Stress and deformation heterogeneity in individual grains within polycrystals subjected to fully reversed cyclic loading

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Abstract

The influence of spatial variability of the crystal stresses on the evolution of intragrain lattice misorientations during cyclic loading of a polycrystalline copper alloy is examined using a combination of simulation and experiment. The experiments consist of measuring the mechanical responses of deforming individual crystals using high-energy x-ray diffraction and *in situ* mechanical loading. The simulations are based on a crystal-based finite element formulation which is used to compute stress distributions and lattice reorientations in virtual polycrystals subjected to the same loading history. The hybrid methodology produces a picture of the evolving microstructural state during cyclic plasticity. For four target grains, comparisons are made between the diffracted peak intensity distributions as recorded by the experimental detector and those computed from simulation using a virtual diffractometer. Based on the comparisons, a relationship is presented between intragrain lattice misorientations and broadening of the diffraction peaks from individual grains. Stress triaxiality within grains is examined and regions with positive triaxiality throughout the tension/compression loading history are identified as potential locations for void growth.

1 Introduction

In polycrystalline metals, the stress distribution at the crystal level is influenced by a complex interplay of factors such as the orientations of the crystal lattices, the elastic and plastic mechanical properties, the interactions between neighboring crystals, and the type of loading conditions.

Due to the anisotropic nature of the mechanical behavior at the crystal level, spatial heterogeneity of the stress and deformation often is observed within polycrystalline materials, even under macroscopically homogenous loading conditions such as uniaxial tension [1]. Experimental observations have shown that under a broad range of deformation modes, and for a variety of metal alloys, spatial variations can arise within grains and lead to grain subdivision, as characterized by regions within a grain with different lattice orientations [2–7]. Such subdivisions are a consequence of the deformation heterogeneity present within grains, as confirmed through detailed comparisons between the experimental data and finite element simulations of polycrystals [8–10].

While the specific mechanisms can differ, it is generally well accepted that microcracks can initiate within a crystal, or at the boundary between crystals, due to non-reversible slip processes associated with cyclic plasticity [11–13]. Locations which accumulate more damage or are more highly stressed can serve as defect or crack initiation sites. Although it is recognized that stress states in polycrystals are heterogeneous and that slip processes can spawn defect initiation sites, our understanding is largely qualitative and is insufficient to accurately predict where a life-ending defect will form in a polycrystalline sample during cyclic loading. This shortcoming has been due, in part, to our inability to quantify and verify crystal stress distributions together with the changes in microstructure that they induce. However, advances in both experimental and simulation capabilities have greatly improved our ability to examine grains within the interior of polycrystals while they are under external load. Here we apply a coordinated combination of high-energy x-ray diffraction and finite element simulations to study the behavior of individual grains within a polycrystalline sample subjected to fully reversed cyclic loading.

High-energy x-ray diffraction techniques enable non-destructive characterization of the microstructural and micromechanical response of grains within the bulk of a deforming polycrystal [14, 15]. Various diffraction techniques have been developed to determine the spatial position, morphology, lattice orientation and lattice strains for individual grains within a polycrystal [15–17]. In particular, current x-ray diffraction techniques that employ monochromatic beams and *in situ* specimen loading provide the ability to measure average elastic strains within grains during deformation. However, these methods currently do not provide spatially-resolved stress distributions within those grains.

Crystal-based finite element simulations, in conjunction with forward modeling of diffraction peaks, offer the capability to estimate the stress

distributions within grains, and thus help to complete the mechanical description from the diffraction experiments in a physically consistent manner. Polycrystal plasticity provides a theory that links constitutive response to key microstructural features which can be embedded within a finite element model. Finite element methods provide solutions that simultaneously satisfy compatibility and equilibrium within an aggregate of grains under applied loads. Using a finite element formulation, grains within a deforming aggregate can be resolved with sufficient definition to capture the spatial distributions of stress and deformation across the grains, and thus facilitate the investigation of heterogeneities that arise from grain interactions. In the context of finite element simulations, forward modeling consists of simulating the passage of an x-ray beam through a virtual specimen, computing the diffraction condition based on the microstructure within the specimen volume, and then projecting the diffracted beam onto a surface that coincides with the detector in an experiment (thus defining a diffraction peak). The spatial position of the grain, its shape, misorientations of its crystallographic lattice, and the elastic strain state all can be captured in the intensity distributions of the diffraction peaks via this procedure, performed with software called a virtual diffractometer. The virtual diffractometer framework developed previously [18] is used here to simulate the diffraction peaks from individual grains embedded within fully three-dimensional virtual polycrystals.

The focus of this paper is to quantify the influence of the spatial distribution of the crystal stresses on the evolution of intragrain lattice misorientations during cyclic loading of an Okegawa Mold Copper (OMC) sample subjected to fully reversed cyclic loading. Diffraction peak intensities obtained by a high-energy x-ray diffraction (HEXD) experiment are presented for four target grains along with the cyclic response of an analogous virtual polycrystal simulated using the crystal-based finite element formulation. Comparisons are made between the measured and computed peak profiles, the latter having been generated using the virtual diffractometer. Having critiqued the similarities and differences in the measured and computed peak broadening, we proceed to examine the stress and deformation heterogeneity of four target grains within the sample in terms of their relationship to broadening of the simulated diffraction peaks. We provide only a brief summary of the experiments and data, and refer the reader to a related paper that addresses the experimental aspects of the investigation [19].

2 Experimental Methodology

A uniaxial, cyclic loading history was applied in strain control to an OMC mechanical loading specimen for a total of six complete cycles. Three fully-reversed cycles were conducted with a strain amplitude of 0.3%, followed by another three fully-reversed cycles with a strain amplitude of 0.5%. The material response measured over the course of the test is shown in Figure 1(a) in the form of an axial stress versus axial strain record along with the simulated record for the same load history (discussed later). At several points in the loading history (indicated by symbols in the figure), diffraction measurements were performed to acquire data for selected target grains. The orientations of these grains with respect to the loading direction of the sample are shown in Figure 1(b) within the basic fundamental triangle of an inverse pole figure. The Taylor factor distribution for axisymmetric extension is also shown in the figure. The Taylor factor is formally defined in Section 4.2, but in brief, it is a measure of the magnitude of the stress required to plastically deform a crystal as a function of its orientation. The orientations of these grains provide for a broad range of strengths under the nominal stress state applied in the experiment, which is reflected in their mechanical responses to the cyclic loading. Further, the diffraction measurements also indicate that microstructural changes induced by the loading cycles with larger strain amplitude of 0.5% are much more pronounced than those observed over the course of the smaller strain amplitude (0.3%) loading cycles. The experimental setup to perform the diffraction measurements is discussed in more detail in Section 2.1. A description of how diffracted intensities from crystals are produced and an example of the type of diffraction data obtained from the experiment are presented in Section 2.2.

2.1 HEXD experimental technique

The HEXD experiment depicted in Figure 2(a) consists of a rotating crystal method conducted in transmission, employing high energy synchrotron x-rays ($E \geq 50$ keV) and high speed area detectors to measure diffracted intensities from individual grains within polycrystalline bulk materials. The OMC sample was mounted on an ω -rotation stage, where ω is the rotation about the sample axis, $\mathbf{Y}_s$, and is perpendicular to the incoming beam. Using the experimental configuration illustrated, the detector was positioned at a distance from the sample such that a number of average quantities were determined for individual grains, including the positions of their centers of mass, lattice orientations, and lattice strain tensors [15, 17]. In our experi-

ment, a monochromatic x-ray beam with energy, $E = 80.725$ keV, an energy bandwidth of $\Delta E/E < 5 \times 10^{-3}$ keV, and a beam size of $400\mu\text{m} \times 400\mu\text{m}$ was employed. The sample to detector distance, D , was 1.122 m. Experiments were conducted at beamline 1-ID-C at the Advanced Photon Source (APS).

Diffraction measurements were taken on four target grains within the sample at various points in the loading history, as denoted in Figure 1(a). At these points in the loading history, the center of mass of each target grain was positioned on the rotation axis of the sample and diffraction images were collected while the sample was rotated continuously in ω . This translation effectively defines an individual sample coordinate system ($\mathbf{X}_s, \mathbf{Y}_s, \mathbf{Z}_s$) for each grain. Detector images were acquired as the sample was rotated through a total of 300° in ω . The rotation was discretized into 0.25° ω -intervals, so that each detector image acquired corresponds to the integrated intensities through a 0.25° ω -rotation.

2.2 Observed diffraction peaks

A perfect crystal is composed of regularly spaced atoms which act as scattering sites for x-rays. When an incident x-ray beam strikes a crystal, scattering of the x-rays by the atoms occurs. Due to the periodic arrangement of these atoms, x-rays scattered in certain directions will be in-phase and constructive interference of the x-rays will occur in these directions. A diffracted beam is composed of a large number of scattered x-rays undergoing constructive interference in a particular direction. The directions of these diffracted beams are governed by Bragg's law:

$$\lambda = 2d \sin \theta \quad (1)$$

where λ is the wavelength of the incident x-ray beam, d is the lattice plane spacing for a particular diffracting plane of atoms, and 2θ is the angle between the incident beam and the diffracting plane.

In a diffraction experiment using a monochromatic x-ray beam, when a diffracted beam strikes a detector, a diffraction peak is observed at a well-defined position with its own intensity distribution and shape. Each diffraction peak on the detector is uniquely identified by the set of angles, $(2\theta, \eta, \omega)$, and has a corresponding position, intensity distribution and shape. If a grain were to have a sufficiently perfect lattice arrangement, the diffraction peaks have a very narrow spread in intensity. However, when a grain undergoes deformation, changes occur in its lattice arrangement, which are manifest as changes to the positions and intensity distributions of its diffraction peaks.

Peak #	$(h\ k\ l)$	$2\theta^\circ$	η°	ω°
1	(-1 -1 1)	4.22	-146.97	39.08
2	(-1 -1 1)	4.22	-33.03	-145.95
3	(1 1 -1)	4.22	33.03	34.05
4	(1 1 -1)	4.22	146.97	-140.92
5	(0 -2 2)	6.89	-161.40	4.18
6	(0 2 2)	6.89	-125.80	-111.17
7	(-2 0 2)	6.89	-66.11	-130.63
8	(0 2 2)	6.89	-54.20	57.08
9	(0 -2 2)	6.89	-18.60	176.92
10	(0 2 -2)	6.89	18.60	-3.08
11	(0 -2 -2)	6.89	54.20	-122.92
12	(2 0 -2)	6.89	66.11	49.37
13	(0 -2 -2)	6.89	125.80	68.83
14	(0 2 -2)	6.89	161.40	-175.82
15	(-1 3 -1)	8.08	-167.12	-177.40
16	(-3 1 1)	8.08	-127.51	122.93
17	(-3 1 1)	8.08	-52.49	-70.31
18	(-3 -1 1)	8.08	-35.68	-112.65
19	(3 1 -1)	8.08	35.68	67.35
20	(3 -1 -1)	8.08	52.49	109.69
21	(1 -1 -3)	8.08	102.23	142.32
22	(-1 1 -3)	8.08	152.02	152.28
23	(-1 -3 -1)	8.08	155.98	55.08
24	(1 -3 1)	8.08	167.12	2.60
25	(-2 -2 2)	8.44	-146.90	41.59
26	(-2 -2 2)	8.44	-33.10	-148.47
27	(2 2 -2)	8.44	33.10	31.53
28	(2 2 -2)	8.44	146.90	-138.41

Table 1: Diffraction peaks monitored within Grain 4 during the HEXD experiments listing the lattice plane family ($\{hkl\}$) and the pre-deformation values of the centroid $(2\theta, \eta, \omega)$ for each peak. Figure 2(b) depicts these $(2\theta, \eta)$ values schematically on a detector. The Peak # corresponds to the FWHM data columns numbered left to right for Grain 4 as depicted in Figures 6 – 9. Similar mappings are used for the other target grains.

An example of a diffraction image captured on the detector at a particular sample rotation angle, ω , is shown in Figure 3, along with a close-up

view of a single diffraction peak from the detector image. The diffraction peaks shift during elastic deformation, then start to broaden when plasticity begins, leading to a larger, more diffuse intensity distribution. The diffraction peaks can also shift and broaden in the ω -dimension, where a diffraction event from a single set of planes can produce diffracted intensity on multiple detector frames. In general, shifts and broadening in the radial (2θ) direction are associated with lattice strains, while changes in the distributions in the η and ω directions are related to lattice orientation evolution.

3 Simulation Methodology

The intent of the finite element simulations of virtual polycrystals is to complement the experiments by aiding in the interpretation of the observed trends. This is done in two stages: first, we make quantitative comparisons of measured and computed diffraction patterns, and second, we explore the full-field information available only through simulation. Simulations were performed on a virtual polycrystal which mimicked the loading of the cyclic test. Using the simulation results, synthetic diffraction images were generated that are comparable to those measured by the HEXD technique.

In this section we describe the simulation framework and the methodology for constructing the virtual diffraction images. An overview of the finite element framework is given first in Section 3.1 together with details regarding the instantiation of a virtual specimen. The virtual specimens are constructed to be representative of the diffraction volume of the physical specimen. In Section 3.2, the constitutive equations are laid out in detail together with those assumptions that are most relevant to the interpretation of the results. Section 3.3 describes the framework of the virtual diffractometer, which is a procedure for generating synthetic diffraction peaks from simulation data.

3.1 Finite element framework

The finite element formulation is capable of modeling quasi-static, inelastic deformations of polycrystalline solids. It is a velocity-based formulation that enforces the weak form of the balance of linear momentum for smooth motions. Following standard finite element procedures, the domain is divided first into grains and then the grains are discretized with elements. In this context, the domain, $\mathcal{B}$, refers to the union of all grains that collectively define a virtual polycrystal (the intersection of grains is required to be null).

The grains may be irregular in shape and size, and exhibit well-defined interfaces that are smooth surfaces that remain coherent throughout the motion. The formulation used here employs a standard isoparametric mapping for discretizing the polycrystal domain into elements and for representing the solution variables over those elements [20]. The mapping of the coordinates of points are provided by the elemental interpolation functions, $\left[\mathbf{N}(\xi, \eta, \zeta) \right]$, and the coordinates of the nodal points, $\{x^{\text{np}}\}$:

$$\{x\} = \left[\mathbf{N}(\xi, \eta, \zeta) \right] \{x^{\text{np}}\} \quad (2)$$

where (ξ, η, ζ) are local coordinates within an element. The same mapping functions are used for the solution (trial) functions which, together with the nodal point values of the velocity, $\{v^{\text{np}}\}$, specify the velocity field over the elemental domains:

$$\{v\} = \left[\mathbf{N}(\xi, \eta, \zeta) \right] \{v^{\text{np}}\} \quad (3)$$

The motion derived from this isoparametric representation accommodates large strains and arbitrary rotations in a fully three-dimensional framework.

In the simulations presented later, two virtual specimens (designated as Specimen 1 and Specimen 2, henceforth) were instantiated as Voronoi tessellations using **Neper** [21]. To be representative of the diffraction volume that was illuminated in the HEXD experiment, the cube-shaped specimens were 0.5 mm on each side. The specific shapes of the target grains and the exact details of their neighborhoods are not known from the experiment, and thus no attempt was made to replicate these attributes of the physical specimen. Emerging high-energy x-ray diffraction methods provide the non-destructive capability to more precisely quantify grain boundaries within a polycrystalline sample [22, 23] prior to applying mechanical loads. Such approaches eventually will facilitate closer comparisons between experiments and simulations for actual specimens tested, but were not yet available for the simulations presented here. In the presence of this uncertainty in the shape and neighborhood of the target grains, two instantiations were considered to gauge the sensitivity of the results to polycrystal representation, at least in a limited way.

To instantiate the virtual specimens, the spatial locations of 100 grain nucleation points used by **Neper** to form the Voronoi tessellation were randomly positioned within the specimen volume. Each specimen had a distinct set of nucleation points, thereby giving the two samples completely different arrangements of the 100 grains. The grains each were discretized with several thousand 10-node tetrahedra (isoparmetric) elements, resulting in

meshes with approximately 500,000 elements over the full specimen volume. Four grains within the interior of each virtual specimen were selected and were assigned the orientations of the four target grains measured in the experiment. (See Figure 1(b) for the orientations of these grains with respect to the loading direction of the sample.) The remaining grain orientations were randomly assigned from the orientation distribution function (ODF) of the material, which had been measured experimentally. Table 2 gives the volume fraction of the four target grains, the numbers of elements used to discretize them, and the relative volume of the individual elements. The grains were discretized with thousands of elements to facilitate quantifying the development of the intragrain lattice misorientations with deformation. Note that the target grains of Specimen 1 have somewhat larger volumes than average while the target grains in Specimen 2 all have volumes that are closer to the average. The level of discretization, however, is relatively uniform (there are more elements in larger grains). The grain size differences did not appear to alter the overall trends in the predicted peak broadening, as will be shown later.

Specimen	Target Grain	Volume Fraction	Elements	Volume Fraction/Element
1	1	0.0139	6527	2.13×10^{-6}
1	2	0.0139	7648	1.77×10^{-6}
1	3	0.0136	8135	1.67×10^{-6}
1	4	0.0213	10580	2.01×10^{-6}
2	1	0.0095	5459	1.74×10^{-6}
2	2	0.0102	5535	1.84×10^{-6}
2	3	0.0109	5475	1.99×10^{-6}
2	4	0.0111	5335	2.08×10^{-6}

Table 2: Relative size and level of discretization of target grains in the virtual specimens

With the domain defined and a kinematically-admissible motion represented over the domain, a solution is sought that best satisfies the balance laws from among those admitted by the discretization. This is accomplished by requiring a weighted residual on the balance of linear momentum over the domain vanish:

$$R_u = \int_{\mathcal{B}} \psi \cdot (\text{div} \boldsymbol{\sigma}^T + \boldsymbol{\iota}) \, d\mathcal{B} = 0 \quad (4)$$

where R_u is the residual, $\boldsymbol{\sigma}$ is the Cauchy stress, $\boldsymbol{\iota}$ is the body force, and ψ are the weights. The residual is manipulated in the customary manner

(integration by parts and application of the divergence theorem) to obtain the weak form:

$$R_u = - \int_{\mathcal{B}} \text{tr} \left(\boldsymbol{\sigma}'^T \text{grad} \boldsymbol{\psi} \right) d\mathcal{B} + \int_{\mathcal{B}} \pi \text{div} \boldsymbol{\psi} d\mathcal{B} + \int_{\partial \mathcal{B}} \boldsymbol{t} \cdot \boldsymbol{\psi} d\Gamma + \int_{\mathcal{B}} \boldsymbol{\iota} \cdot \boldsymbol{\psi} d\mathcal{B} \quad (5)$$

which, among other things, exposes the surface tractions, $\boldsymbol{t}$. In preparation for introducing the constitutive equations, the Cauchy stress has been split into its deviatoric and spherical components: $\boldsymbol{\sigma}'$ and π , respectively. The simulation involves computing the motion of the polycrystal over the duration of the loading history, which is accomplished by dividing the history into discrete time steps and solving Eq. (5) at each step for the velocity field. With the velocity known, the geometry and state are updated. For numerical stability, implicit methods are employed in constructing the time discretization. Further, once the constitutive equations are introduced, the resulting set of equations are highly nonlinear. An adaptive strategy has been implemented that combines Newton-Raphson and Picard iterations to reach a converged solution. Additional description of the finite element formulation can be found in [24–26].

3.2 Crystal-scale constitutive equations

The material behavior is quantified with a set of constitutive equations, here written at the level of the single crystal. The behavior includes both elastic (recoverable strains upon removal of the stress) and plastic (non-recoverable strains upon removal of the stress) responses. The particular constitutive equations are chosen to represent the behavior of OMC copper. In the regime of plastic strain rate and temperature of the experiments, crystallographic slip is the dominant mechanism of inelastic deformation. Consequently, neither twinning nor deformation associated with diffusional mechanisms is included. Similarly, no criteria for fracture are considered. Based on the strain rates observed in the experiment, heat generated by deformation is conducted away in times short in comparison to the experiment and the specimen temperature is assumed to remain at its initial, uniform value. Evolution of relevant state descriptors, namely the slip system strengths and the crystal lattice orientations, are included. The set of equations are summarized in the following subsections, starting with the kinematic decomposition. The equations for the elastic and plastic responses follow discussion of the kinematic decomposition and are broken into two parts: fixed state relations and evolution relations.

3.2.1 Elastoplastic kinematic decomposition

The motion of the virtual polycrystal is a smooth mapping of all points within the domain, $\mathcal{B}$, as defined by the trial functions given in (3). Over the deformation history, the current coordinates, $\mathbf{x}$, advance under the motion, and may be written as a mapping, χ , from the reference coordinates, $\mathbf{X}$:

$$\mathbf{x} = \chi(\mathbf{X}) \quad (6)$$

The deformation gradient is defined locally in terms of the mapping as:

$$\mathbf{f} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \quad (7)$$

The deformation gradient includes both elastic and plastic parts, which must be separated via a kinematic decomposition to introduce equations for each. The decomposition is not strictly derivable from the mapping, but rather involve assumptions regarding the crystal mechanical behavior. Consequently, it is part of constitutive model. The decomposition employed for volumes within single crystals consists of a sequence of three parts: a plastic part, a rotation and an elastic part, given as:

$$\mathbf{f} = \mathbf{f}^e \mathbf{f}^* \mathbf{f}^p = \mathbf{v}^e \mathbf{r}^* \mathbf{f}^p \quad (8)$$

These are shown schematically in Figure 4. Each part of the decomposition brings the material point to a new configuration, starting with reference coordinates, $\mathbf{X}$, and finishing at the current coordinates, $\mathbf{x}$. The elastic part is a pure stretch which, by assuming small elastic strains, can be approximated with:

$$\mathbf{v}^e = \mathbf{I} + \mathbf{e}^e \quad (9)$$

where

$$\|\mathbf{e}^e\| \ll 1 \quad (10)$$

The plastic part involves both stretch and rotation as a consequence of being a linear combination of slip modes, each of which is simple shear. The distinct rotation in $\mathbf{f}^*$ (or equivalently, $\mathbf{r}^*$) is the rotation beyond that included in $\mathbf{f}^p$ that is needed for consistency with the overall mapping given by Equation 6.

To cast the kinematic decomposition in rate form, the velocity gradient first is written in terms of the deformation gradient and its time-rate-of-change:

$$\mathbf{l} = \dot{\mathbf{f}} \mathbf{f}^{-1} \quad (11)$$

where the velocity gradient is subsequently decomposed into the deformation rate and spin. The deviatoric deformation rate is obtained by subtracting the volumetric part from the total:

$$\mathbf{d}' = \mathbf{d} - \frac{1}{3} \text{tr } \mathbf{d} \mathbf{I} \quad (12)$$

Substituting Equation 8 into Equation 11 and separating the deformation rate into its volumetric and deviatoric parts with Equation 12 gives:

$$\text{tr}(\mathbf{d}) = \text{tr}(\dot{\mathbf{e}}^e) \quad (13)$$

and

$$\mathbf{d}' = \dot{\mathbf{e}}^{e'} + \hat{\mathbf{d}}^{p'} + \mathbf{e}^{e'} \hat{\mathbf{w}}^p - \hat{\mathbf{w}}^p \mathbf{e}^{e'} \quad (14)$$

in which the small elastic strain approximation from Equation 9 has been invoked. The spin becomes:

$$\mathbf{w} = \hat{\mathbf{w}}^p + \mathbf{e}^{e'} \hat{\mathbf{d}}^{p'} - \hat{\mathbf{d}}^{p'} \mathbf{e}^{e'} \quad (15)$$

where, again, small elastic strains are assumed. In Equations 14 and 15, the hat over $\mathbf{w}^p$ and $\mathbf{d}^{p'}$ indicates mapping to configuration $\hat{\mathcal{B}}$ using $\mathbf{r}^*$, as indicated in Figure 4:

$$\hat{\mathbf{d}}^{p'} = \mathbf{r}^* \mathbf{d}^{p'} \mathbf{r}^{*\text{T}} \quad (16)$$

$$\hat{\mathbf{w}}^p = \mathbf{r}^* \mathbf{w}^p \mathbf{r}^{*\text{T}} \quad (17)$$

It is important to note that these equations are capable of accommodating the kinematic nonlinearities associated with both large strains and arbitrary rotations, provided that the elastic strains remain small. Given that the elastic stiffness is orders of magnitude larger than the strength for the copper alloy considered here, that assumption remains valid throughout.

3.2.2 Fixed state constitutive relations

The stress is now related to the kinematic quantities appropriate for the elastic and plastic responses through fixed-state relations. Both the elastic and plastic responses are intimately connected to the crystallographic lattice, which is parameterized within each element of every grain using a Rodrigues vector, $\mathbf{r}$, [27, 28]:

$$\mathbf{r} = \mathbf{n} \tan \frac{\phi}{2} \quad (18)$$

Here, $\mathbf{n}$ is the axis of the rotation that maps base vectors attached to the sample frame to base vectors attached to the crystallographic axes and ϕ is the rotation angle about $\mathbf{n}$.

For the elastic deformations, the fixed-state relation is simply Hooke's law, written using the $\hat{\mathcal{B}}$ configuration as a reference volume:

$$\boldsymbol{\tau} = \mathcal{C}(\mathbf{r})\mathbf{e}^e \quad (19)$$

where the Kirchhoff stress, $\boldsymbol{\tau}$, is written in the $\hat{\mathcal{B}}$ configuration as:

$$\boldsymbol{\tau} = \beta \boldsymbol{\sigma} \quad \text{where} \quad \beta = \det(\mathbf{v}^e) \quad (20)$$

Here, the anisotropic behavior stemming from the crystal symmetry is indicated by the orientation dependence of the elastic stiffness.

The plastic response is nonlinear and rate-dependent (viscoplastic). It is assumed to be isochoric and independent of the mean stress. The fixed-state relation is a combination of several equations that describe crystallographic slip on a limited number of slip systems (commonly called restricted slip), with each slip system, α , being defined by a slip plane, $\mathbf{m}^\alpha$, and slip direction, $\mathbf{s}^\alpha$. For the OMC fcc structure, we use the twelve slip systems defined by the $\{111\}$ slip planes and the $\langle 111 \rangle$ slip directions. First are equations for the kinematic decomposition written in terms of slip using the Schmid tensor's symmetric and skew parts:

$$\hat{\mathbf{l}}^p = \hat{\mathbf{d}}^{p'} + \hat{\mathbf{w}}^p \quad (21)$$

where

$$\hat{\mathbf{d}}^{p'} = \sum_{\alpha} \dot{\gamma}^{\alpha} \hat{\mathbf{p}}^{\alpha} \quad \text{and} \quad \hat{\mathbf{w}}^p = \dot{\mathbf{r}}^{\star} \mathbf{r}^{\star\text{T}} + \sum_{\alpha} \dot{\gamma}^{\alpha} \hat{\mathbf{q}}^{\alpha} \quad (22)$$

and

$$\hat{\mathbf{p}}^{\alpha} = \hat{\mathbf{p}}^{\alpha}(\mathbf{r}) = \text{sym}(\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha}) \quad (23)$$

$$\hat{\mathbf{q}}^{\alpha} = \hat{\mathbf{q}}^{\alpha}(\mathbf{r}) = \text{skw}(\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha}) \quad (24)$$

Next is an equation that defines the kinetics of slip, which introduces the rate dependence of plastic flow using a power law expression between the resolved shear stress and the slip system shearing rate:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{|\tau^{\alpha}|}{g^{\alpha}} \right)^{\frac{1}{m}} \text{sgn}(\tau^{\alpha}) \quad (25)$$

The resolved shear stress is scaled by the slip system strengths, g^{α} , which in general may be different for each slip system, but here are the same for all slip systems within a given element. The 'sgn' term forces the shearing to be in the same direction as the shear stress. Finally, the resolved shear

stress is the projection of the crystal stress tensor onto the slip plane and into the slip direction, which is readily computed with the symmetric part of the Schmid tensor:

$$\tau^\alpha = \text{tr}(\hat{p}^\alpha \boldsymbol{\tau}') \quad (26)$$

The equations for slip are combined in a single, nonlinear relation as:

$$\hat{d}^{p'} = \mathcal{M}(\boldsymbol{r}, \dot{\gamma}^\alpha) \boldsymbol{\tau}' \quad (27)$$

After introducing a difference expression for the elastic strain rate, Equations 13, 14, 19 and 27 are combined into equations (one hydrostatic and the other deviatoric) that relate the Cauchy stress to the total deformation rate. These subsequently are substituted into the weak form, Equation 5 [24, 25].

The fixed-state model parameters for the elastic and plastic responses must be specified for the OMC copper being modeled in the simulations. The single crystal elastic moduli for pure copper [29] were taken for the OMC copper alloy, assuming that the minor alloying additions did not appreciably alter the elastic behavior. The fixed-state kinetics parameters for slip are ones used previously for modeling copper as well [18]. The important attribute to preserve is the low value of the rate sensitivity, which was held at $m = 0.01$. The values are shown in Table 3.

C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	m	$\dot{\gamma}_0$ (s ⁻¹)
168.4	121.4	75.2	0.01	1.0

Table 3: Fixed-state, single crystal, material parameters for OMC copper used in the simulations. See Equations 19 and 25 for use in the constitutive equations.

3.2.3 State evolution equations

There are two state variables that are updated as a deformation progresses, the lattice orientation and the slip system strength (also called hardness). The rate of lattice re-orientation follows directly from the Equations 21 and 22, assuming that the slip system shearing rates are known. Written in terms of the Rodrigues vector:

$$\dot{\boldsymbol{r}} = \frac{1}{2} \boldsymbol{\omega} + (\boldsymbol{\omega} \cdot \boldsymbol{r}) \boldsymbol{r} + \boldsymbol{\omega} \times \boldsymbol{r} \quad (28)$$

where

$$\boldsymbol{\omega} = \text{vect} \left(\hat{w}^p - \sum_{\alpha} \dot{\gamma}^\alpha \hat{q}^\alpha \right) \quad (29)$$

Evolution of the slip system strengths is governed by an additional, empirical relationship which follows a modified Voce form, but takes into account differences between monotonic and cyclic loading [30]. The slip system strengths for each crystal, g , evolve according to an isotropic hardening law:

$$\dot{g} = h_0 \left(\frac{g_s(\dot{\gamma}) - g}{g_s(\dot{\gamma}) - g_0} \right) f, \quad g_s(\dot{\gamma}) = g_{s0} \left(\frac{\dot{\gamma}}{\dot{\gamma}_{s0}} \right)^{m'} \quad (30)$$

where $\dot{\gamma} = \sum_{\alpha} |\dot{\gamma}^{\alpha}|$ is the sum of the slip system shearing rates and h_0 , g_0 , g_{s0} , m' are slip system hardening parameters. For cyclic loading, the model tracks the accumulated slip system shear strains on individual slip systems and the net crystal shearing rates within each crystal during a cycle. The quantity f in Eq. (30) is dependent on the number of active slip systems, n_a , contributing to hardening within a crystal:

$$f = \sum_{\beta=0}^{n_a} |\dot{\gamma}^{\beta}| \quad (31)$$

The α -slip system is considered to be contributing to hardening if the accumulated shear strain on the slip system since the last change in shearing direction, $\Delta\gamma^{\alpha}$, exceeds a critical value, $\Delta\gamma_{\text{crit}}$:

$$\Delta\gamma^{\alpha} = \int_{t_{+/-}}^t |\dot{\gamma}^{\alpha}| dt, \quad \Delta\gamma_{\text{crit}} = a \left(\frac{g}{g_s} \right)^b \quad (32)$$

where a , b are cyclic hardening model parameters and $t_{+/-}$ is the time since the last change in straining direction. The critical accumulated shear strain on a slip system, $\Delta\gamma_{\text{crit}}$, is implemented in the cyclic hardening model to introduce a hiatus in hardening following the reversals in the straining direction during cyclic loading. Using this modification it is possible to capture the pseudosaturation behavior exhibited by the macroscopic stress-strain response with only a minimal modification to the evolution equations of the slip system strengths used for monotonic loading.

The slip system and cyclic hardening parameters used in our simulations are shown in Table 4. These values are sensitive to the alloy being modeled and were chosen to provide a good match between the measured and computed cyclic stress-strain curves shown in Figure 1(a). In comparison to annealed pure copper, OMC copper has higher initial strength, but tends to strain harden much less. The parameters associated with adjusting the monotonic hardening rate to account for pseudosaturation during cyclic loading are similar to those used in [30], but have been adjusted slightly for the OMC copper.

h_0 (MPa)	g_0 (MPa)	g_{s0} (MPa)	m'	$\dot{\gamma}_{s0}$ (s^{-1})	a	b
800	85	285	0.0	5×10^{10}	0.3	4.0

Table 4: Slip system and hardening model parameters for OMC copper.

3.3 Construction of Virtual Diffraction Peaks

The virtual diffractometer framework provides a methodology for generating synthetic diffraction peaks from finite element simulations of the elastoplastic deformations of virtual polycrystals by computationally mimicking a physical diffraction experiment. The framework explicitly deals with the spatial position of a grain, its shape, and various other aspects of its mechanical state in constructing a diffraction peak on a virtual detector. Figure 5 illustrates how it is used to generate synthetic diffraction peaks; a more detailed explanation is available in [18].

The first step in generating an image from a particular grain within the virtual specimen is to determine the diffraction condition for each finite element on its lattice orientation and Bragg’s law (Equation 1). Initially, all elements within a grain have the same lattice orientation, but as the sample is deformed, the lattice orientations evolve independently and will vary over the volume of the grain. If the lattice orientation associated with an element satisfies a particular diffraction condition, the diffracted intensity of the element is projected onto a virtual detector that lies in the path of the diffracted beam. This is done by projecting diffracted x-ray intensity from each point in the direction indicated by the local diffraction conditions.

The next step is to bin the cluster of points from all diffracting elements associated with the grain within the pixels of the detector to obtain integrated intensity values pixel-by-pixel. The superposition of the diffracted intensities from all diffracting elements of the grain forms a diffraction peak across a set of adjoining pixels on the detector. Recall from Section 2.1 that each experimental diffraction image captured on the detector corresponds to the integrated diffracted intensities over an exposure. Correspondingly, the simulated diffracted intensities which fall within a $\Delta\omega$ are also summed.

Finally, a point spread function [31] for the detector used in the experiment is applied to the integrated and summed intensities to obtain the simulated diffraction peak.

4 Results

For the experiments summarized in Section 2, uniaxial tension boundary conditions were applied to the two virtual specimens described in Section 3.1 according to the experimental loading history prescribed in Figure 1(a). This plot shows nominal stresses computed from the measured loads and taken from the resultant forces of the simulation for Specimen 1. The curve computed for Specimen 2 essentially overlays that for Specimen 1. The simulation results were post-processed for both specimens to generate virtual diffraction peaks at several target macroscopic stress levels, which are denoted on the macroscopic stress-strain curve shown in Figure 1(a). Due to length restrictions, peak-to-peak comparisons of the diffraction peak widths are shown only for Specimen 1. The trends are comparable for the two specimens, although details differ, as expected, because each specimen has a distinct grain geometry. Correlations between the peak broadening and the evolving lattice misorientations are given for both specimens.

The results are presented in two steps. First, the measured and computed diffraction peak widths are compared for the four target grains for the diffraction conditions defined by numerous combinations of scattering vector and crystallographic plane. These comparisons give an indication of how well the trends present in the simulations follow those observed in the experiments. Second, the spatial heterogeneities in the stress, the plastic deformation rate, and the lattice orientations computed using the finite element model are shown for the four target grains. The elastic strain (and thus the stress) and lattice orientation appear explicitly in the computation of diffraction intensity and their spatial variations are the sources of broadening of the diffraction peaks.

4.1 Radial and azimuthal peak widths

Using the virtual diffractometer framework described in Section 3.3, diffraction peak widths in the radial and azimuthal directions were computed from the simulated responses for comparison with experimentally measured peak widths. The radial and azimuthal directions correspond to the polar coordinate system whose origin lies at the center of the diffraction pattern (see Figure 2(a) for an illustration of these detector directions). The full width at half the maximum (FWHM) parameter is used to quantify the peak widths in each of the directions. The FWHM is the width of the peak at an intensity that is half of the maximum peak intensity.

The measured and simulated FWHM values in the radial direction are

presented in Figures 6–7, while the FWHM values in the azimuthal direction are presented in Figures 8–9. Comparisons are made in both the tension and the compression phases of the loading cycle, which are presented in separate figures. Each figure shows the evolution of the FWHM values with increasing numbers of loading cycles for all of the peaks examined. The diffraction peaks are grouped according to families of crystallographic planes ($\{hkl\}$) and ordered by increasing η within each group. Table 5 is a guide to the data and gives the macroscopic strain level corresponding to each row of Figures 6–9. The macroscopic strain points corresponding to these rows are also shown in Figure 1(a). Note that the ranges of the FWHM values for the azimuthal and radial plots are quite different. Peak broadening in the radial direction typically is much less than in the azimuthal direction.

The mapping of chart columns to their corresponding diffraction peaks is provided in Table 1 and Figure 2(b) for Grain 4. The other grains have a similar mapping. In Figure 2(b) the detector positions are shown for the peaks in the context of the peaks’ Debye-Scherrer rings. The peak number corresponds to the chart column for Grain 4 in Figures 6–9. Table 1 lists the unique angles, $(2\theta, \eta, \omega)$, together with the corresponding crystallographic planes ($\{hkl\}$). Note that all of the peaks do not appear simultaneously on the detector, but rather are associated with different rotations of angle ω about the sample axis (see Section 2.1).

Row number	Macroscopic strain magnitude	Cycle number
Row 1	0	0
Row 2	0.3%	1
Row 3	0.3%	2
Row 4	0.3%	3
Row 5	0.5%	1
Row 6	0.5%	2
Row 7	0.5%	3

Table 5: Macroscopic strain magnitude and cycle number for the FWHM values. Row numbers refer to Figures 6–9. Strain values are positive in the tension and negative in the compression for each loading cycle.

The radial FWHM values in tension and compression are shown in Figures 6 and 7, respectively. While the correspondence between experiment and simulation clearly is not perfect (and is not expected to be perfect since the virtual sample does not exactly replicate the physical sample), a number of trends are apparent in both the measured and simulated data. First,

the broadening is greater as the order of the peak increases (moving from left to right of the figures). Second, there is a slight trend toward increased FWHM for larger strain amplitudes. For a given peak, greater radial FWHM indicates greater variation of the stress within a grain. Third, tension and compression show approximately the same values for corresponding peaks, indicating the stress variability does not depend strongly on the sign of the stress. Finally, the differences in FWHM values between grains are similar for simulation and experiment. Implications of these observations are discussed later.

The azimuthal FWHM values from the experimental and simulated diffraction peaks in tension and compression are shown in Figure 8 and Figure 9, respectively. Again, several trends emerge in comparing the measured and computed FWHM values. First, the much larger azimuthal FWHM values, relative to the radial FWHM values, is captured by the simulation. Second, as with the radial FWHM values, there is a jump in FWHM between the cycles at 0.5% strain amplitude from those at 0.3% strain amplitude for all grains in tension and compression. Third, there is a substantial difference between tension and compression in the experimental FWHM values, with the compression values in the experiments generally being larger. In contrast, the FWHM values in tension and compression for the simulated peaks are comparable in magnitude. Consequently, the experiments and simulations compare well for tension, but differ for compression, for all grains except Grain 2. Recall that azimuthal peak widths correlate with variations in the lattice orientations within a grain. Thus, in the simulations, the level of intragrain lattice misorientation is roughly the same between tension and compression, but in the experiments, there is a larger difference. Experiments on (pure) copper by the authors indicate that the tension-compression asymmetry is more exaggerated in OMC copper than in copper, pointing to the possible influence of strength-enhancing precipitates present in OMC copper. The implications of these trends are discussed later.

4.2 Computed intragrain distributions

Broadening of simulated diffraction peaks arises from inhomogeneities over the domain of the crystal being interrogated. Without spatial variations in the lattice plane spacing or in the orientation of the lattice, the diffraction peaks for a particular grain would remain sharply defined. Variations in the unit cell dimensions are directly tied to variations in the stress, while variations in the lattice orientation arise principally from variations in the slip-associated deformation processes. Here we examine the distributions of

stress, plastic deformation rate and lattice orientation over the four target grains with an intent to relate these to the relative degrees of peak broadening presented in Section 4.1 for those grains.

4.2.1 Stress heterogeneity

The three-dimensional nature of the crystal-scale stress, even under uniaxial macroscopic loading conditions, is an important outcome from the experiment and simulation. To illustrate the variations of stress state, however, we choose a simple scalar quantity, often employed with phenomenological plasticity: the von Mises effective stress, $\bar{\sigma}$. A scalar effective stress cannot capture the anisotropy needed to describe yielding at the single crystal level, and is not used for that purpose; rather, it is used strictly for visualizing the spatial variations in stress over the crystals. The effective stress, $\bar{\sigma}$, is computed from the deviatoric Cauchy stress as:

$$\bar{\sigma} = \sqrt{\frac{3}{2} \boldsymbol{\sigma}' : \boldsymbol{\sigma}'} \quad (33)$$

The effective stress distributions, plotted for each grain over its surface and on slices cutting through its interior, are shown in Figure 10 for the four target grains. Higher stresses tend to develop near the grain boundaries due to the constraints of the neighboring grains, and especially near triple points where several grains connect. However, the highly stressed domains are not limited strictly to the grain boundaries, but rather penetrate well into the grain interior in some cases. The spatial variations in stress imply variations in elastic strain, which in turn imply variations in the lattice plane spacings that manifest in the radial broadening of the diffracted x-ray beam.

As the color scale for Figure 10 implies, there are significant differences in the average stress observed among the four grains. Grain 3 has the lowest average effective stress, which correlates with its Taylor factor, M . (the same is true for Grain 3 in Specimen 2). The Taylor factor may be computed for a given orientation assuming that the crystal is undergoing the nominal deformation rate from:

$$M = \frac{\bar{\sigma}}{\tau} \quad (34)$$

where τ is the critical resolved shear stress for the active slip systems [32, 33]. The Taylor factor provides an estimate of the magnitude of the deviatoric stress needed to activate a sufficient number of slip systems to accommodate the imposed deformation as a function of the crystal lattice orientation. It

is plotted over the stereographic triangle in Figure 1(b) for axisymmetric extension along with superimposed lattice orientations for the four target grains. On average, the stress to activate slip needed for axisymmetric extension is relatively low for grains oriented with a $\{100\}$ plane normal aligned with the loading axis, as is the case for Grain 3.

4.2.2 Plastic deformation rate heterogeneity

As plastic flow is driven by the deviatoric stress, the presence of gradients in the deviatoric stress over the volume of a grain implies that there will also be gradients in the plastic deformation rate. For the model outlined in Section 3.2, plastic flow occurs by crystallographic slip on a restricted number of slip systems. The plastic deformation rate is the net result of shearing of the active slip systems and is computed from:

$$d^{p'} = \sum_{\alpha} \dot{\gamma}^{\alpha} \hat{p}^{\alpha} \quad (35)$$

The plastic deformation rate, $d^{p'}$, is deviatoric by construction and a scalar effective deformation rate, $\bar{d}^p$, can be defined in a manner analogous to computing the effective stress:

$$\bar{d}^p = \sqrt{\frac{2}{3} d^{p'} : d^{p'}} \quad (36)$$

The spatial distributions of the effective plastic deformation rate over the surface of the grain and on slices through the grain are shown in Figure 11. Although Grain 3 has, on average, the lowest effective stress, it experiences plastic deformation that is comparable to the other target grains (again, this is true in Specimen 2). It should be noted that the stresses are shown for points of the loading cycle at which the crystals are in fully-developed plastic flow and the crystal stresses lie on the single crystal yield surface. The four target grains also exhibit different trends in their spatial distributions of $\bar{d}^p$. Within a given crystal, higher rates of deformation are observed in regions of higher stress. Grain 2 exhibits high plastic deformation close to the grain boundaries whereas Grain 1 exhibits bands of relatively higher plastic deformation spanning across the grain.

4.2.3 Lattice rotations

The lattice rotates in concert with the local deformation over the course of the cyclic loading. As the deformation varies over the volume of a grain

from interactions with their neighbors, so do the lattice rotations. This is evident from the responses of the four target grains, which exhibit the heterogeneities in stress and deformation arising illustrated in Sections 4.2.1 and 4.2.2. The rotation of the lattice orientation accompanying the motion from the initial to the current deformed configurations can be expressed as a Rodrigues vector:

$$\mathbf{w}^d = \tan \frac{\phi^d}{2} \mathbf{n}^d \quad (37)$$

where ϕ^d is the rotation angle and $\mathbf{n}^d$ is the rotation axis. For the purpose of visualizing the spatial distribution of lattice orientations, we focus first on ϕ^d and plot its spatial distribution over the grain volume for each of the target grains. These distributions are shown on the surfaces of the target grains and on slices through them in Figure 12 for +0.5% macroscopic strain on Cycle 3. There are significant spatial variations in the rotation (and thus current lattice orientation) within each grain. The largest rotation of the lattice occurs near the grain boundaries, although significant rotation can also develop within the interior of the grain. Comparing Figure 12 to Figure 11, regions within the grain with high effective deformation rate, $\bar{d}^p$, do tend to correspond to regions of high lattice rotation. The same trends were seen in Specimen 2.

The axes for lattice rotations also can be visualized by plotting the Rodrigues vectors over orientation space (the three components of $\mathbf{r}$ define the coordinates of orientation space). $\mathbf{w}^d$ for each element within a target grain is plotted as a point in Rodrigues space that is positioned at the coordinates of its Rodrigues vector $\mathbf{w}^d$ and is colored by the value of ϕ^d . In the initial undeformed state at zero macroscopic load on Cycle 0, the distribution collapses to a point at the origin. Points become more distant from the origin, and their colors change, as their rotations increase. The distributions for the four target grains are shown in Figure 13 for the final loading cycle (Cycle 3) at +0.5% and -0.5% macroscopic strain. The differences in the distributions between the tension and compression points of the same loading cycle illustrate the lattice rotations as the deformation proceeds between tension and compression. When the stress is reversed during a loading cycle, the slip reverses direction and the lattice rotates in the opposite direction. As the range in ϕ^d is small, the mapping is approximately linear, giving rise to the nearly symmetrical distributions between tension and compression observed in Figure 13. However, the Rodrigues vectors between the tension and compression phase for any given element are not exactly aligned. The misalignments of the rotation axes corresponding to tension and compres-

sion, $((\mathbf{n}^d)_t$ and $(\mathbf{n}^d)_c$, respectively) computed as $\tilde{\beta} = \text{acos}((\mathbf{n}^d)_t \cdot (\mathbf{n}^d)_c)$, are, on average, several degrees, which implies that the slip system activities are not the same for tensile and compression phases of the loading.

It should be noted that the ϕ^d distributions observed here are specific to the type of cyclic hardening model that is used in the simulations. Less symmetric ϕ^d distributions might be expected to result from different hardening models, such as latent or kinematic hardening, or from a model that incorporates a back stress. We return to this point in the discussion.

5 Discussion

5.1 Correlation between misorientations and azimuthal FWHM values

We now examine the relationship between the spread in lattice orientations over a grain and the amount of broadening observed in its diffraction peaks. Over the volume of a grain, spatial variations in the lattice rotations presented in Section 4.2.3 lead to the development of misorientation distributions. As mentioned in Section 1, the evolution of lattice misorientation distributions has been quantified experimentally [2–5, 7], showing that, overall, with increasing inelastic deformation, both the mean and standard deviation of the misorientation distribution increase. Evolution of a misorientation distributions is closely linked to the spreading of diffraction peaks. However, it is difficult to apply the average trend quantified in a distribution function to specific grains due to the difficulty in quantifying the influence of the crystallographic neighborhood on the local deformation and thus lattice rotation.

A common approach in quantifying misorientation within grains is to construct the misorientation tensor, $\mathbf{A}$, from a set of misorientation vectors, $\mathbf{w}^m$, as:

$$\mathbf{A}^{-1} = \sum_{i=1}^{n_e} \varphi^i ((\mathbf{w}^m)^i \times (\mathbf{w}^m)^i) \quad (38)$$

where n_e is the number of orientations in the set, which equals the number of finite elements within a grain, and φ^i is the volume fraction attributed to each element [34, 35]. The Rodrigues misorientation vector, $\mathbf{w}^m$, represents the misorientation between the lattice orientation within an element and the average orientation over all the elements that discretize the grain. It is given by:

$$\mathbf{w}^m = \tan \frac{\phi^m}{2} \mathbf{n}^m \quad (39)$$

where ϕ^m is the misorientation angle and $\mathbf{n}^m$ is the misorientation axis. Note that the misorientation is computed from the average orientation over all the elements, in contrast to the rotation discussed in Section 4.2.3 which was computed from the initial orientation of the same element. A useful measure of the extent or size of the misorientation set is the first invariant of A^{-1} :

$$\theta^m = \sqrt{\text{tr}(A^{-1})} \quad (40)$$

Larger values of θ^m imply larger spatial variations of the lattice orientations over a grain. This is important here because the differing lattice orientations introduced by non-uniform deformations present different diffraction conditions for the virtual diffractometer and thus diffract the beam in different directions. The diffraction peak on the detector, therefore, covers a larger area, leading to a larger azimuthal peak width (more azimuthal broadening).

For both Specimens 1 and 2, values of θ^m for the four target grains are plotted in Figure 14 as a function of the simulated average azimuthal FWHM. The values are taken from Figure 8 for the tensile phase of the loading cycle. The trend is interesting in several aspects. First, the correlation is strong for both specimens. Second, these correlations exist even though correlations between other attributes of the grains or their mechanical responses did not correlate with the azimuthal FWHM. That is, metrics like grain size, average lattice orientation, or average stress did not correlate well with the azimuthal FWHM. Thus, the collective evolution of the azimuthal FWHM for each peak within a crystal is a key indicator of deformation-induced grain subdivision, which is sensitive many aspects of the grain's properties and its neighborhood. In principle, therefore, one could interpret a specific misorientation distribution, such as one of those shown in Figure 12 and Figure 13, within the context of distributions of dislocations and provide a link between azimuthal broadening and the evolution of dislocation densities. This link is suggested by Korsunsky and coworkers [36] in comparing the streaking of an observed microdiffraction spot to spots computed both a dislocation dynamics simulation and a finite element model and by Ice and Barabash [37] in comparing a simple models of slip system activity to simulate the spreading of Laue patterns during plastic deformation.

The examination of azimuthal broadening is completely distinct from classic line broadening analysis, the latter being explicitly linked to radial broadening [38–40], often of complete Debye-Scherrer rings. Correlations of radial broadening with attributes of the microstructure, such as dislocation density, are possible through modeling, as reported in [41, 42]. In [41], increases in the radial FWHM were shown to correlate with the increase

in slip system strength for aluminum and stainless steel alloys. Further, the variances in lattice strains over all crystals contributing to a particular reflection were found to be insufficient to account for the radial broadening. A similar result was reported by Kanjarla et al [42]. (The latter study also reports that bi-modal strain distributions develop, but these arise at strain levels exceeding the small strain limitation of their model.) Although useful insight has been drawn from these correlations, the existence of complete Debye-Scherrer rings in a diffraction image implies that the measurement necessarily represents an average over many diffracting crystals. This negates the opportunity to examine evolving intragrain lattice misorientations via azimuthal broadening, as is possible with individual spots via the distributions shown in Figure 12 and Figure 13, because (1) the overlying spots of many grains that collectively comprise a Debye-Scherrer ring cannot readily be deconvolved and (2) some features of the evolving microstructure affect lattice orientation to a greater extent than lattice spacing. By analyzing the broadening in both radial and azimuthal directions a more complete examination of issues like the computed stress variation being too little account for observed radial broadening is possible, as was done in Wong et al [18].

5.2 Tension/compression FWHM asymmetry

The simulated azimuthal FWHM values compare better with the experimental azimuthal FWHM values for the tensile stages of the loading cycle than they do for the compression stages. As seen in Figures 8 and 9, the experimental azimuthal FWHM values in compression are considerably larger than those in tension at corresponding strain levels. In contrast, the simulated values are comparable between tension and compression – a trend confirmed by the similarities in the volumes encompassed by the orientations in Rodrigues space shown in Figure 13. In this particular experiment, tension is the initial loading direction, while compression is imposed on load reversal. Larger experimental FWHM values in compression suggest that greater reorientation of the lattice takes place in the experiments when the loading is reversed than is computed in the simulation. This in turn suggests that the equations for slip outlined in Section 3.2 do not adequately represent the physical system in this respect.

Differences in the mechanical response between forward and reverse loading have long been recognized as central to cyclic loading and fatigue, and have been modeled at the continuum scale with the addition of kinematic hardening to isotropic hardening theories [13, 43]. The basic construct for a

yield surface with combined isotropic and kinematic hardening utilizes two state variables: an isotropic variable that controls the size of the yield surface and a tensorial variable (the backstress) that regulates the center of the yield surface. Each variable has its own evolution equation. Asymmetry in yielding is provided by the backstress, which is supported in the material through the presence of structural heterogeneities arising from deformation, such as dislocation structures. The concept of kinematic hardening has been more recently applied to equations for slip at the crystal scale though often times using methods developed for the macroscopic scale. An approach reported by several investigators [44, 45] involves modifying Equation 25 so that the slip system shearing rate is driven by the difference between the resolved shear stress, τ^α , and a slip system backstress, τ_{bs}^α . This modification facilitates modeling the yield asymmetry observed in cyclic loading, but at the modeling expense of an additional set of scalar state variables that must be initialized and evolved. (Note that in the forms used [44, 45] the backstress is not a tensor quantity, but rather a set of scalars). Wollmer-shauer and coworkers [46] employed combined isotropic/kinematic hardening, crystal-scale, equations to model neutron diffraction experiments involving cyclic loading of stainless steel samples. They showed that when both the kinematic and isotropic variables are allowed to evolve, good agreement is achieved for the macroscopic stress and the lattice strains for several crystallographic reflections in the loading direction.

Alternatives exist to the traditional macroscopic scale combined isotropic and kinematic hardening model construct. Several of those alternatives have been made to include the effects that dislocations have on the yield surface at the crystal scale. One is to modify the kinematic decomposition to admit a configuration defined by the presence of dislocations within the differential volume depicted schematically in Figure 4 [47]. There is an elastic strain tensor associated with that configuration arising from the dislocation content which can induce yield asymmetries [48]. Another approach is to explicitly include the dislocations in the form of a field [49]. The evolution of this field is driven by deformation and also can induce yield asymmetry. Yet other approaches include higher-order strain gradients with dependence on the presence of dislocations to account for size effects as seen in [50]. Expansions of the higher-order strain gradient approaches introduce latent hardening to model slip-system interactions [51, 52]. The latent hardening can lead to an increase in macroscale hardening over standard models and also induce yield asymmetry. A serious issue that arises with the use of any of these models is the verification that the state or field variables are evolving correctly and that their influence on the deformation is correctly

quantified. This verification has been impeded by an inability to measure the variables directly, or even to correlate them uniquely with a signal that can be measured independently. Herein lies the opportunity associated with coordinating diffraction data for individual crystals of a polycrystalline sample with modeling studies that query the behavior of state variables designed to capture behaviors observed complex loadings typical of low cycle fatigue testing.

5.3 Identification of potential void growth sites

The relationship between void growth and stress triaxiality has been established in the classical treatment of ductile fracture [53]. The stress triaxiality, Ψ , is defined as:

$$\Psi = \frac{\sigma_{kk}/3}{\bar{\sigma}} \quad (41)$$

where σ_{kk} is the trace of the stress tensor. According to the classical treatment, if the stress triaxiality is positive, existing voids tend to grow. Thus, the value of the stress triaxiality can be used to identify regions within a grain and points along the loading history which are more conducive to void growth. Since fatigue cracks initiate at the crystal level, variation in stress triaxiality at the scale of individual grains is an important consideration during cyclic loading [54]. During fully-reversed cyclic loading however, regions within the grain experience alternating excursions of positive and negative mean stress or stress triaxiality. The stress triaxiality at +0.5% macroscopic strain and -0.5% macroscopic strain on Cycle 3 are shown in Figures 15 and 16, respectively. The most severe situations arise on the tensile stage of the loading cycle, often near grain boundaries. Similar domains of elevated stress are seen in the deviatoric stress distributions plotted in Figure 10.

The stress triaxiality distributions provide an important complement to the distributions of lattice misorientations, which identify regions where large packing defects are implied by large misorientations. The coincidence of positive triaxiality with high misorientations and high local plastic deformation rate has been suggested as a criterion for candidate sites for fatigue crack initiation [55]. To apply this criterion here we required that the misorientation be greater than 0.35° and the effective deformation rate be greater than $1.7 \times 10^{-3} \frac{1}{s}$. These limits were chosen to limit the total volume of the target grains satisfying criterion to a small fraction of their total volumes and thus to identify those sites most favorable for defect initiation. According to this filter, Grain 1 has likely locations for defect initiation in both Specimens 1 and 2. The sites lie in the vicinity of the grain boundary near

edges between facets, as shown in Figures 17 and 18. Shading indicates domains where both conditions are simultaneously satisfied and define the only regions that meet the potential damage site criterion for both the misorientation and plastic deformation rate. Because the grain shape is different and the orientations of neighboring grains are different, the precise locations of the sites cannot be the same. In contrast to Grain 1, Grains 3 and 4 do not have likely sites in either of the specimens, while Grain 2 has likely sites in Specimen 1 but not in Specimen 2. The reason why these regions are experiencing this most severe set of conditions depends on many factors, including the lattice orientation (and with it, the Taylor factor and directional modulus), the relative stiffness and strength of neighboring grains, and the arrangement of facets, to name a few. The consequence of the coincident sites, however, is that hydrostatic tension is present over domains where packing defects are plentiful as necessary to accommodate large lattice misorientations. Thus, the heterogeneity of slip has nucleated voids that could grow under the conditions of hydrostatic tension.

6 Conclusions

Using a crystal-based finite element model and a virtual diffractometer framework, the cyclic deformation of an OMC copper specimen was simulated and diffraction peaks were generated from the virtual specimen. The heterogeneity of the stress and of the deformation at the scale of individual grains were examined by comparing the evolution of diffraction peak widths from four target grains in the specimen to trends observed via high energy x-ray diffraction experiments. In particular, radial and azimuthal peak broadening were compared at two strain amplitudes. In general, azimuthal broadening is much larger than radial broadening – a trend captured in the simulations. There is a marked increase in the broadening for loading cycles at $\pm 0.5\%$ strain amplitude over cycles at $\pm 0.3\%$ strain amplitude due to the greater extent of plastic strain at the larger strain amplitudes. The azimuthal FWHM values showed greater tension/compression asymmetry in the experimental observations than was predicted by simulations. This is attributed to the relative simplicity of the evolution equation used to model strain hardening of the slip systems. The results further demonstrate that azimuthal broadening grows with intra-grain lattice misorientations such that the volume encompassed by the orientations in Rodrigues space correlates with the change in FWHM in the azimuthal direction. Thus, the greater the misorientations within a grain, the greater the azimuthal broad-

ening of the diffraction peaks from that grain. The link provided between the misorientation distributions predicted by the finite element model and the azimuthal FWHM values could be exploited to estimate the evolution of dislocation densities in a manner independent of that employed in classic line broadening analysis.

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References

- [1] D.P. Mika and P.R. Dawson. Polycrystal plasticity modeling of intracrystalline boundary textures. *Acta Materialia*, 47(4):1355–1369, 1999.
- [2] H Chandra, JD Embury, and UF Kocks. On the formation of high angle grain boundaries during the deformation of aluminum single crystals. *Scripta Metallurgica*, 16(5):493–497, 1982.
- [3] R Ørsund, J Hjelen, and E Nes. Local lattice curvature and deformation heterogeneities in heavily deformed aluminium. *Scripta metallurgica*, 23(7):1193–1197, 1989.
- [4] D. Kuhlmann-Wilsdorf and Niels Hansen. Geometrically necessary, incidental and subgrain boundaries. *Scripta Metallurgica et Materialia*, 25(7):1557 – 1562, 1991.
- [5] B. Bay, N. Hansen, D.A. Hughes, and D. Kuhlmann-Wilsdorf. Overview no. 96 evolution of f.c.c. deformation structures in polyslip. *Acta Metallurgica et Materialia*, 40(2):205 – 219, 1992.
- [6] D. Raabe, M. Sachtleber, Z. Zhao, F. Roters, and S. Zaefferer. Micromechanical and macromechanical effects in grain scale polycrystal

- plasticity experimentation and simulation. *Acta Materialia*, 49(17):3433 – 3441, 2001.
- [7] Bo Jakobsen, Henning F. Poulsen, Ulrich Lienert, Jonathan Almer, Sarvjit D. Shastri, Henning O. Sørensen, Carsten Gundlach, and Wolfgang Pantleon. Formation and subdivision of deformation structures during plastic deformation. *Science*, 312(5775):889–892, 2006.
  - [8] N. R. Barton and P. R. Dawson. On the spatial arrangement of lattice orientations in hot rolled multiphase titanium. *Modeling and Simulation in Materials Science and Engineering*, 9:433–463, 2001.
  - [9] P. R. Dawson, D. P. Mika, and N. R. Barton. Finite element modeling of lattice misorientations in aluminum alloys. *Scripta Materialia*, 47:713 – 717, 2002.
  - [10] R. Quey, P. R. Dawson, and J. H. Driver. Grain orientation fragmentation in hot-deformed aluminum: experiments and simulations. *Journal of the Mechanics and Physics of Solids*, 60:509–524, 2012.
  - [11] W. A. Wood. Formation of fatigue cracks. *Philosophical Magazine*, 3(692–699), 1958.
  - [12] N. F. Mott. A theory of the origin of fatigue cracks. *Acta Metallurgica*, 6(195–197), 1958.
  - [13] S. Suresh. *Fatigue of Materials*. Cambridge University Press, second edition, 1998.
  - [14] H. F. Poulsen. *Three-Dimensional X-Ray Diffraction Microscopy*. Springer, 2004.
  - [15] U. Lienert, M.C. Brandes, J.V. Bernier, J. Weiss, S.D. Shastri, M.J. Mills, and M.P. Miller. In situ single-grain peak profile measurements on ti-7al during tensile deformation. *Materials Science and Engineering: A*, 524(1–2):46 – 54, 2009.
  - [16] Jette Oddershede, Søren Schmidt, Henning Friis Poulsen, Henning Os-holm Sørensen, Jonathan Wright, and Walter Reimers. Determining grain resolved stresses in polycrystalline materials using three-dimensional X-ray diffraction. *Journal of Applied Crystallography*, 43(3):539–549, Jun 2010.

- [17] J V Bernier, N R Barton, U Lienert, and M P Miller. Far-field high-energy diffraction microscopy: a tool for intergranular orientation and strain analysis. *The Journal of Strain Analysis for Engineering Design*, 46(7):527–547, 2011.
- [18] S. L. Wong, J.-S. Park, M. P. Miller, and P. R. Dawson. A framework for generating synthetic diffraction images from deforming polycrystals using crystal-based finite element formulations. *Computational Materials Science*, 77:456–466, 2013.
- [19] M. Obstalecki, S. L. Wong, P. R. Dawson, and M. P. Miller. Quantitative analysis of crystal scale deformation heterogeneity during cyclic plasticity using high-energy x-ray diffraction and finite-element simulation. *Acta Materialia*, 75:259–272, 2014.
- [20] Erik G. Thompson. *An Introduction to the Finite Element Method*. 1st edition. Wiley, 2005.
- [21] R. Quey, P.R. Dawson, and F. Barbe. Large-scale 3d random polycrystals for the finite element method: Generation, meshing and remeshing. *Computer Methods in Applied Mechanics and Engineering*, 200(17–20):1729–1745, 2011.
- [22] S. F. Li and R. M. Suter. Adaptive reconstruction method for three-dimensional orientation imaging. *Journal of Applied Crystallography*, 46(2):512–524, 2013.
- [23] S. Schmidt, U. L. Olsen, H. F. Poulsen, H. O. Srensen, E. M. Lauridsen, L. Margulies, C. Mauricec, and D. Juul Jensen. Direct observation of 3-d grain growth in Al?0.1% Mn . *Scripta Materialia*, 59:491–494, 2008.
- [24] E. B. Marin and P. R. Dawson. On modelling the elasto-viscoplastic response of metals using polycrystal plasticity. *Computer Methods in Applied Mechanics and Engineering*, 165(1-4):1–21, 1998.
- [25] E. B. Marin and P. R. Dawson. Elastoplastic finite element analyses of metal deformations using polycrystal constitutive models. *Computer Methods in Applied Mechanics and Engineering*, 165(1-4):23–41, 1998.
- [26] P. Dawson and D. Boyce. Finite element polycrystals: Theory, formulation, implementation and examples. Technical report, Sibley School of Mechanical and Aerospace Engineering, Cornell University, 2014.

- [27] F. C. Frank. Orientation mapping. *Metallurgical Transactions A*, 19(3):403–408, 1988.
- [28] A. Kumar and P. R. Dawson. Computational modeling of f.c.c. deformation textures over rodrigues’ space. *Acta Materialia*, 48(10):2719–2736, 2000.
- [29] A. Kelly and G. W. Groves. *Crystallography and Crystal Defects*. Addison-Wesley Publishing Company, 1970.
- [30] H. Turkmen, M. Miller, P. Dawson, and J. Moosebrugger. A slip-based model for strength evolution during cyclic loading. *Journal of Engineering Materials and Technology*, 126:329–338, 2004.
- [31] John H. Lee, C. Can Aydiner, Jonathan Almer, Joel Bernier, Karena W. Chapman, Peter J. Chupas, Dean Haeffner, Ken Kump, Peter L. Lee, Ulrich Lienert, Antonino Miceli, and German Vera. Synchrotron applications of an amorphous silicon flat-panel detector. *Journal of Synchrotron Radiation*, 15(5):477–488, Sep 2008.
- [32] W. F. Hosford. *The Mechanics of Crystals and Textured Polycrystals*. Oxford Science Publications, 1993.
- [33] U. F. Kocks, C. N. Tome, and H.-R. Wenk. *Texture and Anisotropy*. Cambridge University Press, 1998.
- [34] J.-Ch. Glez and J.H. Driver. Orientation distribution analysis in deformed grains. *J. Appl. Crystallogr.*, 34:280–288, 2001.
- [35] N. R. Barton and P. R. Dawson. A methodology for determining average lattice rotations and its application to the characterization of grain substructure. *Metallurgical and Materials Transactions*, 32A:1967–1975, 2001.
- [36] A.M. Korsunsky, F. Hofmann, B. Abbey, X. Song, J. P. Belnoue, Mucuta C., and I. Dolbnya. Analysis of the internal structure and lattice (mis)orientation in individual grains of deformed CP nickel polycrystals by synchrotron x-ray micro-diffraction and microscopy. *International Journal of Fatigue*, 126:329–338, 2011.
- [37] G.E. Ice and R.I. Barabash. Chapter 79 white beam microdiffraction and dislocations gradients. volume 4 of *Dislocations in Solids*, pages 261–362. Elsevier, 2007.

- [38] M Wilkens. The determination of density and distribution of dislocations in deformed single crystals from broadened x-ray diffraction. *Physical Status Solidi (A)*, 2:359–370, 1970.
- [39] M Wilkens, K. Herz, and H Mughrabi. An X-Ray Diffraction Study of Cyclically and of Unidirectionally Deformed Copper Single Crystals. *Zeitschrift für Metallkunde*, 71(6):376–384, jun 1980.
- [40] T Ungt’ar, H Mughrabi, and M Wilkens. An X-Ray line-broadening study of dislocations near the surface and in the bulk of deformed copper single crystals. *Acta Metall. (USA)*, 30(10):1861–1867, 1982.
- [41] P. R. Dawson, D. E. Boyce, and R. Rogge. Correlation of diffraction peak broadening and crystal strengthening in finite element simulations. *Materials Science and Engineering A*, 399(1-2):13–25, 2005.
- [42] A.K. Kanjarla, R.A. Lebensohn, L. Balogh, and C. N. Tome. Study of internal lattice strain distribution in stainless steel using a full-field elasto-viscoplastic formulation based on fast Fourier transforms. *Acta Materialia*, 60:3094–3106, 2012.
- [43] Donald C. Stouffer and L. Thomas Dame. *Inelastic Deformation of Metals*. 1st edition. Wiley, 1996.
- [44] L. Méric and G. Cailletaud. Single crystal modeling for structural calculations: Part 2 – finite element implmentation. *Journal of Engineering Materials and Technology*, 113:171–182, 1991.
- [45] C.-H. Goh, J. M. Wallace, R. W. Neu, and D. L. McDowell. Polycrystal plasticity simulations of fretting fatigue. *International Journal of Fatigue*, 23:S423–S435, 2001.
- [46] J. A. Wollmershauser, B. Clausen, and S. R. Agnew. A slip system-based kinematic hardening model application to in situ neutron diffraction of cyclic deformation of austenitic stainless steel. *International Journal of Fatigue*, 42:1–133, 2012.
- [47] C. S. Hartley. A method for linking thermally activated dislocation mechanisms of yielding with continuum plasticity theory. *Philosophical Magazine*, 83:3783–3808, 2003.
- [48] J. M. Gerken and P. R. Dawson. A crystal plasticity model the incorporates stresses and strains due to slip gradients. *Journal of the Mechanics and Physics of Solids*, 56:1651–1672, 2008.

- [49] A. Archarya. A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of the Mechanics and Physics of Solids*, 49:761784, 2001.
- [50] Morton E. Gurtin, Lallit Anand, and Suvrat P. Lele. Gradient single-crystal plasticity with free energy dependent on dislocation densities. *Journal of the Mechanics and Physics of Solids*, 55:1853–1878, 2007.
- [51] C.J. Bayley, W.A.M. Brekelmans, and M.G.D. Geers. A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity. *International Journal of Solids and Structures*, 43:7268–7286, 2006.
- [52] Swantje Bargmann, B. Daya Reddy, and Benjamin Klusemann. A computational study of a model of single-crystal strain-gradient viscoplasticity with an interactive hardening relation. *International Journal of Solids and Structures*, 51:2754–2764, 2014.
- [53] J. R. Rice and D. M. Tracey. On the ductile enlargement of voids in triaxial stress fields. *Journal of the Mechanics and Physics of Solids*, 17(3):201–217, 1969.
- [54] A. J. Beaudoin, M. Obstalecki, R. Storer, W. Tayon, J. Mach, P. Kene-sei, and U Lienert. Validation of a crystal plasticity model using high energy diffraction microscopy. *Modelling and Simulation in Materials Science and Engineering*, 20(024006), 2012.
- [55] N. R. Barton and P. R. Dawson. Modeling defect origins from lattice misorientations in polycrystalline metals. *International Journal of Forming Processes*, 5:191–203, 2002.

Figure

(b) Orientations of target grains with respect to the loading axis.

Figure 1: (a) Measured and computed stress-strain behavior for the cyclic loading history. (b) Stereographic triangle showing the orientations of the four target grains with respect to the loading axis. Color background gives the Taylor factor for axisymmetric extension.

Figure 2: (a) Schematic of the HEXD experiment at APS beamline 1-IDC depicting the geometric relationships between the incident and diffracted x-ray beam, the sample and the area detector. Three relevant coordinate systems are defined. One is the fixed laboratory system ($\mathbf{X}_l, \mathbf{Y}_l, \mathbf{Z}_l$). The ($\mathbf{X}_s, \mathbf{Y}_s, \mathbf{Z}_s$) is fixed within the specimen and the detector coordinate system ($\mathbf{X}_d, \mathbf{Y}_d, \mathbf{Z}_d$) is fixed on the detector. ((b) Approximate $(2\theta, \eta)$ positions of the centroids of the diffraction spots collected for grain 4 before deformation. Full $(2\theta, \eta, \omega)$ information for each spot is given in Table 1.

Figure 3: Example of a diffraction peak that appears on an area detector. To quantify position and spread of the intensity, the peak is integrated in the radial, then the azimuthal directions to obtain diffracted intensity profiles in the azimuthal and radial directions, respectively.

Figure 4: Kinematic decomposition for motion by a combination of plastic slip, rotation and elastic straining.

Figure 5: Schematic of how the virtual diffractometer is used to generate diffracted intensities from each element within a grain and then how the diffracted intensity is projected onto a virtual detector. Reproduced from [18]

Figure 6: Experimental and simulated radial FWHM values in tension for Grains 1-4. The corresponding macroscopic strain and cycle number for each row can be obtained from Table 5. Reflections from a particular set of lattice planes are separated by vertical black bars. The left to right column numbers for Grain 4 correspond to Peak #'s in Table 1

Figure 7: Experimental and simulated radial FWHM values in compression for Grains 1-4. The corresponding macroscopic strain and cycle number for each row can be obtained from Table 5. The left to right column numbers for Grain 4 correspond to Peak #’s in Table 1

Figure 8: Experimental and simulated azimuthal FWHM values in tension for Grains 1-4. The corresponding macroscopic strain and cycle number for each row can be obtained from Table 5. The left to right column numbers for Grain 4 correspond to Peak #'s in Table 1

Figure 9: Comparison of the experimental and simulated azimuthal FWHM values in compression. The corresponding macroscopic strain and cycle number for each row can be obtained from Table 5. The left to right column numbers for Grain 4 correspond to Peak #’s in Table 1

Grain 1
Von Mises stress

Grain 2
Von Mises stress

Grain 3
Von Mises stress

Grain 4
Von Mises stress

(d) Grain 4

Figure 10: The distribution of effective stress, $\bar{\sigma}$, for each grain on the final cycle (+0.5% macroscopic strain on Cycle 3). The left column in each figure shows the value of $\bar{\sigma}$ over the surface of the grain. The second, third and fourth columns in each figure show the distributions of $\bar{\sigma}$ on slices through the grain. Each slice is plotted on the x-y plane in the sample coordinate system defined for each grain at $z = -0.005$ mm, $z = 0$ mm and $z = 0.005$ mm, where z is the position with respect to the grain centroid.

(d) Grain 4

Figure 11: Plastic deformation rate magnitude distribution, $\bar{d}^P$, for each grain on the final cycle (+0.5% macroscopic strain on Cycle 3). The left column in each figure shows the value of $\bar{d}^P$ for each element on the surface of the grain. The second, third and fourth columns in each figure shows $\bar{d}^P$ on slices through the grain. Each slice is plotted on the x-y plane in the sample coordinate system defined for each grain at $z = -0.005$ mm, $z = 0$ mm and $z = 0.005$ mm, where z is the position with respect to the grain centroid.

Grain 1
Misorientation

Grain 2
Misorientation

Grain 3
Misorientation

Grain 4
Misorientation

(d) Grain 4

Figure 12: Rotation angle, ϕ^d , of each element within a grain on the final cycle (+0.5% macroscopic strain on Cycle 3). For each grain, the origin of Rodrigues space is defined as the initial undeformed lattice orientation; hence, $\phi^d = 0$ implies that the lattice orientation is unchanged from the initial orientation. The left column in each figure shows ϕ^d for each element on the surface of the grain. The second, third and fourth columns in each figure show the ϕ^d distribution on slices through the grain. Each slice is plotted on the x-y plane in the sample coordinate system defined for each grain at $z = -0.005$ mm, $z = 0$ mm and $z = 0.005$ mm, where z is the position with respect to the grain centroid.

Figure 13: Rotations, $\mathbf{w}^d$, associated with each element within a grain plotted in Rodrigues space for the tension and compression load points on the final cycle (+0.5% macroscopic strain and -0.5% macroscopic strain on Cycle 3). $\mathbf{w}^d$ is plotted as a point in Rodrigues space that is positioned at the coordinates of its Rodrigues vector $\mathbf{w}^d$ and is colored by the value of ϕ^d . In the initial undeformed state, the distribution will appear as a single point at the origin of Rodrigues space.

Figure 14: Correlation between the misorientation set size, θ^m , and the simulated mean azimuthal FWHM.

(d) Grain 4

Figure 15: Stress triaxiality at +0.5% macroscopic strain on Cycle 3.

Grain 1
Stress triaxiality at -0.5%

Grain 2
Stress triaxiality at -0.5%

Grain 3
Stress triaxiality at -0.5%

Grain 4
Stress triaxiality at -0.5%

(d) Grain 4

Figure 16: Stress triaxiality at -0.5% macroscopic strain on Cycle 3.

(a) Positive triaxiality and high misorientation

(b) Positive triaxiality and high plastic deformation rate magnitude

Figure 17: Locations of defect initiation sites suggested by the coincidence of positive triaxiality, high lattice misorientation, and high plastic deformation rate magnitude Grain 2 in Specimen 1.

(a) Positive triaxiality and high misorientation

(b) Positive triaxiality and high plastic deformation rate magnitude

Figure 18: Locations of defect initiation sites suggested by the coincidence of positive triaxiality, high lattice misorientation, and high plastic deformation rate magnitude for Grain 2 in Specimen 2.