Computational Homogenization and Micromechanical Analysis of Textured Polycrystalline Materials

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ABSTRACT

We present a numerical methodology for the thermomechanical analysis of real polycrystalline material microstructures obtained using electron backscatter diffraction techniques. The asymptotic expansion homogenization method is used in conjunction with the finite element method to perform comprehensive micromechanical analyses and determine the effective thermoelastic properties of polycrystalline materials. Smooth grain boundaries are generated from the discretely sampled electron backscatter diffraction data of real polycrystalline materials. The microscale displacements, strains and stresses are related to the macroscale temperature change and strains through 21 distinct characteristic functions. The three-dimensional equilibrium equations at the microscale yield a system of partial differential equations for the characteristic functions which are solved using the finite element method. The effective properties of the polycrystalline material are obtained from the single-crystal thermoelastic properties, crystallographic orientations of the crystallites and the characteristic functions. The proposed methodology is demonstrated by considering electron backscatter diffraction maps of zinc, stainless steel, and natural quartzite rock. Results are presented for homogenized properties such as elastic stiffnesses, thermal expansion coefficients, and seismic wavespeeds, as well as for microscale stress distributions resulting from different macroscale loading conditions. The bulk thermoelastic properties are compared with those obtained using the Voigt, Reuss, Voigt-Reuss-Hill and self-consistent methods. Details are provided regarding a freely available software package that has been developed for the thermomechanical analysis of polycrystalline materials based on the proposed numerical framework.

Keywords: Homogenization; heterogeneous materials; bulk properties; microtexture; polycrystalline microstructure; electron backscatter diffraction.

1 Introduction

A large class of technologically important materials, including metals and ceramics, as well as natural materials, such as rocks and ice, are polycrystalline. As such, there is a need for numerical tools that can be used to perform detailed microstructural analysis of polycrystalline materials. Several methods currently exist for the calculation of effective thermoelastic properties of

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polycrystalline materials given the single-crystal properties and crystallographic orientations of the grains. Previous work on the analysis of polycrystalline materials can be broadly classified into three categories, namely theoretical averaging methods, mean field theories and full-field methods. Examples of theoretical averaging methods include the Voigt [1] and the Reuss [2] methods which are based on the iso-strain and iso-stress assumptions, respectively. It has been shown that the Voigt and the Reuss methods provide upper and lower bounds, respectively, for the bulk elastic stiffnesses [3]. Various theoretical averaging schemes that lie between the two bounds have been proposed, including the Voigt-Reuss-Hill (VRH) arithmetic average [3,4] and the geometric mean [5]. Although these averages closely approximate laboratory-determined bulk elastic properties in some instances, they lack physical justification since they do not account for grain shapes, grain distributions or grain-to-grain interactions. Mean-field theories, such as the self-consistent method [6–9], were developed in an effort to better approximate the response of polycrystalline materials. In the self-consistent method, the average stresses within the grains are obtained by modeling each grain as a separate ellipsoidal inclusion that is embedded within a homogeneous equivalent medium with physical properties that correspond to that of the bulk polycrystalline material. Full-field methods have been developed for the simulation of microscale stress distributions since grain-scale stress concentrations can cause damage or crack initiation. In this context, the finite element (FE) method has been used for the stress analysis of computer-generated polycrystalline microstructures, such as 3D Voronoi polycrystals [10–13]. Numerical simulations of the brittle fracture of polycrystalline materials have been performed using advanced FE techniques and Voronoi microstructures [14,15]. Lebensohn [16] has developed a formulation based on the fast Fourier transform for the viscoplastic analysis of 3D polycrystals. Bishop et al. [17] have performed direct numerical simulations wherein polycrystalline microstructures were embedded throughout a macroscale structure.

Most polycrystalline materials exhibit a pattern of preferred orientations of the crystals, commonly referred to as texture or fabric. In the case of engineered materials, texture is the result of processing history whereas the texture of rocks is due to their natural evolution. It is well known that the texture of polycrystalline materials has a significant influence on bulk properties such as elastic modulus, thermal expansion coefficient, yield strength and fracture toughness. Currently available mainstream methods for collecting crystallographic orientation data can be classified into two distinct categories, namely macrotexture and microtexture techniques. Macrotexture techniques, such as X-ray goniometry and neutron diffraction, enable the determination of bulk texture [18]. They can provide useful information regarding the average orientation data for a large volume of a polycrystalline material. A disadvantage of macrotexture methods is that they cannot capture the detailed spatial variation of crystallographic orientation within a polycrystalline sample. Microtexture techniques, such as electron backscat-

ter diffraction (EBSD), allow for the measurement of the local orientations of the individual crystals within a polycrystalline sample. In recent years, EBSD has become the most popular technique for the measurement of local crystal orientations due to the availability of automated systems which can index patterns at sub-micron spatial resolutions [19,20]. It is now possible to generate detailed microstructural orientation and phase maps using EBSD and to identify individual grains using advanced post-acquisition data analysis software. Subsequently, the bulk properties of the polycrystalline sample can be calculated from the EBSD phase and orientation data using one of the available homogenization schemes. The Voigt, Reuss and VRH are the most widely used methods for the calculation of bulk properties from texture data due to their inherent simplicity and ease of implementation [4,21]. These averaging methods take into account the crystallographic orientations and phase modal fractions but they disregard the shapes and arrangement of the grains, two factors which have been shown to influence the bulk properties of polycrystalline materials [22,23]. Furthermore, these averaging methods are incapable of supplying information in regard to microscale stress and strain distributions induced by macroscale loads.

Numerical methodologies for the analysis of polycrystalline materials have been demonstrated on computer-generated Voronoi-microstructures [10–15]. Much progress has been made in recent years in developing methodologies for the simulation of realistic polycrystalline microstructures [24]. For example, Li et al. [25] have simulated the nano-indentation of polycrystalline aluminum using a Voronoi microstructure with crystallographic orientations imported from EBSD. Dunne et al. [26] reconstructed the grain morphology and crystallographic orientations of a small region of a nickel-base alloy from EBSD data and used it to perform crystal plasticity analyses. Schuh et al. [27] have developed a Monte Carlo method for the construction of physically realistic grain boundary networks. Simulated microstructures are useful for sensitivity studies that seek to understand the influence of microstructural variables on macroscale properties [23]. In light of the increasing use of automated EBSD systems for materials characterization, there is a need for robust methodologies for the detailed microstructural analysis of real polycrystalline material microstructures obtained from EBSD data. It is possible to analyze heterogeneous microstructures using a standard finite element formulation with either displacement or traction boundary conditions [11]. However, it has been shown that periodic boundary conditions exhibit faster convergence of bulk elastic stiffnesses than either displacement or traction boundary conditions [11,28]. Furthermore, the calculation of bulk elastic stiffnesses using displacement or traction boundary conditions necessitates the solution of multiple finite element models for prescribed displacements or unit loads.

Presented herein is a computational framework for the microstructural analysis of real polycrystalline materials that have been indexed using EBSD techniques. Smooth grain boundaries

are generated from the discretely sampled EBSD data points and microscale analyses are performed using asymptotic expansion homogenization (AEH) and the FE method. AEH is a rigorous multiscale technique for the detailed micromechanical analysis of heterogeneous materials in which the bulk properties and stress-strain distributions are obtained by solving the three-dimensional equilibrium equations at the microscale [29–31]. The AEH method explicitly accounts for the elastic interaction between microstructural heterogeneities and has previously been used for the analysis of fiber- and particle-reinforced composite materials [31–35], as well as the nonlinear creep of polyphase lithospheric rocks [36]. Here, the AEH method is used for the microstructural analyses of polycrystalline materials since it provides precise microscale stresses by taking into account the elastic interaction between anisotropic grains. The present formulation, which incorporates periodic boundary conditions, allows us to calculate the homogenized elastic stiffnesses of complex polycrystalline material microstructures accurately with fewer elements than either displacement or traction boundary conditions. The computational scheme presented here can be used to (1) perform comprehensive microstructural analysis of polycrystalline materials subjected to mechanical and thermal loads, (2) precisely calculate bulk thermoelastic properties, and (3) analyze complex microstructures using high-quality FE meshes that conform to the grain boundaries. In addition, a freely available software package for use by materials and Earth scientists has been developed for the analysis of polycrystalline microstructures based on the proposed methodology.

The AEH-FE methodology is demonstrated by considering an EBSD map of a rolled zinc specimen. After numerical convergence characteristics have been established, the bulk elastic moduli and thermal expansion coefficients are compared with the Voigt, Reuss, VRH and self-consistent methods. Next, the microstructural stress analysis procedure is illustrated using a duplex stainless steel sample. In the last example, we compute the seismic wave speeds and grain-scale stresses in a natural quartzite rock using macroscale loading conditions consistent with the published state of stress at depth adjacent to the San Andreas fault in California, USA.

2 Multiscale Analysis of Polycrystalline Materials

A formulation based on the AEH method [29–31] for the multiscale analysis of polycrystalline materials is presented in this section. Fig. 1(a) depicts a polycrystalline aggregate of macroscale dimension L . The response of the polycrystalline material at the microstructural level is studied using a representative volume element of size ℓ shown in Fig. 1(b). Although the AEH method is insensitive to the size of the representative volume element, i.e., it is scale-independent, it assumes a clear separation between the two length-scales with the ratio $\epsilon = \ell/L$ being much

less than unity. The AEH method assumes local periodicity of the heterogeneous material at the lower length scale [29].

Polycrystalline materials are composed of individual grains/crystallites of varying size, phase and crystallographic orientations (i.e., orientation of lattice planes relative to a fixed coordinate system). Grain boundaries represent the interfaces between adjacent grains whose misorientation (i.e., the difference in crystallographic orientation) exceeds a certain threshold angle. The individual grains and crystallographic orientations of a polycrystalline sample can be mapped using the EBSD technique (see Sec. 3).

The location of a point within the microstructure is specified using a y_1 - y_2 - y_3 analysis coordinate system as shown in Fig. 1(b). The orientation of the crystal at a point within the microstructure is specified by a local crystal coordinate system a - b - c whose orientation varies from grain to grain. The orientation of the crystal coordinate system relative to the analysis coordinate system is specified using three Euler angles that represent a set of rotations required to bring the y_1 - y_2 - y_3 coordinate system into coincidence with the a - b - c crystal coordinate system. While there exist several different definitions of Euler angles that are used in the physical sciences, the Bunge Euler angles $\{\varphi_1, \Phi, \varphi_2\}$ [37] are the most widely applied in texture analysis. The sequence of rotations in Bunge's description is 1) rotation by an angle φ_1 about the y_3 -axis, followed by 2) rotation Φ about the rotated y_1 -axis, and then 3) final rotation φ_2 about the rotated y_3 -axis. The angles φ_1 and φ_2 both range from 0 to 2π whereas Φ ranges from 0 to π .

The physical properties of crystallites, such as elastic stiffnesses and thermal expansion coefficients, are typically specified in the crystal coordinate system. In order to perform an analysis, the physical properties must first be transformed from the crystal coordinate system to the common analysis coordinate system using tensor transformation techniques (see Appendix A).

2.1 Microstructural analysis using the AEH method

The constitutive equation for a linear thermoelastic material can be expressed as follows [38]

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - \beta_{ij}T, \quad (1)$$

where σ_{ij} are the components of the Cauchy stress tensor, ε_{kl} are the components of the infinitesimal strain tensor, T is the temperature change from the stress-free reference configuration, C_{ijkl} are the components of the fourth-order elastic stiffness tensor and β_{ij} are the stress-temperature moduli which are related to the thermal expansion coefficients α_{ij} through the relationship $\beta_{ij} = C_{ijkl}\alpha_{kl}$. Lowercase Latin indices range over the values 1, 2, 3 and a repeated index implies summation over the range of the index. Due to the spatial variation of crystallographic orientations in a polycrystalline material, the elastic stiffnesses C_{ijkl} , thermal expansion

coefficients α_{ij} and stress-temperature moduli β_{ij} are in general functions of the spatial coordinates $\mathbf{y} = (y_1, y_2, y_3)$, i.e., $C_{ijkl} = C_{ijkl}(\mathbf{y})$, $\alpha_{ij} = \alpha_{ij}(\mathbf{y})$ and $\beta_{ij} = \beta_{ij}(\mathbf{y})$. It is assumed that the microstructure consists of grains that are perfectly bonded together with traction and displacement continuity across the grain-boundary interfaces between adjacent grains.

The displacement of a material point in a polycrystalline microstructure is decomposed into two parts: 1) a macroscale displacement that represents the average displacement of the entire microstructure, and 2) a superimposed microscale displacement fluctuation due to the elastic interaction between neighboring grains of different phase or crystallographic orientations. The displacement is then expressed as [29–31],

$$u_i(\mathbf{y}) = \bar{u}_i + \epsilon \hat{u}_i(\mathbf{y}) + O(\epsilon^2), \quad (2)$$

where $\bar{u}_i$ are the components of the average macroscale displacement and $\hat{u}_i(\mathbf{y})$ are the microscale displacement fluctuations. In the case of a linear thermoelastic material, the displacement fluctuations at a point are assumed to be proportional to the average macroscale strains $\bar{\varepsilon}_{kl}$ and average macroscale temperature change $\bar{T}$, and can be written as [39],

$$\hat{u}_i(\mathbf{y}) = \chi_i^{kl}(\mathbf{y})\bar{\varepsilon}_{kl} + \psi_i(\mathbf{y})\bar{T}, \quad (3)$$

where $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$ are position-dependent proportionality constants that are commonly referred to as the characteristic functions. The eighteen characteristic functions $\chi_i^{kl}(\mathbf{y})$ represent the microscale fluctuations in the displacement components u_i for a unit macroscale strain $\bar{\varepsilon}_{kl}$. Likewise, the three characteristic functions $\psi_i(\mathbf{y})$ represent the microscale fluctuations in the displacement components u_i for a unit temperature change.

Spatial differentiation of the microscale displacement field $u_i(\mathbf{y})$ in (2) with respect to coordinates $\mathbf{y}$ yields the following microscale infinitesimal strains $\varepsilon_{ij}(\mathbf{y})$ in the limit $\epsilon \rightarrow 0$:

$$\varepsilon_{ij}(\mathbf{y}) = \bar{\varepsilon}_{ij} + \frac{1}{2} \left(\frac{\partial \chi_i^{kl}(\mathbf{y})}{\partial y_j} + \frac{\partial \chi_j^{kl}(\mathbf{y})}{\partial y_i} \right) \bar{\varepsilon}_{kl} + \frac{1}{2} \left(\frac{\partial \psi_i(\mathbf{y})}{\partial y_j} + \frac{\partial \psi_j(\mathbf{y})}{\partial y_i} \right) \bar{T}. \quad (4)$$

The corresponding microscale stresses $\sigma_{ij}(\mathbf{y})$ are obtained using the constitutive equation (1) and microscale strains $\varepsilon_{ij}(\mathbf{y})$ from (4),

$$\sigma_{ij}(\mathbf{y}) = \left[C_{ijkl}(\mathbf{y}) + C_{ijpq}(\mathbf{y}) \frac{\partial \chi_p^{kl}(\mathbf{y})}{\partial y_q} \right] \bar{\varepsilon}_{kl} - \left[\beta_{ij}(\mathbf{y}) - C_{ijkl}(\mathbf{y}) \frac{\partial \psi_k(\mathbf{y})}{\partial y_l} \right] \bar{T}. \quad (5)$$

Insertion of (5) into the three-dimensional equilibrium equations $\partial \sigma_{ij}(\mathbf{y}) / \partial y_j = 0$ yields the following system of partial differential equations for the characteristic functions $\chi_i^{kl}(\mathbf{y})$ and

$\psi_i(\mathbf{y})$,

$$\frac{\partial}{\partial y_j} \left(C_{ijpq}(\mathbf{y}) \frac{\partial \chi_p^{kl}(\mathbf{y})}{\partial y_q} \right) = - \frac{\partial C_{ijkl}(\mathbf{y})}{\partial y_j}, \quad (6)$$

$$\frac{\partial}{\partial y_j} \left(C_{ijkl}(\mathbf{y}) \frac{\partial \psi_k(\mathbf{y})}{\partial y_l} \right) = \frac{\partial \beta_{ij}(\mathbf{y})}{\partial y_j}. \quad (7)$$

In the AEH method, the characteristic functions $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$ are subject to periodic boundary conditions.

The average macroscale stresses $\bar{\sigma}_{ij}$ are obtained by integrating the microscale stresses over the microstructural domain Y ,

$$\bar{\sigma}_{ij} = \frac{1}{|Y|} \int_Y \sigma_{ij}(\mathbf{y}) dY, \quad (8)$$

where $|Y|$ represents the volume of the microstructural domain. Substitution of the microscale stresses from (5) into (8) yields the following macroscale constitutive relation

$$\bar{\sigma}_{ij} = \bar{C}_{ijkl} \bar{\varepsilon}_{kl} - \bar{\beta}_{ij} \bar{T}, \quad (9)$$

where $\bar{C}_{ijkl}$ are the homogenized or effective elastic stiffnesses and $\bar{\beta}_{ij}$ are the homogenized stress-temperature moduli. The homogenized elastic stiffnesses and stress-temperature moduli are computed from the spatially varying elastic stiffnesses and characteristic functions as follows:

$$\bar{C}_{ijkl} = \frac{1}{|Y|} \int_Y \left(C_{ijkl}(\mathbf{y}) + C_{ijpq}(\mathbf{y}) \frac{\partial \chi_p^{kl}(\mathbf{y})}{\partial y_q} \right) dY, \quad (10)$$

$$\bar{\beta}_{ij} = \frac{1}{|Y|} \int_Y \left(\beta_{ij}(\mathbf{y}) - C_{ijkl}(\mathbf{y}) \frac{\partial \psi_k(\mathbf{y})}{\partial y_l} \right) dY. \quad (11)$$

Upon solving (6) and (7) for the characteristic functions $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$, the microscale strains $\varepsilon_{ij}(\mathbf{y})$, the microscale stresses $\sigma_{ij}(\mathbf{y})$, the homogenized elastic stiffnesses $\bar{C}_{ijkl}$ and the homogenized stress-temperature moduli $\bar{\beta}_{ij}$ of the polycrystalline material are determined using (4), (5), (10) and (11), respectively.

The AEH formulation presented in this section is applicable to arbitrary 3D microstructures. However, analysis of 3D microstructures requires the use of advanced mapping techniques, as well as significant computational resources for generating finite element meshes and solving full 3D models. For the purposes of our work, we consider 2D microstructures in which the grain boundaries are projected in the third direction in order to generate a 3D geometry. Consequently, the characteristic functions and thermomechanical fields do not vary in the third direction. By retaining all three components of the characteristic functions and restricting them

to vary in the y_1 - y_2 plane only, all nonzero components of the 3D homogenized thermoelastic properties can be computed using a 2D finite element model. In addition, microscale stress and strain distributions can be determined using (4) and (5), respectively, for prescribed macroscale strains and temperature change. In the case of prescribed macroscale stresses and temperature change, the macroscale strains $\bar{\varepsilon}_{kl}$ are first obtained from the homogenized stiffnesses $\bar{C}_{ijkl}$, stress-temperature moduli $\bar{\beta}_{ij}$ and the macroscale constitutive relations (9). Subsequently, the microscale stresses $\sigma_{ij}(\mathbf{y})$ are calculated using (5).

2.2 Finite Element Solution

In order to determine the homogenized stiffnesses $\bar{C}_{ijkl}$, the homogenized stress-temperature moduli $\bar{\beta}_{ij}$ and the microscale strains $\varepsilon_{ij}(\mathbf{y})$ and stresses $\sigma_{ij}(\mathbf{y})$, it is necessary to first solve (6) and (7) for the characteristic functions $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$. In the present work, the partial differential equations (6) and (7) are solved numerically using the FE method. We begin by multiplying (6) and (7) by test functions $v_i(\mathbf{y})$ and integrating over the microstructural domain Y to obtain the weak form of the partial differential equations for $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$,

$$\int_Y C_{ijpq}(\mathbf{y}) \frac{\partial \chi_p^{kl}(\mathbf{y})}{\partial y_q} \frac{\partial v_i(\mathbf{y})}{\partial y_j} dY = - \int_Y C_{ijkl}(\mathbf{y}) \frac{\partial v_i(\mathbf{y})}{\partial y_j} dY, \quad (12)$$

$$\int_Y C_{ijkl}(\mathbf{y}) \frac{\partial \psi_k(\mathbf{y})}{\partial y_l} \frac{\partial v_i(\mathbf{y})}{\partial y_j} dY = \int_Y \beta_{ij}(\mathbf{y}) \frac{\partial v_i(\mathbf{y})}{\partial y_j} dY. \quad (13)$$

The microstructural domain Y is discretized using an FE mesh of six-noded isoparametric triangular elements with quadratic shape functions (see Sec. 4). We choose the following FE discretization for the characteristic functions $\chi_i^{pq}(\mathbf{y})$ and $\psi_i(\mathbf{y})$, and test function $v_i(\mathbf{y})$,

$$[\chi_i^{kl}(\mathbf{y}), \psi_k(\mathbf{y}), v_i(\mathbf{y})] = N_a(\mathbf{y}) [d_{ai}^{kl}, g_{ak}, b_{ai}], \quad (14)$$

where $N_a(\mathbf{y})$ is the FE shape function (e.g. see [40]) corresponding to node $a = 1, \dots, 6$, and d_{ai}^{kl} , g_{ak} and b_{ai} are the nodal values of the functions $\chi_i^{kl}(\mathbf{y})$, $\psi_k(\mathbf{y})$ and $v_i(\mathbf{y})$, respectively. Substituting (14) into (12) and noting that the resulting equation must hold for all test functions $v_i(\mathbf{y})$ yields the linear system of equations

$$K_{PQ} d_Q^{kl} = F_P^{kl}, \quad (15)$$

where K_{PQ} and F_P^{kl} are referred to in FE terminology as the global stiffness matrix and global force vectors, respectively, and indices $P = ID(a, i)$ and $Q = ID(b, j)$ map the degree of freedom i and element node numbers a and b to their corresponding global equation number and

global degree of freedom, respectively. Equation (15) represents the assemblage of contributions from all elements in the FE mesh, i.e.,

$$K_{PQ} = \mathbf{A}_{e=1}^{N_e} \left[\mathbf{e}_i^T \left(\int_{Y^e} \mathbf{B}_a^T \mathbf{C} \mathbf{B}_b dY \right) \right] \mathbf{e}_j, \quad F_P^{kl} = \mathbf{A}_{e=1}^{N_e} \left[-\mathbf{e}_i^T \int_{Y^e} \mathbf{B}_a^T \mathbf{C}^{kl} dY \right]. \quad (16)$$

where $\mathbf{A}$ is the FE assembly operator [40], $\mathbf{C}$ is a 6×6 contracted matrix of elastic stiffnesses C_{ijkl} , $\mathbf{B}_a$ is a 6×3 matrix containing the spatial derivatives of the shape functions for node a [33], $\mathbf{e}_i$ are the unit normals in the i direction expressed as a 3×1 array, N_e is the number of elements in the mesh, and $\mathbf{C}^{kl}$ is the J^{th} column of $\mathbf{C}$; J being the contraction of kl .

Insertion of (14) into (13) and noting that the equation must hold for all test functions $v_i(\mathbf{y})$ yields the linear system of equations

$$K_{PQ} g_Q = H_P, \quad (17)$$

where the elements of the global stiffness matrix K_{PQ} are the same as in (16)₁, H_P are the elements of the global force vector,

$$H_P = \mathbf{A}_{e=1}^{N_e} \left[\mathbf{e}_i^T \int_Y \mathbf{B}_a^T \boldsymbol{\beta} dY \right]. \quad (18)$$

and $\boldsymbol{\beta} = [\beta_{11}, \beta_{22}, \beta_{33}, \beta_{23}, \beta_{13}, \beta_{12}]^T$ is a column array of stress-temperature moduli.

The nodal values d_{ai}^{kl} and g_{ak} are obtained by solving the linear systems of equations (15) and (17). The periodic boundary conditions are enforced using a mesh in which the boundary node locations are mirrored on the opposite edges of the domain and assigned the same node number and degrees of freedom. Since the periodicity conditions require that the nodal values d_{ai}^{kl} and g_{ak} be equal at all four corners, they are set equal to zero without loss of generality. The values of the characteristic functions $\chi_i^{kl}(\mathbf{y})$ and $\psi_i(\mathbf{y})$ at an arbitrary point $\mathbf{y}$ in the domain are obtained using the corresponding nodal values d_{ai}^{kl} and g_{ak} and the element shape functions $N_a(\mathbf{y})$ in (14). Subsequently, the characteristic functions are used to calculate the microscale strains, stresses and homogenized properties.

3 Microstructure characterization using EBSD

Electron backscatter diffraction is a scanning electron microscope (SEM) technique that is used for the identification of phase and crystallographic orientations of crystallites in a polycrystalline sample. The principal components of the system are shown in Fig. 2a. A polished sample is placed in the SEM chamber at a specific angle to the incident electron beam. The electrons

diffract through the crystal lattice planes and generate a number of bands on a phosphor screen. These bands, known as Kikuchi bands [41], form an EBSD pattern which, in principle, uniquely defines the identity and orientation of the diffracting crystal [19, 20, 42]. The EBSD pattern is recorded using a camera (typically equipped with a low-light charge-coupled device image sensor) and subsequently transferred to a computer where it is indexed and used to determine crystal orientations in the sample. Automated methods and predefined scanning grids can be used to rapidly collect EBSD patterns over sample microstructures. Indexing algorithms vary with manufacturer, but the end result is the same – determination of the phase and orientation of the crystal at each gridpoint, usually with an angular uncertainty $<1\%$. To improve the reliability of the indexing procedure, chemical data can be collected simultaneously with the backscatter diffraction patterns [43]. The chemical data are used to identify the phase and the diffraction pattern to determine the orientation. Some materials, such as most metals and the minerals quartz and olivine, index well, with success rates $>90\%$. Cleanup algorithms can correct mis- or unindexed points, which usually result from surface blemishes or, in geological materials, difficulty in discriminating between orientations of low-symmetry phases with similar EBSD patterns. The goal of all cleanup procedures is to more accurately reproduce the microstructure, yet the operator must take care not to overcorrect the analytical results by using cleanup procedures too aggressively.

Once the EBSD phase and orientation data have been collected over a predefined scanning grid, they are rendered in the SEM display view after correcting for the tilt of the sample. The coordinates (x_{pix}, y_{pix}) of an EBSD sampling point are specified relative to the top left corner of the image in the SEM display view, as shown in Fig. 2b. The orientation of the crystal coordinate system at each EBSD sampling point is specified relative to a sample coordinate system denoted by R - T - N , where R represents the reference direction, T the transverse direction and N the normal direction. The crystal orientations are specified using the Bunge Euler angles $\{\varphi_1, \Phi, \varphi_2\}$ which represent a set of rotations required to bring the R - T - N sample reference coordinate system into coincidence with the a - b - c crystal coordinate system (the so-called *passive* description). Upon completion of an EBSD scan, a data file is created which contains the three Euler angles $(\varphi_1, \Phi, \varphi_2)$, the spatial coordinates (x_{pix}, y_{pix}) and phase number for each EBSD sampling point, as shown in Fig. 2c.

In most EBSD systems, the N -axis is oriented normal to the surface of the sample and the R - T axes lie in the plane of the sample. In general, the R - T - N sample reference coordinate system need not coincide with the y_1 - y_2 - y_3 analysis coordinate system described earlier in Sec. 2. In the present work, we denote the orientation of the R -axis relative to the horizontal (y_1) axis in the plane of the sample by the angle Θ . The default value of Θ for EBSD systems is typically $0^\circ, 90^\circ, 180^\circ$ or 270° , although it can be user-defined if necessary. At each EBSD

sampling point the thermoelastic properties in the analysis coordinate system are obtained from the properties in the crystal coordinate system through tensor transformation (see Appendix A).

4 Numerical Implementation

Since the AEH method is scale-independent (see Sec. 2), we normalize the y_1 -coordinates of EBSD sample points so that they range from 0 to 1 and scale the y_2 -coordinates in order to preserve the initial aspect ratio of the EBSD map. Normalization of the sample coordinates simplifies certain aspects of the numerical implementation, such as grain boundary smoothing and meshing routines.

4.1 Grain Boundary Smoothing

In our analyses, we smooth coarse (i.e., pixelated) EBSD grain boundaries for the following reasons. Firstly, pixelated boundaries produce artificial stress concentrations that are absent in natural or engineered microstructures (e.g., stress concentrations along straight inclined boundaries). Smooth grain boundaries relieve these stress concentrations to an extent (while maintaining those which actually exist in locations such as triple junctions) and therefore appear to more accurately represent grain boundaries in actual rocks, metals, and other materials. Secondly, many elements are typically needed in an FE mesh in order to discretize pixelated grains due to the large number of corners. Since computation time and required memory increase with the number of elements in the FE mesh, pixelated grain boundaries can inhibit the analyses of larger microstructures containing many grains.

We have developed a computational technique that uses radial basis functions (RBFs) and contouring routines to smooth pixelated grain boundaries. For an EBSD map of pixelated data, grains are initially defined as sets of contiguous pixels with the same phase and orientation. In the process of isolating the individual grains, we locate points within the domain where more than two grain boundaries intersect (e.g., triple junctions), and any points along the domain edges that are shared by two or more grain boundaries. These points are needed in order to match element nodes on opposite boundaries of the domain for the enforcement of periodicity. Since the regions defining grains are initially sets of contiguous pixels, their boundaries are represented by polygons with pixelated edges (see grain A in Fig. 3a). Without significantly altering their areas, we smooth the polygonal boundaries using a contouring method which employs RBFs. In essence, a grid of points is first created over the microstructural domain. For a given polygonal grain, points which lie on the interior are assigned a value of unity, points which lie outside are assigned a value of zero and points at triple junctions are assigned a value

of $1/2$. RBFs are then constructed in order to generate a surface plot by interpolating values on a denser grid of points (see Fig. 3b). Contouring routines are subsequently used to determine the contour which has a value of $1/2$, and this contour is taken as the smooth grain boundary. As shown in Fig. 3c, the resulting smooth grain boundary passes through any triple-junction points that exist along the original pixelated boundary. Once each grain has been considered, neighboring grain boundaries are matched in order to remove any existing overlaps and voids. The smooth grain boundaries thus obtained pass between EBSD sampling points of neighboring grains and are relatively insensitive to the exact choice of smoothing parameters. The degree to which the smoothing process represents the true grain boundaries depends on the spatial resolution of the EBSD analysis. Higher resolution data will lead to a better approximation, but also to increased time and computational resources.

4.2 Finite Element Mesh Generation

We have developed a Delaunay triangulation algorithm that can generate FE meshes for complex polycrystalline microstructures. The goal of the algorithm is to 1) generate elements whose edges conform to grain boundaries, 2) capture fine features of arbitrary grain shapes, and 3) achieve high-quality elements which vary in size throughout the mesh. We have employed an adapted version of the meshing routine DISTMESH2D, developed by Persson and Strang [44].

In the finite element analyses presented in this paper, both conforming and nonconforming meshes are used. Conforming meshes preserve the discontinuous boundaries between neighboring grains, while nonconforming meshes do not. However, both types of meshes have their advantages. Conforming meshes typically allow for accurate calculation of homogenized material properties, as well as stress and strain distributions, with fewer elements than nonconforming meshes. However, creating conforming meshes for large microstructures with many grains requires significant computational resources, and therefore nonconforming meshes may provide a more reasonable alternative. Nonconforming meshes can be created easily by constructing a grid of triangular elements and subsequently determining which grains the element centroids lie within. Conforming meshes require the identification of grain boundaries before the insertion of finite elements. Our method for creating conforming meshes is described below.

In order to capture the fine details of a polycrystalline domain using finite elements, as well as produce a periodic mesh that conforms to grain boundaries, it is first necessary to construct a mesh size function [76]. Once constructed, the mesh size function returns the appropriate element size (i.e., lengths of its edges) based on the grain geometry in the polycrystalline domain at any desired location. We generate our mesh size functions using an adapted version of the meshing software DISTMESH2D [76]. Two contributing factors are considered when constructing the mesh size function, namely, the curvature of the grain boundaries and the medial

axes of the grains. Consideration of these factors allows us to capture fine features such as thin geometrical sections and grain boundaries exhibiting significant curvature. Upon determining the curvatures of grain boundaries and their medial axes, a gradient limiting technique is used to smooth the mesh size function and enforce periodicity on the polycrystalline domain edges. A more thorough explanation regarding mesh size functions can be found in Persson [76]. Once it is determined, the mesh size function is applied in order to generate an initial distribution of nodes from which a crude preliminary mesh is constructed (see Fig. 3d). DISTMESH2D is then used to create an intermediate nonuniform mesh that does not yet conform to grain boundaries (Fig. 3e). The purpose of the intermediate mesh is to distribute element nodes appropriately based on the variation of the mesh size function throughout the polycrystalline domain. An adapted version of DISTMESH2D is then used iteratively to create a conforming mesh by collectively meshing all grains while at the same time matching nodes along the boundaries of neighboring grains, as well as those which lie along the domain edges. The iterative process continues until all elements within the domain attain sufficient quality based on their edge lengths, or until the user ends the process manually. As shown in Fig. 3f, the resulting mesh conforms to the grain boundaries and captures the fine features of the material geometry. Furthermore, the mesh is periodic along the polycrystalline domain edges. Once the conforming mesh is constructed, nodes are inserted at element edge midpoints in order to generate 6-noded triangular elements.

5 Results and discussion

Our implementation of the AEH-FE method has been validated in prior studies in which the homogenized thermoelastic properties were found to be in good agreement with experimental data for random two-phase material systems [33] and fiber-reinforced composites [35, 45]. In addition, microscale stress distributions compared well with those obtained using other numerical techniques [35, 45, 46]. The aforementioned studies were limited to computer-generated microstructures composed of two-phase isotropic or transversely isotropic constituents. In the present work, the AEH-FE methodology has been extended to the homogenization and stress analysis of real polycrystalline microstructures determined using EBSD. The AEH-FE homogenized thermoelastic properties are compared with those obtained using the Voigt, Reuss, VRH and self-consistent methods. In addition, grain-scale stress distributions are presented for prescribed macroscale mechanical and thermal loads. Details of the different analytical homogenization methods and their application to polycrystalline materials are given in Appendix B.

EBSD crystal orientation maps presented in this section have been obtained using the

EDAX-TSL EBSD detector on the Tescan Vega II Scanning Electron Microscope located at the School of Earth and Climate Sciences at the University of Maine. Diffraction patterns were recorded at a working distance of 25 mm using a 20 kV acceleration voltage and a ~ 11 nA beam current with the beam striking the uncoated sample at an incident angle of 20° . The patterns were processed using EDAX-TSL OIM Data Collection 5 software. A post-acquisition cleanup procedure was employed to accurately identify phases, optimize the quality of the orientation data, and prepare the dataset for numerical analysis. Individual grains were identified based on phase information and a misorientation angle threshold of 10° at grain boundaries.

5.1 Convergence study and comparison with analytical homogenized properties for a rolled zinc sheet

In this section, we investigate convergence characteristics of the AEH-FE method using the EBSD map of a rolled zinc sample. We have chosen to study zinc because of its highly-anisotropic elastic and thermal expansion properties. Zinc monocrystals exhibit hexagonal symmetry about their c -axes and have 5 independent elastic constants [47,48] with the following values: $C_{11} = C_{22} = 158.25$ GPa, $C_{33} = 61.6$ GPa, $C_{12} = 31.51$ GPa, $C_{13} = C_{23} = 47.44$ GPa, $C_{44} = C_{55} = 40.0$ GPa and $C_{66} = (C_{11} - C_{12})/2 = 63.37$ GPa [49–51]. The independent thermal expansion coefficients are $\alpha_1 = \alpha_2 = 14.1 \times 10^{-6}/^\circ C$ and $\alpha_3 = 63.9 \times 10^{-6}/^\circ C$ [52]. After establishing convergence of the AEH-FE homogenized properties, we compare the results with those determined using the Voigt, Reuss, VRH, and self-consistent estimates.

The zinc sample used in our study was taken from a hot-rolled zinc sheet purchased from McMaster-Carr (Robbinsville, NJ; Part No: 1007T11). The sample was first polished to remove any pre-existing surface deformations and scratches. Next, a $1000 \mu\text{m} \times 1000 \mu\text{m}$ region was indexed in a square grid pattern using a step size of $1 \mu\text{m}$. The resulting EBSD map contains approximately one million data points arranged in a square grid pattern with a total of 6,071 distinct grains identified in post-acquisition cleanup. The inverse pole figure map for the sample, along with the R and T directions for the Euler angles, are shown in Fig. 4a. The rolling direction of the zinc sample coincides with the horizontal (y_1) axis while the direction transverse to rolling coincides with the vertical (y_2) axis. The equal area, lower hemisphere discrete pole figure of the c -axis is shown in Fig. 4b. The pole figure map is qualitatively similar to previously published data [53] for rolled zinc samples.

FE analyses of EBSD maps which contain many grains (e.g., Fig. 4a) require significant computational effort in order to generate meshes that conform to grain boundaries. Furthermore, resulting meshes contain a large number of elements, making it computationally expensive to assemble and solve the resulting global system of equations (16). Therefore, we start by considering a small portion of the larger EBSD map and perform a convergence study using

conforming meshes. Later, we will present an efficient strategy for the analysis of larger EBSD maps. We consider a $400\ \mu\text{m} \times 400\ \mu\text{m}$ cropped region, shown in Fig. 5a, taken from the center of the larger map in Fig. 4a. Fig. 5b shows the inverse pole figure map of the cropped region with a single average orientation assigned to each grain. The cropped region has a total of 818 grains. The individual grains and their smoothed boundaries are shown in Fig. 5c in which different colors are used solely to distinguish different grains and have no special significance. A finite element mesh containing 36,302 elements was generated for the microstructure shown in Fig. 5c, a small portion of which is magnified and displayed in Fig. 5d. In what follows, we define the mesh density by the average number of elements per grain, i.e., the total number of elements N_e divided by the total number of grains N_g . By this definition, the representative mesh in Fig. 5d has a density of $N_e/N_g \simeq 44$ elements/grain.

For the cropped zinc map shown in Fig. 5b, we perform a series of analyses using increasingly finer meshes and plot AEH-FE homogenized properties as functions of the mesh density N_e/N_g . The convergence of Young's moduli E_1 and E_2 , shear modulus G_{12} and thermal expansion coefficient α_1 are shown in Fig. 6. The homogenized properties converge fairly rapidly and are found to be within 0.5% of their respective converged values at a mesh density of approximately 8 elements/grain. Table 1 lists the converged homogenized properties along with the corresponding analytical estimates. As expected, the VRH and self-consistent properties are closer to the AEH-FE values than either the Voigt or the Reuss bounds.

The Young's modulus parallel to the rolling direction ($E_1 = 110.6$ GPa) is found to be lower than the Young's modulus transverse to the rolling direction ($E_2 = 117.2$ GPa). This apparent anisotropy is consistent with previously published experimental and analytical values for rolled zinc sheets [54], and can be attributed to the rolling texture. The degree of anisotropy typically depends on the amount of deformation (i.e., thickness reduction) achieved during the rolling process. It is instructive to study the directional dependence of the homogenized Young's modulus and thermal expansion coefficient in the plane of the rolled zinc sample. The directional Young's modulus is computed using the expression $E_\theta = 1/S_{11}(\theta)$ where $\mathbf{S}(\theta)$ is the rotated compliance tensor in a coordinate system whose 1-axis is oriented at an angle θ to the rolling direction in the plane of the sample (see Fig. 5b). As depicted in Fig. 7a, the AEH-FE value of E_θ lies between those of the VRH and self-consistent estimates for all values of θ , decreasing slightly from the initial value of E_1 at $\theta = 0^\circ$ and then gradually increasing until a value of E_2 is reached at $\theta = 90^\circ$. Values of E_θ determined using the Reuss, VRH and self-consistent estimates exhibit a similar decrease at low angles whereas the value obtained using the Voigt estimate appears to increase monotonically.

The directional thermal expansion coefficient α_θ is plotted in Fig. 7b as a function of θ . The directional thermal expansion coefficient α_θ decreases with increasing angle θ , consistent with

previously published experimental data for rolled zinc alloy samples [55]. The AEH-FE and self-consistent methods exhibit a similar variation of α_θ vs. angle θ although the AEH-FE value is approximately 3% larger than the self-consistent value. The thermal expansion coefficient α_1 in the rolling direction obtained using the Reuss average is 10.4% larger than the Voigt average (see Table 1). However, in the case of the transverse thermal expansion coefficient α_2 , the Reuss average is 2.4% smaller than the Voigt average. This phenomenon can be attributed to the texture of the rolled zinc sample since it is not observed when the crystallographic orientations of the crystallites are randomized. The reversal in the Voigt and Reuss averages is reflected in the directional thermal expansion coefficient α_θ (Fig. 7b). Dunn and Ledbetter have observed that in certain cases the Reuss average for the thermal expansion coefficient is larger while in other cases the Voigt average is larger. As such, the Voigt and Reuss averages do not provide upper and lower bounds for the thermal expansion coefficients. Rigorous bounds for the thermal expansion coefficients have been presented by Rosen and Hashin [56] and Gibiansky and Torquato [57].

As mentioned previously for EBSD maps containing many grains, the generation of a finite element mesh that conforms to the grain boundaries can be a time consuming process. Therefore, it is advantageous to develop a method that uses a non-conforming mesh to compute the homogenized properties. In order to assess the accuracy of AEH-FE results obtained using a non-conforming mesh, we consider the cropped zinc map shown in Fig. 5b with a single average crystallographic orientation assigned to each grain. We use a structured triangular mesh to discretize the analysis domain as shown in Fig. 8a. Since the mesh does not conform to grain boundaries, the triangular elements generally contain EBSD data points from different grains. Therefore, we first perform an element-level homogenization using one of the analytical schemes such as the VRH estimate. The homogenized properties obtained for each element are assigned to all quadrature points within the element. Subsequently, the AEH-FE method is used to compute the homogenized properties of the entire map. The homogenized Young's modulus E_1 , shear modulus G_{12} and thermal expansion coefficient α_1 obtained using the aforementioned procedure are shown in Fig. 8b-d, as functions of the mesh density for different element-level homogenization schemes. It is found that the homogenized properties computed using a non-conforming mesh and the VRH or self-consistent element-level homogenization schemes converge towards the corresponding AEH-FE values obtained earlier using a conforming mesh. However, more elements are required in the non-conforming mesh in order to achieve the same accuracy as the conforming mesh. The non-conforming mesh with VRH element-level homogenization converges faster than any of the other element-level homogenization methods. These results demonstrate that it is possible to obtain accurate homogenized properties using a non-conforming mesh and an appropriate element-level homogenization method. Having es-

tablished the convergence characteristics of a non-conforming mesh using the cropped zinc map in Fig. 5b with a single average orientation assigned to each grain, we use the same procedure to study convergence in the case of EBSD data points that have the original crystallographic orientations (see Fig. 5a). The converged results for both conforming and non-conforming meshes are listed in Table 2 along with analytical estimates. It is observed that the homogenized properties for the case of original crystallographic orientations are in good agreement with those obtained for a single average crystallographic orientation per grain (cf. Table 1).

In our next study, we examine the influence of EBSD map size on the homogenized properties by performing a series of analyses on portions of the large zinc map shown in Fig. 4a. We start with a small $100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$ cropped region at the center of the map (i.e., region A in Fig. 9a) and increase both the width and height of the region in increments of $100\text{ }\mu\text{m}$ all the way up to the full $1000\text{ }\mu\text{m} \times 1000\text{ }\mu\text{m}$ map shown as region E in Fig. 9a. In each analysis, the original crystallographic orientations at data points are used and a non-conforming mesh with a density of ~ 50 elements/grain is generated. The Young's modulus E_1 and thermal expansion coefficient α_1 are plotted in Fig. 9b and Fig. 9c vs. the number of grains in each of the cropped regions. It is found that roughly 1,400 grains are needed to obtain homogenized properties that are within 1% of their respective converged values listed in Table 3.

5.2 Stress analysis of a duplex stainless steel specimen

In this next example, we use the AEH-FE method to perform stress analyses on a sample of 2205 duplex stainless steel for prescribed macroscopic loads. The nominal chemical composition of the sample is 21%-23% chromium, 4.5%-6.5% nickel, 2.5%-3.5% molybdenum with other alloying elements such as manganese and nitrogen. The stainless steel sample has a two-phase microstructure consisting of nearly equal proportions of austenite and ferrite. Austenite has a face-centered cubic crystal structure while ferrite has a body-centered cubic crystal structure. The thermoelastic properties of ferrite and austenite monocrystals are listed in Table 4 [58]. Due to the directional-dependence of the elastic properties, cubic materials are generally anisotropic even though the properties normal to the three crystal symmetry planes are identical. The degree of anisotropy is usually characterized by the Zener index $A = 2C_{44}/(C_{11} - C_{12})$ [59]. By definition, the Zener index equals unity for an isotropic material. The austenite and ferrite phases are considered highly anisotropic since their Zener indices are 3.77 and 2.41, respectively.

The 2205 duplex stainless steel sample used in our study has been taken from a hot-rolled sheet purchased from McMaster-Carr (Robbinsville, NJ; Part No: 3623T33). After polishing a portion of the sheet, a $400\text{ }\mu\text{m} \times 400\text{ }\mu\text{m}$ region of the sheet was indexed in a square grid pattern using a step size of $1\text{ }\mu\text{m}$. The inverse pole figure and lower hemisphere discrete pole

figure maps are shown in Fig. 10a with a single average orientation assigned to each grain. Fig. 10b displays a phase map containing grains with smoothed boundaries. Grain interiors are shaded based on their phases and Euler angles. The volume fractions of ferrite and austenite in the indexed region are 50.5% and 49.5%, respectively. Using a 10° misorientation threshold, the resulting EBSD map contains a total of 1,402 grains. The converged thermoelastic properties for the duplex stainless steel sample have been determined through a series of AEH-FE analyses and are listed in Table 5 along with the Voigt, Reuss, VRH, and self-consistent approximations. It is found that the Voigt approximation significantly overestimates the AEH-FE elastic properties while the Reuss approximation significantly underestimates the properties. However, the VRH and self-consistent approximations are in reasonable agreement with the AEH-FE values. The AEH-FE Young's modulus in the rolling direction $E_1 = 199.0$ GPa is in good agreement with the published value of $E = 200$ GPa at 20°C [60]. The AEH-FE Young's modulus in the transverse direction $E_2 = 211.0$ GPa is larger than E_1 due to the rolling texture. It is also found that the AEH-FE Poisson's ratio $\nu_{12} = 0.2933$ and shear modulus $G_{12} = 76.74$ GPa are in good agreement with the published values of $\nu = 0.3$, $G = E/[2(1 + \nu)] = 76.9$ GPa.

We now use the AEH-FE method to perform elastic stress analyses on the 2205 duplex stainless steel sample for prescribed macroscale mechanical and thermal loads. Convergence of the microscale stresses is first determined by applying an average macroscale axial tensile stress of $\bar{\sigma}_{11} = 1$ MPa. We track the microscale normal stress $\sigma_{11}(\mathbf{y})$ and shear stress $\sigma_{12}(\mathbf{y})$ at points A and B shown in Fig. 10b as the mesh is refined and plot the values as functions of the mesh density (see Fig. 11). It is observed that the stresses converge when the mesh density exceeds roughly 100 elements/grain. For the mesh containing 180,600 elements with a density of 130 elements/grain, the distributions of microscale normal stress $\sigma_{11}(\mathbf{y})$ and shear stress $\sigma_{12}(\mathbf{y})$ are plotted in Fig. 12a and Fig. 12b, respectively. It is found that the peak value of $\sigma_{11}(\mathbf{y})$ can be as high as 2.1 times the macroscale value $\bar{\sigma}_{11}$. Next, we consider the distributions in microscale stresses for a macroscale temperature change of $\Delta T = 1^\circ\text{C}$. In this case, the macroscale deformation of the polycrystalline sample is unconstrained and free to expand in all directions. This is achieved by setting the macroscale stresses $\bar{\sigma}_{ij}$ equal to zero. The amplified microscale deformation of the sample due to the temperature increase is shown in Fig. 13a. The warping of the boundaries can be attributed to microstructural heterogeneities and the anisotropic properties of ferrite and austenite. The corresponding distribution of microscale normal stress $\sigma_{11}(\mathbf{y})$ is depicted in Fig. 13b. Since the thermal expansion coefficient of austenite is greater than ferrite, and the grain boundaries are assumed to be perfectly bonded, a temperature increase induces a dominantly compressive stress in the austenite grains while inducing a dominantly tensile stress in the ferrite grains. The peak microscale stresses $\sigma_{11}(\mathbf{y})$ in austenite and ferrite are 2.87 MPa and 2.70 MPa, respectively, while the average values

in austenite and ferrite are -1.04 MPa and 1.06 MPa, respectively. The distributions of microscale normal stress $\sigma_{22}(\mathbf{y})$ and shear stress $\tau_{12}(\mathbf{y})$ are shown in Fig. 13c and Fig. 13d, respectively. The phase averaged normal stress σ_{22} and shear stress τ_{12} in the austenite and ferrite are of opposite signs since the prescribed macroscale normal stress $\bar{\sigma}_{22}$ and shear stress $\bar{\tau}_{12}$ are zero. The mismatch in thermal expansion coefficients of austenite and ferrite, coupled with the crystallographic orientations and phase geometry, produces relatively large microscale stresses in the duplex stainless steel sample.

5.3 Analysis of natural quartzite microstructure

In this final example, we demonstrate that the AEH-FE computational framework can be used to study seismic wave propagation and determine grain-scale stress distributions in natural polycrystalline materials. A sample of quartzite rock, collected from the Norumbega fault system in Maine, USA, is considered. The Norumbega represents the roots of a right-lateral, large displacement, strike-slip fault system that was active until approximately 290 million years before present [61]. Exhumation and erosion of the fault system have since exposed rocks that were deformed at temperatures greater than approximately 300 degrees C, above which quartz deforms by viscous creep mechanisms. The Norumbega shows abundant evidence of seismogenic history [62, 63], and it represents an excellent ancient analog for the San Andreas fault system in California, USA, with similar kinematics [64] and dimensions [65]. The sample comes from the Sandhill Corner shear zone [63, 64], which is the largest strand of the Norumbega system. A $904 \mu\text{m} \times 588 \mu\text{m}$ region of the polished quartzite rock was indexed in a square grid pattern using a step size of $2 \mu\text{m}$. After cleanup, the resulting EBSD map contains 2,959 quartz grains, each of which was assigned a single average crystallographic orientation. The orientation map and pole figure are shown in Fig. 14a and Fig. 14b, respectively.

Single-crystal α -quartz exhibits trigonal symmetry with 6 independent elastic constants [48, 66]. The density and elastic stiffnesses for α -quartz are assumed to be $\rho = 2648.5 \text{ kg/m}^3$, $C_{11} = C_{22} = 86.8 \text{ GPa}$, $C_{33} = 105.75 \text{ GPa}$, $C_{12} = 7.04 \text{ GPa}$, $C_{13} = C_{23} = 11.91 \text{ GPa}$, $C_{44} = C_{55} = 58.2 \text{ GPa}$, $C_{14} = C_{56} = -18.04 \text{ GPa}$, $C_{24} = -C_{14} \text{ GPa}$, $C_{66} = (C_{11} - C_{12})/2 = 39.88 \text{ GPa}$ [67]. As evidenced by the directional Young's modulus plot in Fig. 14c, single-crystal α -quartz is moderately anisotropic due to its trigonal crystal structure. The maximum and minimum directional Young's moduli for quartz are 130 GPa and 70 GPa, respectively.

Seismic wave propagation is strongly influenced by the mineralogy and microstructure of rocks [23, 68, 69]. Since the wave length of seismic waves is larger than the microstructural dimensions of rocks, it is possible to analyze seismic wave propagation in the Earth's crust by using the homogenized elastic stiffnesses and densities of its constituents. The seismic wave

speeds are computed using the Christoffel equation [70],

$$\det[\bar{C}_{ijkl}n_jn_l - \bar{\rho}V^2\delta_{ik}] = 0, \quad (19)$$

where $\bar{C}_{ijkl}$ are the homogenized elastic stiffnesses, $\bar{\rho}$ is the homogenized density, n_i are the components of the unit vector $\mathbf{n}$ which define the wave propagation direction, and V is the wave speed. The Christoffel equation (19) yields three real wave speeds [71], namely a quasi P wave denoted by V_P and two quasi S waves denoted by V_{S1} and V_{S2} ($V_{S1} > V_{S2}$). The quasi P wave corresponds to the longitudinal mode of vibration while the two quasi S waves correspond to transverse shear modes. In the case of an elastically anisotropic rock, the P and S wave speeds depend on the propagation direction $\mathbf{n}$. For the quartzite sample shown in Fig. 14a, the AEH-FE bulk elastic stiffnesses $\bar{C}_{ijkl}$ are calculated using (10) and the corresponding wave speeds are shown as functions of propagation direction in Fig. 15a-c. The longitudinal wave speed varies from $V_P^{\min} = 5.62$ km/s to $V_P^{\max} = 6.29$ km/s. The resulting seismic anisotropy $AV_P = [(V_P^{\max} - V_P^{\min}) / 0.5(V_P^{\max} + V_P^{\min})] \times 100\%$ is found to be 11.2%. The seismic anisotropy can be attributed to the crystallographic preferred orientation and elastic stiffnesses of the quartz grains. The two quasi S waves also exhibit directional dependence. The shear wave split time, defined as $\Delta t_S = 1/V_{S2} - 1/V_{S1}$, measures the difference in arrival times of the two S waves per unit propagation distance. Shear wave splitting is recognized by seismologists as an important indicator of seismic anisotropy. The directional dependence of the shear wave split time is shown in Fig. 15d.

In the next study, we analyze the grain-scale stress distributions in the quartzite sample (Fig. 14a) for loading conditions consistent with the state of stress at depth adjacent to the San Andreas fault. The effective macroscale normal and shear stresses on a plane parallel to the fault, as well as the inclination of the maximum principal direction to the fault strike, were reported by Townend [72] for a depth of 7.5 km. Using these values and the corresponding hydrostatic pressure, the nonzero macroscale ambient stresses in the analysis reference frame are estimated to be $\bar{\sigma}_{11} = -173.6$ MPa, $\bar{\sigma}_{22} = -360$ MPa, $\bar{\sigma}_{12} = 90$ MPa, and $\bar{\sigma}_{33} = -130$ MPa, corresponding to principal stresses of $\bar{\sigma}_1^p = -130$ MPa, $\bar{\sigma}_2^p = -137$ MPa and $\bar{\sigma}_3^p = -396.4$ MPa (see Fig. 16). For these loading conditions, an AEH-FE stress analysis is performed using a conforming finite element mesh with 346,438 elements. As shown in Fig. 17a, the resulting distribution of longitudinal stress σ_{11} parallel to the fault is compressive throughout the sample and varies from -298 MPa to -32.2 MPa. The peak value of the microscale shear stress τ_{12} (Fig. 17b) is 186 MPa, which is roughly double the corresponding macroscale value of 90 MPa. It is observed that the microscale principal stress σ_1^p is tensile in some grains, even though all three macroscale principal stresses are compressive (see Fig. 17c). The maximum microscale shear stress $\tau_{\max} = (\sigma_1^p - \sigma_3^p)/2$, shown in Fig. 17d, attains a peak value that is nearly twice

the corresponding macroscale value of 133.2 MPa. At the scale of individual grains, tensile principal stresses and large shear stresses have important implications as they can cause brittle damage through microfracturing. This is especially true during coseismic events that introduce large dynamic stresses to the ambient state [73, 74].

6 Toolbox for the analysis of polycrystalline microstructures

The AEH-FE methodology presented here is useful for accurately calculating the homogenized elastic and thermal properties of polycrystalline materials and computing distributions in strains and stresses. However, numerical implementation of the mathematical formulation is elaborate and time consuming. Therefore, we have developed a freely-available software package using Matlab which allows researchers to more conveniently study polycrystalline materials using the AEH-FE framework. The front-end of the software package is a stand-alone Matlab-based graphical user interface (GUI). The GUI offers users a number of analysis tools while at the same time providing simplicity and ease of use (see Fig. 18). Users can perform analyses on polycrystalline samples in order to (1) determine homogenized, i.e., effective elastic and thermal properties, (2) compute effective wavespeeds and plot directional distributions using equal-area projections and 3D spheres, and (3) visualize detailed distributions of stresses and strains via contour plots. In the current version of the software, the user can provide an EBSD data file with extension .ang or .ctf containing data point coordinates, Bunge Euler angles, and phase numbers for a polycrystalline sample. Alternatively, the user can provide an indexed grayscale or true color image of a computer-generated or natural microstructure in one of several different image formats. For each phase in the sample, the user should provide a formatted text file containing the phase density, elastic stiffnesses and thermal expansion coefficients. Once the EBSD data file or image is loaded into the GUI, the user can assign the appropriate property file to each phase in the microstructure. After meshing the microstructure using our adapted version of DISTMESH2D [76], the user can run the AEH homogenization analysis to obtain the effective material properties and plot the microscale stresses and strains for prescribed macroscale loads. In addition to EBSD microstructures, it is possible to analyze computer-generated microstructures, such as those obtained using Voronoi tessellation, by sampling the microstructure using a fine rectangular grid and subsequently importing the data into the GUI. The software package and a user manual are currently available for download at the following address: <http://umaine.edu/mecheng/faculty-and-staff/senthil-vel/software/>

7 Conclusions

We have developed a robust numerical methodology for the thermomechanical analysis of textured polycrystalline materials using asymptotic expansion homogenization and finite element analysis. The methodology can be used to perform comprehensive microscale stress-strain analyses and to accurately compute bulk thermoelastic properties of real polycrystalline material microstructures obtained using EBSD techniques. We have developed a specialized meshing algorithm that can generate high-quality conforming meshes, allowing for the finite element analysis of complex polycrystalline microstructures.

The methodology has been demonstrated by considering EBSD maps of zinc, duplex stainless steel, and natural quartzite. In the analyses of zinc and stainless steel, the Young's moduli in the direction transverse to the rolling direction were found to be greater than the Young's moduli parallel to the rolling direction. The homogenized properties of zinc and stainless steel were both found to be in good agreement with their corresponding published values. In the zinc analysis, it was shown that the homogenized properties calculated using a nonconforming mesh approached the converged values for a conforming mesh as the number of elements was increased. As such, a nonconforming mesh can be used instead of a conforming mesh if the nonconforming mesh contains a sufficient number of elements. Nonconforming meshes may be more practical when analyzing EBSD maps containing a large number of grains since the generation of conforming meshes requires increased computational resources. In the analysis of duplex stainless steel, the Voigt and Reuss approximations were found to significantly overestimate and underestimate the AEH-FE homogenized properties, respectively. Therefore, for certain microstructures, the Voigt and Reuss approximations do not provide accurate representations of the material properties. In the microscale stress analysis of stainless steel subjected to a unit temperature increase, significant compressive and tensile stresses were induced in the austenite and ferrite phases, respectively, due to the mismatch in thermal expansion coefficients. The natural quartzite sample, when subjected to macroscale compressive loads in all three principal directions, displayed microscale tensile stresses in certain grains. Large grain-scale tensile stresses could facilitate inelastic deformation mechanisms such as microfracture-driven damage, and may contribute to the initial stage of failure leading to earthquakes.

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Appendix A: Tensor Transformation of Thermoelastic Properties

In order to perform thermomechanical analyses of polycrystalline materials, the elastic stiffnesses and thermal expansion coefficients must first be transformed from the crystal coordinate system to a common analysis coordinate system. In what follows, we use the contracted notation to represent the elastic stiffness tensor and thermal expansion coefficients [48]. The elastic stiffnesses and thermal expansion coefficients in the crystal coordinate system are represented by the 6×6 matrix $\mathbf{C}_c$ and 6×1 column array $\boldsymbol{\alpha}_c = [\alpha_{11}, \alpha_{22}, \alpha_{33}, 2\alpha_{23}, 2\alpha_{13}, 2\alpha_{12}]^T$, respectively.

The orientation of the crystal coordinate system relative to the sample coordinate system is specified using three Bunge Euler angles $\{\varphi_1, \Phi, \varphi_2\}$. They represent a set of rotations required to bring the R - T - N sample coordinate system into coincidence with the a - b - c crystal coordinate system. The direction cosines matrices for the three successive rotations are,

$$\mathbf{a}_{\varphi_1} = \begin{bmatrix} \cos \varphi_1 & \sin \varphi_1 & 0 \\ -\sin \varphi_1 & \cos \varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{a}_{\Phi} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{bmatrix}, \mathbf{a}_{\varphi_2} = \begin{bmatrix} \cos \varphi_2 & \sin \varphi_2 & 0 \\ -\sin \varphi_2 & \cos \varphi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A1})$$

The overall direction cosines matrix $\mathbf{a}$ for the transformation of physical properties from the crystal coordinate system to the sample coordinate system is,

$$\begin{aligned} \mathbf{a} &= (\mathbf{a}_{\varphi_2} \mathbf{a}_{\Phi} \mathbf{a}_{\varphi_1})^{-1} = \mathbf{a}_{\varphi_1}^T \mathbf{a}_{\Phi}^T \mathbf{a}_{\varphi_2}^T \\ &= \begin{bmatrix} \cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \varphi_2 - \sin \varphi_2 \cos \varphi_2 \cos \Phi & \sin \varphi_1 \sin \Phi \\ \sin \varphi_1 \cos \varphi_2 + \cos \varphi_1 \sin \varphi_2 \cos \Phi & -\sin \varphi_1 \sin \varphi_2 + \cos \varphi_1 \cos \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \Phi \\ \sin \varphi_2 \sin \Phi & \cos \varphi_2 \sin \Phi & \cos \Phi \end{bmatrix}. \end{aligned} \quad (\text{A2})$$

The elastic stiffnesses $\mathbf{C}_s$ and thermal expansion coefficients $\boldsymbol{\alpha}_s$ in the sample coordinate systems are obtained using Bond matrices $\mathbf{M}$ and $\mathbf{N}$ [75],

$$\mathbf{C}_s = \mathbf{M} \mathbf{C}_c \mathbf{M}^T, \quad \boldsymbol{\alpha}_s = \mathbf{N} \boldsymbol{\alpha}_c, \quad (\text{A3})$$

where $\mathbf{M}$ and $\mathbf{N}$ are 6×6 matrices that are constructed from the direction cosines matrix $\mathbf{a}$ [71].

In general, the R - T - N sample reference coordinate system need not coincide with the y_1 - y_2 - y_3 analysis coordinate system (see Sec. 3). In most EBSD systems the R - T axes lie in the plane of the sample with the R -axis oriented at an angle Θ relative to the horizontal (y_1) axis (see Fig. 2). A second transformation is required to obtain the elastic stiffnesses $\mathbf{C}$ and thermal expansion coefficients $\boldsymbol{\alpha}$ in the analysis coordinate system,

$$\mathbf{C} = \hat{\mathbf{M}} \mathbf{C}_s \hat{\mathbf{M}}^T, \quad \boldsymbol{\alpha} = \hat{\mathbf{N}} \boldsymbol{\alpha}_s, \quad (\text{A4})$$

where the Bond matrices $\hat{\mathbf{M}}$ and $\hat{\mathbf{N}}$ are constructed from the direction cosines matrix $\hat{\mathbf{a}}$ which relates the sample and analysis coordinate systems,

$$\hat{\mathbf{a}} = \begin{bmatrix} \cos \Theta & -\sin \Theta & 0 \\ \sin \Theta & \cos \Theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A5})$$

Appendix B: Analytical Averaging Methods and the Self-Consistent Scheme

In this appendix we provide an overview of commonly used analytical schemes for the homogenization of bulk thermoelastic properties of polycrystalline materials. The microstructure is assumed to contain N grains and the volume fraction of grain r is denoted by $V^{(r)}$. The elastic stiffnesses, thermal expansion coefficients and stress-temperature moduli of the r^{th} grain are denoted by $\mathbf{C}^{(r)}$, $\boldsymbol{\alpha}^{(r)}$ and $\boldsymbol{\beta}^{(r)}$, respectively.

B1. Voigt average

The Voigt average [1] is based on the assumption that the microstructural strains in all grains are identical to the macroscale strains, i.e. $\boldsymbol{\epsilon}^{(r)} = \bar{\boldsymbol{\epsilon}}$. The following expressions for the homogenized stiffnesses and stress-temperature moduli are obtained by volumetrically averaging the microscale stresses $\boldsymbol{\sigma}^{(r)} = \mathbf{C}^{(r)}\bar{\boldsymbol{\epsilon}}$ and relating them to the macroscale strains and temperature change,

$$\mathbf{C}^V = \sum_{r=1}^N V^r \mathbf{C}^{(r)}, \quad \boldsymbol{\beta}^V = \sum_{r=1}^N V^r \boldsymbol{\beta}^{(r)}. \quad (\text{B1})$$

The Voigt average for the thermal expansion coefficients are obtained from the elastic stiffnesses and stress-temperature moduli using the expression $\boldsymbol{\alpha}^V = (\mathbf{C}^V)^{-1} \boldsymbol{\beta}^V$.

B2. Reuss average

The Reuss average [2] is based on the iso-stress assumption. The microstresses $\boldsymbol{\sigma}^{(r)}$ are assumed to be constant throughout the microstructural domain and equal to the macroscale average stresses $\bar{\boldsymbol{\sigma}}$. The Reuss estimates for the elastic compliances and thermal-expansion coefficients are obtained by averaging the microscale strains and relating them to the average stresses and temperature change,

$$\mathbf{S}^R = \sum_{r=1}^N V^{(r)} \mathbf{S}^{(r)}, \quad \boldsymbol{\alpha}^R = \sum_{r=1}^N V^{(r)} \boldsymbol{\alpha}^{(r)}, \quad (\text{B2})$$

where $\mathbf{S}^{(r)} = (\mathbf{C}^{(r)})^{-1}$ are the elastic compliances of the grains. The Reuss estimates for the elastic stiffness tensor and stress-temperature moduli are $\mathbf{C}^R = (\mathbf{S}^R)^{-1}$ and $\boldsymbol{\beta}^R = \mathbf{C}^R \boldsymbol{\alpha}^R$, respectively.

B3. Voigt-Reuss-Hill average

The Voigt-Reuss-Hill estimates are obtained by averaging the Voigt and Reuss elastic stiffnesses and thermal expansion coefficients as follows [3, 4, 52],

$$\begin{aligned} \mathbf{C}^{VRH} &= \frac{1}{2}(\mathbf{C}^V + \mathbf{C}^R), \\ \boldsymbol{\alpha}^{VRH} &= \frac{1}{2}(\boldsymbol{\alpha}^V + \boldsymbol{\alpha}^R). \end{aligned} \quad (\text{B3})$$

B4. Self-consistent scheme

The self-consistent scheme is a mean-field approach in which each individual grain is modeled as a separate inclusion that is embedded within a homogeneous equivalent medium whose properties correspond to that of the bulk polycrystalline aggregate. When the polycrystalline aggregate is subjected to a homogeneous macroscale strain field $\boldsymbol{\varepsilon}_0$, the average microscale strains $\boldsymbol{\varepsilon}^{(r)}$ for the r^{th} grain are formally related to the macroscale strain field through the following localization relations,

$$\boldsymbol{\varepsilon}^{(r)} = \mathbf{A}^{(r)} \boldsymbol{\varepsilon}_0, \quad (\text{B4})$$

where $\mathbf{A}^{(r)}$ is the mechanical strain concentration tensor [77]. The average strains $\bar{\boldsymbol{\varepsilon}}$ for the polycrystalline aggregate are obtained by volumetric averaging of the strains over all grains,

$$\bar{\boldsymbol{\varepsilon}} = \sum_{r=1}^N V^{(r)} \boldsymbol{\varepsilon}^{(r)} = \left[\sum_{r=1}^N V^{(r)} \mathbf{A}^{(r)} \right] \boldsymbol{\varepsilon}_0. \quad (\text{B5})$$

The average stresses $\bar{\boldsymbol{\sigma}}$ for the polycrystalline aggregate are obtained by volumetrically averaging the average the stresses $\boldsymbol{\sigma}^{(r)} = \mathbf{C}^{(r)} \mathbf{A}^{(r)} \boldsymbol{\varepsilon}_0$ over all grains,

$$\bar{\boldsymbol{\sigma}} = \sum_{s=1}^N V^{(s)} \boldsymbol{\sigma}^{(s)} = \left[\sum_{s=1}^N V^{(s)} \mathbf{C}^{(s)} \mathbf{A}^{(s)} \right] \boldsymbol{\varepsilon}_0. \quad (\text{B6})$$

Substitution of $\boldsymbol{\varepsilon}_0$ from (B5) into (B6) yields the following relationship between the average stresses $\bar{\boldsymbol{\sigma}}$ and average strains $\bar{\boldsymbol{\varepsilon}}$,

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbf{C}} \bar{\boldsymbol{\varepsilon}},$$

where $\bar{\mathbf{C}}$ is the the bulk stiffness tensor for the polycrystalline aggregate,

$$\bar{\mathbf{C}} = \left[\sum_{s=1}^N V^{(s)} \mathbf{C}^{(s)} \mathbf{A}^{(s)} \right] \left[\sum_{r=1}^N V^{(r)} \mathbf{A}^{(r)} \right]^{-1}. \quad (\text{B7})$$

Levin [78], Rosen and Hashin [56] and Hashin [79] derived general expressions for the bulk thermal expansion coefficients of polycrystalline aggregates which can be expressed in terms of the strain concentration tensor as follows,

$$\bar{\boldsymbol{\alpha}} = (\bar{\mathbf{C}})^{-1} \sum_{r=1}^N V^{(r)} (\mathbf{A}^{(r)})^T \mathbf{C}^{(r)} \boldsymbol{\alpha}^{(r)}. \quad (\text{B8})$$

It is possible to evaluate the bulk stiffness tensor $\bar{\mathbf{C}}$ and the bulk thermal expansion coefficients $\bar{\boldsymbol{\alpha}}$ using (B7) and (B8) if the average strain concentration tensor $\mathbf{A}^{(r)}$ is known. In the self-consistent scheme the strain concentration tensor is obtained by modeling each grain as an ellipsoidal inclusion that is embedded within an infinite homogeneous equivalent medium with

elastic stiffnesses $\bar{\mathbf{C}}$ and thermal expansion coefficients $\bar{\boldsymbol{\alpha}}$. It has been shown that the strain concentration tensor can be obtained explicitly for ellipsoidal inclusions [9, 80],

$$\mathbf{A}^{(r)} = [\mathbf{I} + \mathbf{P}(\mathbf{C}^{(r)} - \bar{\mathbf{C}})]^{-1}, \quad (\text{B9})$$

where $\mathbf{P}$ is the Hill tensor [81], $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the identity tensor and δ_{ik} is the Kronecker delta. In the present work, we idealize each grain as a spherical single-crystal inclusion. The components of the Hill tensor are obtained through an integration over a unit sphere [82, 83],

$$P_{ijkl} = \frac{1}{4\pi} \int_{|\mathbf{x}|=1} \Gamma_{ijkl}(\mathbf{x}) da = \frac{1}{4\pi} \int_0^\pi \left(\sin \theta \int_0^{2\pi} \Gamma_{ijkl}(\mathbf{x}) d\phi \right) d\theta, \quad (\text{B10})$$

where

$$\Gamma_{ijkl}(\mathbf{x}) = \frac{1}{4} ([\mathbf{K}^{-1}(\mathbf{x})]_{ik}x_jx_l + [\mathbf{K}^{-1}(\mathbf{x})]_{jk}x_ix_l + [\mathbf{K}^{-1}(\mathbf{x})]_{il}x_jx_k + [\mathbf{K}^{-1}(\mathbf{x})]_{jl}x_ix_k), \quad (\text{B11})$$

$x_1 = \sin \theta \cos \phi$, $x_2 = \sin \theta \sin \phi$, $x_3 = \cos \theta$ and $K_{pq}(\mathbf{x}) = \bar{C}_{pqkl}x_jx_l$ is the acoustic tensor. In the present work, the components of the Hill tensor P_{ijkl} are obtained numerically [84] by evaluating the double integral in (B10) using 32-point Gaussian quadrature [85].

We use an iterative solution process to calculate the bulk stiffness tensor $\bar{\mathbf{C}}$ since the strain concentration tensor $\mathbf{A}^{(r)}$ depends on $\bar{\mathbf{C}}$. We begin the iterative solution process using a trial value for $\bar{\mathbf{C}}$. In the present work, we use the VRH stiffness tensor $\mathbf{C}^{VRH}$ as the trial value. The Hill tensor $\mathbf{P}$ is evaluated numerically using (B10) and (B11). Next, the strain concentration tensor $\mathbf{A}^{(r)}$ is obtained for all grains using (B9) and the bulk elastic stiffness tensor $\bar{\mathbf{C}}$ and thermal expansion coefficients $\bar{\boldsymbol{\alpha}}$ are updated using (B7) and (B8). The updated bulk elastic stiffness tensor $\bar{\mathbf{C}}$ is used as the initial value in the next iteration. The process is repeated until the bulk elastic stiffness tensor $\bar{\mathbf{C}}$ and thermal expansion coefficients $\bar{\boldsymbol{\alpha}}$ converge. The final converged values are taken to be the self-consistent stiffness tensor $\mathbf{C}^{SC}$ and self-consistent thermal expansion coefficients $\boldsymbol{\alpha}^{SC}$ of the polycrystalline aggregate.

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FIGURE CAPTIONS

Fig. No.	Title
1.	Schematic of a bulk polycrystalline aggregate and a polycrystalline material element consisting of a representative microstructure obtained using EBSD. The polycrystalline microstructure consists of four mineral phases shown in yellow, red, blue and green with different shades used to represent different crystallographic orientations.
2.	(a) Principal components of an SEM-EBSD system, (b) SEM display view of a polycrystalline sample and $R-T-N$ sample coordinate system, and (c) EBSD data file with Euler angles, spatial coordinates and phase information for each sampling point.
3.	Procedure for generating a finite element mesh which conforms to grain boundaries: (a) initial pixelated grain boundary, (b) radial basis function surface plot generated by assigning unity to points inside grain A and zero to points outside, (c) smoothed grain boundary, (d) mesh generated using initial distribution of nodes, (e) intermediate non-conforming mesh containing elements with sizes computed using mesh size function, and (f) final conforming mesh.
4.	(a) EBSD inverse pole figure map and (b) equal area lower hemisphere pole figures for the c -axis of the zinc map shown in (a).
5.	(a) 400x400 EBSD inverse pole figure map for a rolled zinc sheet, (b) inverse pole figure map with a single average orientation assigned to each grain, (c) smoothed grain boundaries, and (d) a magnified view of elements in a representative finite element mesh that conforms to grain boundaries.
6.	Convergence of homogenized properties vs. number of elements per grain using a conforming mesh for a 400x400 zinc map, (a) Young's modulus E_1 , (b) Young's modulus E_2 , (c) shear modulus G_{12} , and (d) thermal expansion coefficient α_1 .
7.	Directional variation of (a) Young's modulus E_θ and (b) thermal expansion coefficient α_θ vs. angle θ for the 400x400 zinc map shown in Fig. 6b.
8.	Convergence of homogenized properties vs. number of elements per grain using a regular non-conforming mesh for a 400x400 zinc map, (a) representative mesh (800 triangular elements), (b) Young's modulus E_1 , (b) shear modulus G_{12} and (d) thermal expansion coefficient α_1 .
9.	Convergence of homogenized properties with increasing image size using a regular non-conforming mesh for a zinc map, (a) full map with boxed sections showing different image sizes, (b) Young's modulus E_1 , (c) shear modulus G_{12} and (d) thermal expansion coefficient α_1 .

10. 2205 Stainless steel sample: (a) EBSD inverse pole figure map and equal area lower hemisphere pole figures for the c -axis of austenite and ferrite phases, and (b) phase map showing individual grains of varying color based on Euler angles.
11. Convergence of microscale stresses at two points for a macroscopic stress of $\sigma_{11} = 1$ MPa: (a) microscale stress σ_{11} at **A**, (b) microscale stress σ_{11} at **B**, (c) microscale stress τ_{12} at **A**, and (d) microscale stress τ_{12} at **B**.
12. Converged microscale stress distributions a) σ_{11} and b) τ_{12} for a macroscopic stress of $\bar{\sigma}_{11}=1$ MPa.
13. Thermal stress analysis for 1 deg temperature change: (a) amplified deformed shape, (b) microstress σ_{11} , (c) microstress σ_{22} , and (c) microstress τ_{12} .
14. (a) EBSD inverse pole figure for the quartzite sample, (b) equal area lower hemisphere pole figures of the c -axis of α -quartz and (c) directional Young's modulus for single-crystal α -quartz .
15. Equal area wave speed plots for quartzite sample. (a) V_P , (b) V_{S1} , (c) V_{S2} and (d) Δt_s .
16. Map-view orientations of macroscale principal stresses at a point near the San Andreas Fault and the stresses in the analysis coordinate system.
17. Resulting grain-scale stress distributions in the quartzite sample for the San Andreas ambient stress state: (a) normal stress σ_{11} , (b) shear stress τ_{12} , (c) principal stress σ_1^p , and (d) maximum shear stress $\tau_{\max}$.
18. AEH-EBSD Toolbox graphical user interface.

Figure 1

Fig. 1. (a) Schematic of a bulk polycrystalline aggregate and (b) a polycrystalline material element consisting of a representative microstructure obtained using EBSD. The polycrystalline microstructure consists of four mineral phases shown in yellow, red, blue and green with different shades used to represent different crystallographic orientations.

Figure 2

Fig.2. (a) Principal components of an SEM-EBSD system, (b) SEM display view of a polycrystalline sample and $R-T-N$ sample coordinate system, and (c) EBSD data file with Euler angles, spatial coordinates and phase information for each sampling point.

Figure 3

Fig. 3. Procedure for generating a finite element mesh which conforms to grain boundaries: (a) initial pixelated grain boundary, (b) radial basis function surface plot generated by assigning unity to points inside grain **A** and zero to points outside, (c) smoothed grain boundary, (d) mesh generated using initial distribution of nodes, (e) intermediate nonconforming mesh containing elements with sizes computed using mesh size function, and (f) final conforming mesh.

Figure 4

Fig. 4. (a) EBSD inverse pole figure map and (b) equal area lower hemisphere pole figures for the c -axis of the zinc map shown in (a).

Figure 5

Fig. 5. (a) 400x400 EBSD inverse pole figure map for a rolled zinc sheet, (b) inverse pole figure map with a single average orientation assigned to each grain, (c) smoothed grain boundaries, and (d) a magnified view of elements in a representative finite element mesh that conforms to grain boundaries.

Figure 6

Fig. 6. Convergence of homogenized properties vs. number of elements per grain using a conforming mesh for a 400x400 zinc map, (a) Young's modulus E_1 , (b) Young's modulus E_2 , (c) shear modulus G_{12} , and (d) thermal expansion coefficient α_1 .

Figure 7

Fig. 7. Directional variation of (a) Young's modulus E_θ and (b) thermal expansion coefficient α_θ vs. angle θ for the 400x400 zinc map shown in Fig. 6b.

Figure 8

Fig. 8. Convergence of homogenized properties vs. number of elements per grain using a regular non-conforming mesh for a 400x400 zinc map, (a) representative mesh (800 triangular elements), (b) Young's modulus E_1 , (c) shear modulus G_{12} , and (d) thermal expansion coefficient α_1 .

Figure 9

Fig. 9. Convergence of homogenized properties with increasing image size using a regular non-conforming mesh for a zinc map, (a) full map with boxed sections showing different image sizes, (b) Young's modulus E_1 , and (c) thermal expansion coefficient α_1 .

Figure 10

Fig. 10. Stainless steel sample: (a) EBSD inverse pole figure map and equal area lower hemisphere pole figures for the c -axis of austenite and ferrite phases, and (b) phase map showing individual grains of varying color based on Euler angles.

Figure 11

Fig. 11. Convergence of microscale stresses at two points for a macroscopic stress of $\sigma_{11} = 1$ MPa: (a) microscale stress σ_{11} at **A**, (b) microscale stress σ_{11} at **B**, (c) microscale stress τ_{12} at **A**, and (d) microscale stress τ_{12} at **B**.

Figure 12

Fig. 12. Converged microscale stress distributions a) σ_{11} and b) τ_{12} for a macroscopic stress of $\bar{\sigma}_{11}=1$ MPa.

Figure 13

Fig. 13. Thermal stress analysis for 1 deg temperature change: (a) amplified deformed shape, (b) microstress σ_{11} , (c) microstress σ_{22} , and (c) microstress τ_{12} .

Figure 14

Fig. 14. (a) EBSD inverse pole figure for the quartzite sample, (b) equal area lower hemisphere pole figures of the c -axis of α -quartz and (c) directional Young's modulus for single-crystal α -quartz .

Figure 15

Fig. 15. Equal area wave speed plots for quartzite sample. a) V_p , b) V_{s1} , c) V_{s2} , and d) Δt_s .

Figure 16

Fig. 16. Map-view orientations of macroscale principal stresses at a point near the San Andreas Fault and the stresses in the analysis coordinate system.

Figure 17

Fig. 17. Resulting grain-scale stress distributions in the quartzite sample for the San Andreas ambient stress state: (a) normal stress σ_{11} , b) shear stress τ_{12} , c) principal stress σ_1^p , and d) maximum shear stress $\tau_{\max}$.

Figure 18

Fig. 18. AEH-EBSD Toolbox graphical user interface.

Table 1

Method	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	α_1 (10^{-6} K $^{-1}$)	α_2 (10^{-6} K $^{-1}$)
AEH	110.6	117.2	47.42	26.47	23.74
Voigt	118.1 (6.8%)	124.8 (6.5%)	51.45 (8.5%)	25.00 (5.6%)	23.60 (0.6%)
Reuss	101.4 (8.3%)	107.0 (8.7%)	42.64 (10%)	27.60 (4.3%)	23.03 (3.0%)
VRH	109.8 (0.7%)	116.1 (0.9%)	47.04 (0.8%)	26.30 (0.6%)	23.31 (1.8%)
Self-consistent	111.9 (1.2%)	118.2 (0.9%)	48.13 (1.5%)	25.67 (3.0%)	23.20 (2.3%)

Table 1: Effective properties of 400x400 zinc map with one orientation per grain and a conforming mesh. Values in parentheses denote percentage differences from AEH result.

Table 2

Method	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	α_1 ($10^{-6}/\text{K}$)	α_2 ($10^{-6}/\text{K}$)
AEH conforming ($N_E=44,118$)	110.6	117.2	47.40	26.47	23.75
AEH nonconforming ($N_E=115,200$)	110.6	117.1	47.42	26.46	23.76
Voigt	118.1	124.8	51.44	25.00	23.61
Reuss	101.4	107.0	42.62	27.61	23.04
VRH	109.8	116.0	47.03	26.31	23.33
Self-Consistent	111.8	118.2	48.11	25.68	23.21

Table 2: Effective properties of 400x400 zinc map with original orientations.

Table 3

Method	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	α_1 ($10^{-6}/\text{K}$)	α_2 ($10^{-6}/\text{K}$)
AEH (276,768 elements)	112.7	115.7	47.63	25.98	23.93
Voigt	119.6	123.9	51.63	24.74	23.69
Reuss	104.1	105.5	42.82	26.85	23.47
VRH	111.9	114.9	47.23	25.79	23.58
Self-consistent	113.8	117.1	48.31	25.26	23.40

Table 3: Effective properties for a 1000x1000 zinc map using a non-conforming mesh.

Table 4

Material	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	$\alpha_1 (\times 10^{-6} \text{ K}^{-1})$
Austenite	204.6	137.7	126.2	18.0
Ferrite	236.9	140.6	116.0	12.4

Table 4: Monocrystal thermoelastic properties of austenite and ferrite

Table 5

Method	$E_1(\text{GPa})$	$E_2(\text{GPa})$	$E_3(\text{GPa})$	$G_{12}(\text{GPa})$	$G_{13}(\text{GPa})$	$\alpha_1(10^{-6} \text{ K}^{-1})$	$\alpha_2(10^{-6} \text{ K}^{-1})$	$\alpha_3(10^{-6} \text{ K}^{-1})$
AEH	199.0	211.0	208.1	76.74	82.30	15.11	15.28	15.13
Voigt	222.9	233.8	227.1	87.94	92.03	15.11	15.11	15.11
Reuss	172.7	182.4	177.1	65.50	68.45	15.22	15.22	15.22
VRH	198.3	208.6	202.5	76.72	80.24	15.17	15.17	15.17
Self-consistent	200.8	212.3	205.3	77.91	81.97	15.18	15.18	15.18

Table 5: Effective properties for a 400x400 steel map.