences between curves for the simulated aggregates of 20–30 grains should not be large. The lack of significant differences between curves for the same boundary condition indicates that the effect of grain morphology and constitutive parameters is limited. This lack of strong difference may, in part, be a result of the series of calibrations described in Section 3.7. However, a comparison of curves with the same constitutive parameters (same color) and grain morphology (same line style) in Figs. 11a and 11b reveals that the hard boundary condition systematically leads to a higher stress response compared to the soft boundary condition. This higher stress response reflects the additional constraints imposed by the hard boundary condition. Thus, the influence of the boundary condition on the simulated volume-averaged stress-strain responses is clearly stronger than grain morphology and constitutive model after calibrating the model.

4.3. Surface stress

The relative importance of proper grain morphology and constitutive parameters on the simulated mechanical response of polycrystalline aggregates on the stress-strain response discussed above is subtle. To evaluate the influence of the three factors on the local constitutive responses in the CPFE simulations, analysis similar to Section 4.1 was performed for the in-plane components of the surface stress tensor at a strain of 4%. To quantify the point-wise difference in stress between any two cases, termed *A* and *B*, an ‘average relative change’ for each stress component was calculated as:

$$\text{avg. rel. change}(\sigma_{ij}(\mathbf{x})) = \text{sgn}\left(\frac{\sigma_{ij}^A(\mathbf{x})}{\sigma_{ij}^B(\mathbf{x})}\right) \left\{ \left| \frac{\sigma_{ij}^A(\mathbf{x}) - \sigma_{ij}^B(\mathbf{x})}{2\sigma_{ij}^A(\mathbf{x})} \right| + \left| \frac{\sigma_{ij}^A(\mathbf{x}) - \sigma_{ij}^B(\mathbf{x})}{2\sigma_{ij}^B(\mathbf{x})} \right| \right\} \quad (8)$$

Figure 11: Von Mises stress–strain responses of patches for soft (a) and hard (b) boundary condition. Blue and red (or initially higher and lower) curves reflect constitutive parameter sets PS₁ and PS₂, respectively. Solid and dotted lines correspond to three-dimensional (3D) and columnar (quasi-3D) grain morphologies, respectively.

where $\mathbf{x}$ denotes the spatial location, and A, B correspond to two simulations for which one out of the three investigated factors (boundary condition, grain morphology, or constitutive parameters) has been changed with the other two fixed. The average relative change quantifies the significance of a stress difference between a reference σ_{ij}^A and the modified σ_{ij}^B after altering any one of the three aforementioned factors.

Figure 12 presents histograms of the average relative change using bins of width 0.5 (*i.e.* bin increments of 50 %) for both the normal stress components in the loading direction (σ_{22} , top) and transverse to the loading direction (σ_{11} , bottom).⁶ A change of boundary condition, grain morphology, or constitutive model causes about the same small relative variation in σ_{22} , as indicated by the narrow distribution in the top row of Fig. 12. In each case, there are four conditions plotted in the same way as shown in Fig. 10, but they are nearly indistinguishable. This is because $\Delta\sigma_{22}$ is relatively small compared to $\sigma_{22} \approx 0.5$ GPa, which pushes the distribution curves towards the center (zero implies no difference). Furthermore, changes in the sign of σ_{22} are improbable such that no data falls into the left half of any histogram in the top row of Fig. 12.

In contrast, the histograms of the transverse normal stress σ_{11} (Fig. 12 bottom) are much broader because the magnitude of σ_{11} is much smaller than σ_{22} . Hence, relative differences in σ_{11} are larger and differences in the sign occur, as indicated by negative values in the lower set of histograms, where there cannot be data in the open interval $(-2, 0)$.⁷ Also, unlike the distribution of the orientation changes in Fig. 10, where there was almost no discernible change for small variations, the stress differences for all combinations of fixed factors have different levels of probability over the full range. Consequently the differences in the the most highly probable subset of the distribution are examined next.

The spread among the three sets of four curves is identified using the gray bracket (Fig. 12 bottom) for the largest (and most relevant) fraction of small differences in stress. This spread is largest for a change in constitutive parameter set and smallest for a change in the grain morphology. The smaller this spread, the less influential the values chosen for the two fixed factors are, with respect to alteration of the remaining varied factor. As this spread is smallest when the grain morphology is varied, the boundary conditions and constitutive parameters have less of an effect on difference in the local stress state. Hence, as the other two plots show, the different outcomes in surface stress are mostly dominated by the differences in grain morphology, while the influence of boundary conditions and constitutive parameters are less significant and similar.

To further analyze how the stress state is affected by the initial shapes of the grains, the simulated surface stress tensor is visualized using vector field plots for the quasi-3D and 3D microstructure at three levels of strain. The plots

⁶The evaluation of σ_{12} is similar to σ_{11} , so only one is shown.

⁷There is no combination of values for which Eq. (8) yields values in this interval.

Figure 12: Histograms of the average relative change (see Eq. (8)) in surface normal stress along the loading axis (σ_{22} , top row) and transverse to it (σ_{11} , bottom row) when changing the boundary condition (Δ boundary condition, column 1), microstructure (Δ morphology, column 2), or constitutive model parameters (Δ constitutive parameters, column 3). Fractional distribution variation (in the bin of smallest relative changes) among the remaining two variables, *e.g.* boundary condition and constitutive parameter set for a switch of grain morphology (center column), are indicated by brackets for σ_{11} . Shaded interval $(-2, 0)$ corresponds to inaccessible values of average relative changes.

show the value and (projected) direction of principal surface stress averaged over areas of $8 \times 8 \mu\text{m}^2$. Due to the averaging process, some of the finer details of spatial variations in the stress tensor are washed out, especially near grain boundaries. The hard boundary condition and constitutive parameter set PS_1 were used for this analysis since the combination of these two factors resulted in better lattice reorientation prediction, as discussed in Section 4.1.

As shown in Fig. 13, the dominant stress state just after yield ($\bar{\epsilon} = 0.40\%$) is uniaxial tension along the horizontal y -axis, and there is no apparent difference arising from the different grain morphologies. With increasing deformation, subtle differences start to emerge in several locations. For example, at 1.0% tensile strain, the upper central region of the quasi-3D microstructure starts to show a weak compressive stress along the (vertical) x -axis, whereas the same region of the 3D microstructure remains in tension. With increasing strain, the local stress state in the 3D case increasingly differs from the quasi-3D case up to 4% tensile strain, where the magnitude of vertical compression is much greater in the left side of the central grain.

From this analysis of the surface principal stress evolution, it is clear that the effects of grain morphology gradually intensify with increasing strain level, especially in the central grain where the DAXM characterization was more complete. Thus, the correct grain morphology becomes increasingly important with increasing strain.

5. Summary

Starting with a microstructure patch comprising 18 grains on the surface of a Ti-5Al-2.5Sn tensile test sample, two approximations of the true subsurface grain structure were made; a close-to-realistic 3D microstructure based

Figure 13: Principal stress vector field plot comparing the simulated surface stress tensor evolution with strain between realistic and columnar grain structure for constitutive parameter set PS₁ and hard boundary condition.

on information from non-destructive differential aperture X-ray microscopy (DAXM) that resulted in a total of 29 grains, and a simpler quasi-3D microstructure developed by extending the surface grain information into a columnar structure of 18 grains. To assess the influence of the geometric accuracy of the grain microstructure relative to the choice of boundary conditions and constitutive parameters, crystal plasticity finite element (CPFE) deformation simulations of the 3D and quasi-3D microstructures were carried out under two different boundary conditions and two different sets of phenomenological crystal plasticity constitutive parameters. The simulations revealed that in order to accurately simulate heterogeneous deformation processes at the grain scale, a geometrically realistic grain morphology, as well as a physically more meaningful boundary condition, are more important than fine-tuning the constitutive model parameters. With an accurate 3D structure and boundary conditions, it is possible to estimate the local stress tensor in the polycrystalline aggregate with some degree of confidence, which can be used to assist interpretation of experimental results and identify opportunities to improve modeling of heterogeneous deformation.

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