A virtual environment for the interrogation of 3D polycrystalline microstructure including grain size effects

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Abstract

A finite element analysis of the large deformation of three-dimensional polycrystals is presented using pixel-based finite elements as well as finite elements conforming with grain boundaries. The macroscopic response is obtained through volume-averaging laws. A constitutive framework for elasto-viscoplastic response of single crystals is utilized along with a fully-implicit Lagrangian finite element algorithm for modeling microstructure evolution. The effect of grain size is included by considering a physically motivated measure of lattice incompatibility which provides an updated shearing resistance within grains. A domain decomposition approach is adopted for parallel computation to allow efficient large scale simulations. Conforming grids are adopted to simulate flexible and complex shapes of grains. The computed mechanical properties of polycrystals are shown to be consistent with experimental results for different grain sizes.

Key words: Polycrystal Plasticity; Constitutive model; Homogenization; Grain size effect; Finite element method

1 Introduction

Material properties of polycrystalline materials are highly dependent on the underlying microstructural features. Quantitative description of plastic flow by crystallographic slip is a long standing problem in microstructure evolution theories [1]. The thermo-mechanical description of polycrystals is usually

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based on analysis on the macro- and meso-scales. The macro-scale is associated with the homogenized continuum and the meso-scale is characterized by the underlying microstructure. Since rate-dependent methods are computationally intensive, recent work emphasizes the use of rate-independent models [1,2]. Taylor-type transition models have been considered extensively [3–6] by assuming that all grains are subjected to the same deformation. This assumption satisfies compatibility but fails to account for equilibrium across grain boundaries. It poses a stringent kinematic constraint on the grains and thus provides a stiff response. The anisotropic response of the grains to the deformation is not taken into account in the Taylor model. In order to correct this inaccuracy, the overall response of the microstructure at the macro-scale is derived in this work on the basis of homogenization [7], which assumes homogeneous deformation on the boundaries of the microstructure while allowing for non-uniform deformation within the microstructure [8]. This approach is further improved here to allow interrogation of complex 3D microstructures using single-crystal constitutive models [9] and mechanical property calculation through volume-averaging laws.

While the homogenization method allows for heterogeneous deformation inside the microstructure, it does not include the effect of the interactions between neighboring grains. In single crystal and polycrystalline materials exposed to plastic deformation, a dominant source of resistance to deformation is the dislocation density. The evolution of dislocation density is controlled by an additive combination of an athermal hardening component and a dynamic recovery component [10]. In continuum theory of crystal plasticity [11–14], the lattice is assumed to distort only elastically though generally elastic deformation is not compatible with single-valued displacement field. Thus, lattice incompatibility is characterized by the elastic component of the deformation gradient [15]. Grain size effect is included by considering the lattice incompatibility which is closely related to the dislocation density in the grains. In recent work [15–19], a grain size effect model based on dislocation density was developed for mechanical response simulation. We follow a similar approach here with some distinct differences: (a) a rate-independent model is used to accelerate the computational efficiency of the methodology, (b) Voronoi tessellation techniques are implemented for modeling of realistic microstructures with finite elements that conform with grain boundaries instead of pixel elements that are assigned orientations to mimic grains, (c) we simulate varying mean sizes of grains by adjusting the number of grains in a fixed region rather than changing the size of the calculation region, and (d) this work includes the elastic component of the deformation gradient and models incompatibility effects at initial yield and the major portion of the elasto-plastic transition [17]. To allow efficient interrogation of realistic 3D polycrystalline microstructures, domain decomposition algorithms are also considered.

The structure of the paper is as follows. Section 2 introduces the homoge-
nization method and Section 3 provides a summary of the constitutive model considered. The grain size model is reviewed in Section 4. The results obtained from the present computational framework are summarized in Section 5 where both numerical results and experimental data from the literature are used to verify the methodology. The paper concludes in Section 6 with a summary of the developments.

2 Microstructure homogenization method

The approach adopted here for interrogation of microstructures involves finite element based elasto-visco-plastic analysis of microstructures using a constitutive model derived from the continuum slip theory. In this section, the microstructure interrogation and property evaluation scheme is systematically developed using the theory of non-linear homogenization.

Let $y : \mathcal{B}_{\text{ref}} \rightarrow \mathcal{B}$ represent the non-linear deformation map of the microstructure at time $t$, and $F = \nabla_{\text{ref}} y$ the associated tangent map (Fig. 1). $F$ maps points $Y \in \mathcal{B}_{\text{ref}}$ onto points $y(Y, t)$ of the current configuration $\mathcal{B}$. The reference microstructure configuration is considered of volume $V(\mathcal{B}_{\text{ref}})$ and boundary $\partial \mathcal{B}_{\text{ref}}$ with outward normal $\mathbf{N}$. The microstructure at time $t$ of volume $V(\mathcal{B})$ and boundary $\partial \mathcal{B}$ with outward normal $\mathbf{n}$ is attached to the material point $X$ in the macro-continuum. Further, we use superposed bars (e.g. $\bar{F}$) to denote homogenized quantities and angular brackets (e.g. $\langle F \rangle$) to denote volume-averaged quantities.

Fig. 1. The microstructure homogenization technique: Each integration point in the macro-continuum is associated with an underlying microstructure. The microstructure reference configuration ($\mathcal{B}_{\text{ref}}$) and the mapping to the present microstructure configuration ($\mathcal{B}$) are shown in contrast with the homogenized macro-continuum.

The deformation gradient at the macro-scale is represented purely in terms of
the motion of the exterior boundary of the microstructure [7],

$$\bar{F} = \frac{1}{V(B_{ref})} \int_{\partial B_{ref}} y \otimes N dA. \quad (1)$$

The deformation of the microstructure is then related to the homogenized deformation gradient in the macro-continuum based on the assumption,

$$y = \bar{F}Y + \tilde{w}, \quad (2)$$

where the deformation consists of a homogeneous part $\bar{F}Y$ and an inhomogeneous part $\tilde{w}$ referred to as the fluctuation field. As a consequence, we have the relationship, $F = \bar{F} + \tilde{F}$ (with $\tilde{F} = \nabla \tilde{w}$) between the microscopic ($F$) and the macroscopic ($\bar{F}$) deformation gradients. From the homogenization law (Eq. (1)) and the decomposition described above, it can be shown that the superposed field $\tilde{w}$ follows the equation

$$\frac{1}{V(B_{ref})} \int_{\partial B_{ref}} \tilde{w} \otimes N dA = 0. \quad (3)$$

This is satisfied by homogeneous deformation on the boundaries of the microstructure while allowing for non-uniform deformations within the microstructure.

To macroscopic Cauchy stress $\bar{T}$ is taken as a volume-averaged (in the current configuration) of the microstructural counterpart $T$ as follows:

$$\bar{T} = \langle T \rangle = \frac{1}{V(B)} \int_{V(B)} T dV. \quad (4)$$

Alternative stress averaging laws are discussed in [8]. Finally, the equivalent stress for the microstructure in terms of the deviatoric average stress $\bar{T}'$ is computed as

$$\bar{\sigma}_{eff} = \sqrt{\frac{3}{2} \bar{T}' \cdot \bar{T}'}.$$

A multiplicative decomposition, $F = F^e F^p$, is used, where $F^e$ and $F^p$ are the micro-scale elastic and plastic deformation gradients, respectively. A total Lagrangian approach is utilized. An equilibrium state of the microstructure at a certain stage of the deformation process is then assumed with the equations,

$$\nabla_{ref} \cdot P = 0 \text{ in } B_{ref}, \quad (6)$$

$$P^T N = p \text{ on } \partial B_{ref}. \quad (7)$$
The Newton Raphson method is adopted to solve the deformation governing equation. The total Lagrangian algorithm is adopted to implement the integration equation such that

$$\int_{B_0} dP_{ik} \frac{\partial \tilde{u}_i}{\partial X_k} dV_0 = - \int_{B_0} P_{ik} \frac{\partial \tilde{u}_i}{\partial X_k} dV_0.$$  (8)

The tangent moduli (effectively the relation between $dP$ and $du$) are computed from the linearization of the constitutive model described in the next section. The derivation of the tangent moduli follows similar calculations as in [8].

The equivalent strain is computed with the volume-average of the plastic deformation rate following the constitutive laws originally developed in [9]. The plastic velocity gradient is defined as

$$L^p = \dot{F} (F^n_p)^{-1}.$$  (9)

The deviatoric part is

$$D^p = sym (L^p) - \frac{1}{3} tr (L^p) I.$$  (10)

So the average plastic rate of deformation is

$$\bar{D} = \langle D^p \rangle = \frac{1}{V(B)} \int_{V(B)} D^p dV.$$  (11)

Then the equivalent strain can be calculated as

$$\bar{\varepsilon}_{eff} = \int_0^t \sqrt{\frac{2}{3} \bar{D} \cdot \bar{D}} dt.$$  (12)

3 Constitutive model based on continuum slip theory

The rate-independent constitutive problem adopted for a single FCC crystal is described in detail in [1]. The constitutive problem uses a total-Lagrangian description of deformation gradient (with $F_{n+1}$ denoting the deformation gradient at current time with respect to the initial undeformed configuration). In the constitutive model, it is assumed that deformation takes place in a single
crystal through dislocation glide and the evolution of the plastic flow is given by

\[ \dot{F}^p(F^p)^{-1} = L = \sum_{\alpha} \dot{\gamma}^\alpha S^\alpha_0, \]  

(13)

where \( S^\alpha_0 = m^\alpha \otimes n^\alpha \) is the Schmid tensor, \( \dot{\gamma}^\alpha \) is the plastic shearing rate on the slip system \( \alpha \) and \( m^\alpha \) and \( n^\alpha \) are the slip directions and the slip plane normals, respectively in the initial configuration (at \( t = 0 \)).

In crystal plasticity theories, the slip system resistance parameters \( s^\alpha \) are taken to evolve according to

\[ \dot{s}^\alpha(t) = h^{\alpha\beta} \dot{\gamma}^\beta, \]  

(14)

where \( \dot{\gamma}^\beta \) is the shearing rate on slip system \( \beta \), and the matrix \( h^{\alpha\beta} \) describes the rate of increase of the deformation resistance on slip system \( \alpha \) due to shearing on slip system \( \beta \); it describes both self-hardening and latent-hardening of the slip systems. \( h^{\alpha\beta} \) is updated by slip system indicator \( q \) and hardening rate \( h^\beta \) in a single slip direction as follows:

\[ h^{\alpha\beta}(t) = \left[ q + (1 - q) \delta_{\alpha\beta} \right] h^\beta(t), \]  

(15)

where

\[ q = \begin{cases} 
1.0 \text{ for coplanar slip systems,} \\
1.4 \text{ for non-coplanar slip systems,} 
\end{cases} \]

and

\[ h^\beta(t) = h_0 \left[ 1 - \frac{s^\beta(t)}{s_s} \right]^a, \]  

(16)

where \( h_0, a \) and \( s_s \) are slip system parameters that are constant for all slip systems. \( s^\beta \) is the plastic resistance of the slip systems and is updated using the incremental shearing \( \Delta \gamma^\beta \) in each slip system by

\[ s^\alpha(t_{n+1}) = s^\alpha(t_n) + \sum_{\beta \in \text{Active}} h^{\alpha\beta} \Delta \gamma^\beta, \]  

(17)

where \( s^\alpha(t_{n+1}) \) is the updated plastic resistance and \( s^\alpha(t_n) \) is the previous value. \( h^{\alpha\beta} \) are the hardening moduli and \( \Delta \gamma^\beta \) is the incremental shearing on the slip system.

The main process for the incremental update of the constitutive model are briefly reviewed below with more details provided in [1]:

\textbf{Step 1:} Calculate the trial elastic strain \( \dot{E}^e_{\text{trial}} \).
\[ F^{\text{trial}}_e \equiv F (F^p_n)^{-1}, \]  
(18)

\[ C^{\text{trial}}_e \equiv (F^{\text{trial}}_e)^T F^{\text{trial}}_e, \]  
(19)

\[ \dot{E}^{\text{trial}}_e \equiv \frac{1}{2} (C^{\text{trial}}_e - I). \]  
(20)

**Step 2:** Calculate the trial stress

\[ \dot{T}^{\text{trial}} \equiv \mathcal{L}^e \left[ \dot{E}^{\text{trial}}_e \right]. \]  
(21)

Here, \( \mathcal{L}^e \) is the 4th-order elastic tensor. Since everything is calculated in the sample coordinate system in the intermediate configuration, \( \mathcal{L}^e \) should be transformed from crystal coordinate system to sample coordinate system by

\[ \mathcal{L}^e_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} \mathcal{L}'_{mnop}, \]  
(22)

where \( \mathcal{L}'_{mnop} \) is the elastic tensor in crystal coordinate system and \( a_{ij} \) is the component of the transformation matrix.

**Step 3:** Calculate the trial resolved shear stress

\[ \tau^{\text{trial}}_\alpha \equiv \dot{T}^{\text{trial}} \cdot S^\alpha_0, \]  
(23)

where in the Schmid tensor \( S^\alpha_0 \equiv m_0^\alpha \otimes n_0^\alpha \), \( m_0^\alpha \) and \( n_0^\alpha \) should be transformed from the crystal coordinate system to the sample coordinate system.

**Step 4:** Determine the potential active slip systems which satisfy

\[ PA = \left\{ \alpha | \tau^{\text{trial}}_\alpha > s^\alpha(t) \right\}, \]  
(24)

where \( s^\alpha(t) \) is the plastic slip resistance of the slip systems. If the shear stress \( \tau^{\text{trial}}_\alpha \) in a slip direction satisfies this criterion, then plastic movement occurs.

Denote the potential active slip system as

\[ PA = \{ \alpha | \alpha = 1 \ldots m \}. \]  
(25)
Actually, among the $m$ potential active systems, only $n \leq m$ slip systems have positive shear rate. So we define the set of real active system as

$$A = \{\alpha | \alpha = 1 \ldots n, \ n \leq m\} \quad (26)$$

Eliminating the negative shear rates from the initial $m$ potential active systems, only $n$ systems are remained.

*Step 5:* Calculate the shear increments by

$$x^+ = A^+ b, \quad (27)$$

where $A^+$ is the pseudoinverse of the $m \times m$ matrix $A$, defined over all the potentially active slip systems.

$$A^\alpha_\beta = h^\alpha_\beta (t) + \text{sgn} \left( \tau^{\alpha \text{trial}} \right) \text{sgn} \left( \tau^{\beta \text{trial}} \right) S_0^\alpha \cdot L \left[ \text{sym} \left( C^e \text{trial} S_0^\beta \right) \right], \quad (28)$$

$$b^\alpha = \left| \tau^{\alpha \text{trial}} \right| - s^\alpha (t), \quad (29)$$

$$\Delta \gamma^\beta \equiv x^\beta. \quad (30)$$

If for any system the solution $\Delta \gamma^\beta \equiv x^\beta \leq 0$, then the slip system is inactive, so we should remove the corresponding row and column in the $A$ matrix, redefine the reduced potential active slip system, solve $x^+ = A^+ b$ again until all $\Delta \gamma^\beta \equiv x^\beta > 0$. The final size of $x$ is $n$, which is the number of active slip systems.

*Step 6:* Update the plastic deformation gradient.

$$F^p = \left( I + \sum_{\alpha \in \text{Active}} \Delta \gamma^\alpha S_0^\alpha \text{sgn} (\tau^{\alpha \text{trial}}) \right) F^p_n. \quad (31)$$

Since the plastic deformation is volume preserving, $F^p$ should be normalized as

$$|F^p| = (\det F^p)^{-\frac{1}{3}} F^p. \quad (32)$$

*Step 7:* Update the elastic deformation gradient and the PK-II stress $\bar{T}$. 

8
\[ F^e = F (|F^p|)^{-1}, \]  
\[ \bar{E}^e = \frac{1}{2} \left( (F^e)^T F^e - I \right), \]  
\[ \bar{T} = \mathcal{L}^e \left[ \bar{E}^e \right]. \]

**Step 8:** Update the Cauchy stress \( T \) and PK-I stress \( P \).

\[ T = \frac{1}{\det F^e} F^e \bar{T} (F^e)^T, \]  
\[ P = \det(F)TF^{-T}. \]

In the examples considered in Section 5, we use FCC Copper and Nickel crystals as the polycrystal material. In FCC crystal, there are 12 fundamental slip systems which are defined by the normal unit vectors perpendicular to the slip plane (111 directions) and the unit vectors representing the slip directions in the plane (110 directions) [1]. Both slip system directions and elastic tensors are applicable in the crystal coordinate system. Since the deformation and constitutive law are applied in the sample coordinate system, transformation of the coordinate system is needed (Eq. (22)). In Eq. (22), the 4th-rank elastic tensor \( \mathcal{L}^e \) is transformed from the crystal coordinate system to the sample coordinate system by the matrix \( a_{ij} \), which is closely relative to the orientation of the grains. The 3D orientation is expressed in Rodrigues-Frank space [20].

The orientation vector \( r \) is defined by the rotation axis \( n \) and the rotation angle \( \phi \) along \( n \) as

\[ r = n \tan \frac{\phi}{2}. \]

If the orientation is totally random, the rotation axis \( n \) should be a random vector and the rotation angle is a random variable in between \([0, \frac{\pi}{2}]\). To transform this representation into the matrix that rotates the crystal coordinate to the sample coordinate, we use the RF-Quaternion and Quaternion transformation relations. Suppose that the three components of the vector \( r \) are \( u, v \) and \( w \). Then the rotation angle is \( \theta \), so the quaternion is

\[ q = q (q_1, q_2, q_3, q_4) = q \left( u \sin \frac{\phi}{2}, v \sin \frac{\phi}{2}, w \sin \frac{\phi}{2}, \cos \frac{\phi}{2} \right). \]
The components of the transformation matrix are then given as:

\[ a_{ij} = \left( q_4^2 - q_1^2 - q_2^2 - q_3^2 \right) \delta_{ij} + 2q_iq_j + 2q_4 \sum_{k=1}^{3} \delta_{ijk}q_k. \]  \hspace{1cm} (40)

With \( a_{ij} \), we can transform the elastic tensor \( \mathbf{L}^e \) from the crystal coordinate system to the sample coordinate system as shown in Eq. (22).

4 Grain size effect model

In the constitutive model, the deformation gradient was decomposed into a plastic part due to slip in the crystals and an elastic part that accounts for lattice distortion and rotation, \( \mathbf{F} = \mathbf{F}^e \mathbf{F}^p \). The assumption that the lattice only distorts elastically is an approximation that is generally not compatible with a regular displacement field [16]. Thus the elastic component \( \mathbf{F}^e \) (more precisely \( (\mathbf{F}^e)^{-1} \)) has been used as a measure of lattice incompatibility. Consider a single crystal deforming by sliding on a surface, if the deformation is not evenly distributed on the sliding plane, the lattice will be curved and the dislocation that occurs during this process is called geometrically necessary dislocation (GND) [14]. The aim is to use \( (\mathbf{F}^e)^{-1} \) as a measure of dislocation density, so the relation between the incompatibility defined by \( (\mathbf{F}^e)^{-1} \) on \( \mathcal{B} \) and the presence of GND in the crystal has to be constructed.

Since the presence of GND implies lattice incompatibility and the tensor \( (\mathbf{F}^e)^{-1} \) mapping the current configuration \( \mathcal{B} \) which has GND, to the intermediate configuration \( \bar{\mathcal{B}} \), implies the presence of lattice incompatibility, \( (\mathbf{F}^e)^{-1} \) can be taken as measure of the cumulative Burgers vector. Based on this, the cumulative Burgers vector on a closed curve \( \mathcal{C} \) in the current configuration is defined as [15]

\[ b_i = \oint_{\mathcal{C}} (\mathbf{F}^e)^{-1}_{ij} dx_j = \int_{\mathcal{S}} \epsilon^{ijk} (\mathbf{F}^e)^{-1}_{ij,k} r_p dS, \]  \hspace{1cm} (41)

where \( \mathbf{r} \) is the unit normal to a surface \( \mathcal{S} \) whose boundary is the curve \( \mathcal{C} \).

It has been shown in [15,17] that for the cumulative Burgers vector of the dislocations in \( \mathcal{B} \) to be a zero vector, a necessary and sufficient condition in terms of \( (\mathbf{F}^e)^{-1} \) is \( (\mathbf{F}^e)^{-1}_{ij,k} = (\mathbf{F}^e)^{-1}_{ik,j} \). Then, naturally, the lattice incompatibility and presence of GND can be characterized by the tensor \( \mathbf{\Lambda} \) defined as:

\[ \mathbf{\Lambda} = (\mathbf{F}^e)^{-1}_{ij,k} - (\mathbf{F}^e)^{-1}_{ik,j}. \]  \hspace{1cm} (42)
If $\Lambda \neq 0$, GND exists and the magnitude of $\Lambda$ is a measure of how much GND exist. A measure of the dislocation on slip system $\beta$ is given as

$$
\lambda^\beta = \sqrt{\left(\Lambda n_0^\beta\right) \cdot \left(\Lambda n_0^\beta\right)}, \quad (43)
$$

where $n_0^\beta$ is the unit normal of the slip plane.

By Eq. (30), the shear movement of slip system $\beta$ in a time step is $\Delta \gamma^\beta$, so the shearing rate is

$$
|\dot{\gamma}^\beta| = \frac{\Delta \gamma^\beta}{\Delta t}. \quad (44)
$$

Denote the total dislocation density as $\rho$. The evolution of dislocation density [17] can be expressed as

$$
\dot{\rho} \equiv \sum_{\beta \in \text{Active}} \left( k_0 \frac{\lambda^\beta}{b} + k_1 \sqrt{\rho} - k_2 \rho \right) |\dot{\gamma}^\beta|. \quad (45)
$$

The right side of Eq. (45) consists of three terms. The first term considers the relation between lattice incompatibility and dislocation density [17,19,21]. An increment of slip on a given slip system gives rise to the total dislocation density. The measure $\frac{\lambda^\beta}{b}$, where $b$ is the magnitude of the Burgers vector, is interpreted as the density of GND on slip system $\beta$. In the second and third terms [10,22], the evolution of the dislocation density is controlled by the combination of hardening component which describes dislocation storage by a mean free path (the average distance that a dislocation line must move before some portion of the dislocation can be stored) [21] and a dynamic recovery component [19]. The parameters $k_1$ and $k_2$ are defined from experimental observations [22] and have the following forms:

$$
k_1 = \frac{2\theta_0}{\alpha \mu b}, \quad k_2 = \frac{2\theta_0}{\hat{\tau}_s - \hat{\tau}_0}, \quad (46)
$$

where $\mu$ is the elastic shearing modulus of the material, $\theta_0$ is the strain rate of the single crystal in work hardening stage and $\alpha$ is a constant depending on the material. For FCC Nickel, $\theta_0 = \frac{\mu}{200}$, $\alpha = \frac{1}{3}$ and the magnitude $b$ of the Burgers vector is taken as the unit length of a single FCC cell. Finally, $\hat{\tau}_s$ is the saturation stress dependent on the material property and $\hat{\tau}_0$ is the initial yield stress of the material.

Dislocation multiplication and interaction in metals generally results in an increase of the yield stress with plastic strain. The Bailey-Hirsch relation gives
the flow stress and dislocation density as

\[ \hat{\tau} - \hat{\tau}_0 = \alpha \mu b \rho^{\frac{1}{2}}, \quad (47) \]

where \( \hat{\tau} \) is the flow stress used as the plastic resistance. If we can solve \( \hat{\tau} \) in terms of dislocation density \( \rho \) which is closely dependent on grain size, then the criterion for judging whether plastic slip occurs on slip systems will include the grain size effect.

Taking the time derivative of Eq. (47) leads to,

\[ \dot{\hat{\tau}} = \frac{1}{2} \alpha \mu b \rho^{-\frac{1}{2}} \dot{\rho}. \quad (48) \]

In Eq. (48), replace \( \dot{\rho} \) with Eq. (45) and \( \rho^{-\frac{1}{2}} \) with Eq. (47) to finally obtain the following:

\[ \dot{\hat{\tau}} = \frac{k_0 \alpha^2 \mu^2 b}{2(\hat{\tau} - \hat{\tau}_0)} \sum_{\beta \in \text{Active}} \lambda^\beta |\hat{\gamma}^\beta| + \theta_0 \left\{ \frac{\hat{\tau}_s - \hat{\tau}}{\hat{\tau}_s - \hat{\tau}_0} \right\} \sum_{\beta \in \text{Active}} |\hat{\gamma}^\beta|. \quad (49) \]

The flow stress \( \hat{\tau} \) can be calculated as

\[ \hat{\tau}^{n+1} = \hat{\tau}^n + \dot{\hat{\tau}} \Delta t, \quad (50) \]

where \( \hat{\tau}^{n+1} \) and \( \hat{\tau}^n \) are the flow stresses in the current and previous time steps. As discussed above, the updated \( \hat{\tau} \) will be used as the plastic resistance (replacing \( s^a(\tau) \) with \( \hat{\tau} \) in Eq. (17)) to judge whether plastic slip occurs in each time step.

5 Numerical Examples

A parallel implementation of the algorithms above was developed including domain decomposition. The initial grains in the problems considered were introduced using a centroidal voronoi tessellation method [23] starting from a given number of generator points. Using the Voronoi tessellation method, the normal planes located in the middle of neighboring generators are found and consequently taken as grain boundaries. The individual regions surrounded by the grain boundaries represent the grains. An example of using the Voronoi tessellation method to generate the grains from a set of random points is shown in Fig. 2.

An advancing front mesh generation technique is introduced to capture the geometrically complex grain boundaries [25–27]. The input to this method is
Fig. 2. Schematic of Voronoi Tessellation method in a 2-D region: each boundary is the perpendicular bisector of the points on the two sides [24].

a boundary mesh. Starting with the original boundary, element by element is cut off to reduce the domain iteratively. The state of the algorithm is always represented by the advancing boundary front, which starts with a given boundary mesh.

To provide a more concrete example on grain generation and meshing, let us suppose that we want to generate and mesh a five-grain microstructure in a cubic region. At first, we choose five random points whose positions are defined as the voronoi centroids. Secondly, we calculate the inter-boundary planes of any two centroids and find the grain boundaries. The individual regions surrounded by the grain boundaries are taken as the grains. We next start from the first grain and generate triangle meshes on grain boundaries. We next propagate the meshes with tetrahedral elements inside the grains and finally mesh the whole region inside this grain. The last two steps are repeated on the other grains and thus a finite element mesh is developed for the whole region. Finally, for the purpose of finite element calculation, we split the initial tetrahedral elements into brick elements (see Fig. 3).

5.1 Virtual compression test

A compression test is utilized in the following calculations to simulate the microstructure deformation and the mechanical response of the material. A cubic region $1mm \times 1mm \times 1mm$ is compressed in one direction and stretched uniformly in the other two directions. The initial conditions include prescribed velocity gradient $\mathbf{L}$ on the microstructure boundary and assuming that each grain initially has a random orientation. Suppose that the compression rate is $r$ and the time step $\Delta t$. If the region is compressed in the $y$ direction and
stretched in the other two directions, the deformation matrix is

\[
P = \begin{bmatrix}
0.5 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0.5
\end{bmatrix}.
\] (51)

So the velocity gradient matrix \( L \) is given as

\[
L = r \cdot P
\] (52)

The velocity gradient on the boundary of the microstructure can then be obtained by the relation

\[
F = (L \Delta t + I) F_n.
\] (53)

The displacements of the points on the boundaries of the polycrystal are given by

\[
d_i = (F_{ii} - 1) x_i, \quad i = 1, 2, 3,
\] (54)

where \( d_i \) is the displacement in the \( i \)-th direction. The resolved displacements are adopted as the boundary conditions in each time step.

5.2 Verification

This section aims to verify that accuracy of the overall model including the homogenization method and grain size effect model. Let us discretize the domain \( 1mm \times 1mm \times 1mm \) into \( 10 \times 10 \times 10 \) pixel-based elements. Each element
is seen as a grain and is assigned a unique random orientation. For FCC Cu, the elastic tensor $\mathbf{L}^e$ is

$$
\mathbf{L}^e = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix}
$$

(55)

where $C_{11} = 170GPa$, $C_{12} = 124GPa$, $C_{44} = 75GPa$. The parameters used in Eq. (16) are: $a = 2.25$, $s_s = 148Mpa$, $h_0 = 180Mpa$, $s^\beta(0) = 16Mpa$ [1]. In this simulation, a full Lagrangian geometry is utilized without remeshing.

In order to show the accuracy of the proposed homogenization method, simulated results with both the Taylor and homogenization method have been compared with the results given in [1]. As expected, the Taylor method gives stiffer mechanical response than the homogenization method (see Fig. 4). The results obtained with the homogenization method fit better to the results in [1] than the ones using the Taylor model. The largest difference between the two results at strain 1.0 is less than 2%.

To investigate the accuracy of the grain-size model, we next consider FCC Nickel. The components of the elastic stiffness tensor are taken as $C_{11} = 247GPa$, $C_{12} = 147GPa$, $C_{44} = 125GPa$ [28]. The parameters in Eq. (16) are: $a = 5.0$, $s_s = 2400Mpa$, $h_0 = 283Mpa$, $s^\beta(0) = 20.0Mpa$ [16,28,21]. Experiments were performed in [21] to investigate the grain size effect for polycrystal Nickel in terms of dislocation density. The material with 99.99% Nickel was used and the samples were recrystallized to have a grain size range from 20 to 90 $\mu m$. A microstructure with finer grains requires an increased dislocation density to give a certain strain compared with one of coarser grain size. In [21], the data obtained at the grain size of 0.091 $mm$ is of more interest to us. Based on this grain size, $11 \times 11 \times 11$ elements are used in the $1mm \times 1mm \times 1mm$ region. Each element is treated as a grain, so the average grain size can be approximated as 0.091 $mm$. Fig. 5 shows a comparison of the computed results versus the experimental data. Beyond the initial jump to the plastic shear resistance of the slip systems, the stress increases first slowly with the increasing strain and steeper after the square root of strain reaches 0.1. The maximum error between the two curves in Fig. 5 is less than 5%.
5.3 Investigation of the grain size effect

5.3.1 Simulations using pixel based grids

The region of interest is divided into $24 \times 24 \times 24$ elements. Four different mean grain sizes, $1/24 \text{mm}$, $1/12 \text{mm}$, $1/8 \text{mm}$ and $1/6 \text{mm}$, are selected by changing the way of assigning the orientations in the domain. If each element has a unique orientation, the average grain size is just the size of a single element ($1/24 \text{mm}$ in this case). By assigning a cluster of elements composing a continuous region the same orientation, the cluster can be seen as a whole grain and the grain size is the size of this region. With this idea, by assigning an orientation to every 8 elements that constitute a cubic region, the mean grain size becomes $1/12 \text{mm}$. Repeating the same to 27 and 64 elements constituting a cube region, the mean grain sizes of $1/8 \text{mm}$ and $1/6 \text{mm}$ can be obtained.

Fig. 6 shows the results for six grain size cases. As the strain increases, the grain size effect becomes more clarified. This reflects work hardening due to the developing lattice incompatibility and dislocation density on the grain boundaries. As expected, the internal strengthening of the material has a negative correlation with the mean grain size of the microstructure. With smaller grain size, the grain boundaries will increase accordingly, thus a single grain
The relation between the flow stress and the grain size follows the Hall-Petch relation at small strains. The effect of grain size on flow stress is introduced by the enhancement of dislocation concentration during plastic deformation [21]. The increase of grain size correlated dislocation density is not only due to geometric necessary dislocation (GND), but also due to the accumulation of dislocations on the grain boundary. When the dislocations are emitted and reach the grain boundaries, they will ‘pile up’ there because they cannot get through the grain boundaries. Hence, dislocation will accumulate on the grain boundaries and high flow stress will be generated due to the high density of dislocations.

Fig. 7 shows a linear relation between the flow stress and the inverse of grain size at different strains. There are four clusters of data (marked as circles, from [21]), which represent the results at strains 5%, 10%, 15% and 20%. Linear fittings are obtained from these experimental data. As the strain increases, the slope of the line becomes steeper. The simulated results shown with stars are in very good agreement with the experimental data for all cases considered.

Similar results have also been obtained in [17]. The difference in their simula-
Fig. 6. Mechanical response using pixel grids for six grain sizes: 1/24mm, 1/12mm, 1/8mm and 1/6mm using 24 × 24 × 24 elements, 1/36mm and 1/48mm using 36 × 36 × 36 and 48 × 48 × 48, respectively.

The conclusion from the present work is that to model different grain sizes, they retained the elements and grains unaltered but changed the scale of the region in their calculation. However, our model uses the same region for all simulations by changing the number of finite elements utilized. Smaller elements can be seen as smaller grains. By using a set of much finer meshes, our results are in better agreement with the experimental results.

Fig. 8(a) shows the distribution of the equivalent stress in a deformed region at the strain of 0.2 using 36 × 36 × 36 elements. Due to the random initial orientations assigned to the elements, the distribution of the equivalent stress is random. Within the microstructure, the maximal stress is around 900 – 1000Mpa and the minimum about 100 – 200Mpa. The total mechanical response (Fig. 8(a)) at the strain of 0.2 is close to 500Mpa, which is the volume-weighted average of the stress on all the elements.
Fig. 7. A comparison of the calculated results and experimental results in [21] for the 6 grain size cases.

Fig. 8. Equivalent stress of the microstructure with the grain size of 1/36mm: (a) The distribution of equivalent stress in the deformed region at the strain of 0.2; (b) The total mechanical response of the microstructure.

5.3.2 Simulations using grids conforming with grain boundaries

Using pixel grids to represent grains is not physically realistic since grains in a microstructure are geometrically complex and variant and they can hardly
Fig. 9. Schematic of splitting a tetrahedron into bricks: (a) Find the centroid point \( G \), in black) of tetrahedron \( AIJK \), and the centroids (\( H, E, L \) and \( B \), in blue) of \( AIJ, AJK, KJI \) and \( AKI \). Then find the centers (in red) of all the edges. Connect \( G \) and the plane centroids \( H, E, L \) and \( B \), respectively. Then connect \( H, E, L, B \) with the corresponding edge centers in the planes they are located in. (b) Finally, four new brick elements, each of which has 8 vertices and 12 edges, are obtained.

grow up in cubic form. Thus, in order to capture the diversity of grain shapes, a conforming grid generation technique is needed. Of course pixel grids can also be used to conform with grain boundaries, however, the required number of elements needed will be quite high.

We follow the steps below to generate the grains and meshes in the region: (1) Generate a set of seed points in a specified region (1\( mm \) \( \times \) 1\( mm \) \( \times \) 1\( mm \)). We use the Voronoi Tessellation method to generate the grains whose centroids are these seeding points. (2) Use conforming grids generating techniques to mesh the grains with tetrahedral elements that we subsequently split into brick elements (Fig. 9).

With the above mesh generation technique, complex grain boundaries can be captured by the conforming grids and the best quality tetrahedral elements can be adaptively selected. Thus the elements are all optimized and as few elements as possible are used.
5.3.3 Verification study

In Section 5.2, we provided verification of the overall algorithm for the case of pixel based grids. We will here use these results to compare the accuracy of performance of simulations base on conforming grids. We consider a rather simple case of 5 grains. Here we choose 5 arbitrary seeding points in a $1mm \times 1mm \times 1mm$ region. Using the Voronoi Tessellation method, we generate the five grains in the region (Fig. 10).

Fig. 10. Use Voronoi Tessellation method to generate 5 grains in the region from 5 arbitrary seeding points: (a) 5 arbitrary seeding points; (b) The generated 5 grains.

We use conforming and non-conforming grids (Fig. 11) to mesh the microstructure. From Fig. 11(a), it is clear that the grain boundaries have been totally captured. However, nonconforming grids cannot eliminate the steps on grain boundaries. A comparison of using 8000 ($20 \times 20 \times 20$) and $70 \times 70 \times 70$ elements is shown in Figs. 11(b,c).

Fig. 11. The region with 5 grains meshed by conforming and nonconforming grids: (a) Conforming grids; (b) Nonconforming grids with $20 \times 20 \times 20$ elements; (c) Nonconforming grids with $70 \times 70 \times 70$ elements.
As we discussed above, the tetrahedral elements are split into brick elements to avoid locking typical of large plastic deformation problems. Thus the final number of elements will be 4 times of the initial number of elements. For conforming grids, the number of elements utilized can be adjusted by altering the length gradient of the initially generated triangles on grain boundaries. The gradient of triangle edges on grain boundaries reflects the tolerance of their length. A high tolerance means the difference between maximum and minimum triangle edges initially generated on the grain boundaries can be large, i.e., the program can select any triangle in need to capture the grain boundaries with relatively little restriction. A low tolerance means a set of relatively similar triangle should be used to capture the grain boundaries, so more elements will be used due to the restriction on the length of triangle edges. We choose the tolerances of 1.2, 1.1, 1.05 and 1.04, leading to meshes with elements 16388, 31776, 68368 and 87416, respectively (Fig. 12).

![Fig. 12. The 5-grain region meshed by increasing number of elements: (a) 16388; (b) 31776; (c) 68368; (d) 87416.](image)

For non-conforming grids, one example of using 343000 (70 × 70 × 70) elements
is presented. This mesh is considered fine enough to represent a desired level of accuracy (convergent result). For conforming grids, the meshes shown in Fig. 12 are utilized. In Fig. 13, we show the convergence of the conforming grid results using a sequence of refined grids. Note that even when using 16388 elements, the error from the fine non-conforming grid result is only around 2.4% – 2.5% at different strains. When using 68368 and 87416 elements, the errors reduce to 0.5% and 0.4%, respectively at strain 0.05.

![Graph showing stress versus strain response for different mesh sizes](image)

Fig. 13. Computed stress versus strain response for different mesh sizes: (C) refers to conforming grids and (N) to the non-conforming fine grid of 343000 elements.

We next use 91125 pixel based cubic elements (45 × 45 × 45) elements (close to 87416 in conforming grids) to mesh the 5-grain region. In Fig. 14, although the elements used in the conforming grid method are fewer, the obtained result is closer to the converged result obtained using 343000 elements. This proves that, using conforming grids, the result converges faster than using nonconforming grids.

![Graph showing stress versus strain response](image)

In concluding this verification study, we note that in an average, any of the above simulations under the environment of 40 CPUS (2.8 GHz) takes approximately 2 days for completion. Thus using conforming grids is recommended not only for better modeling of grain boundaries but also because less elements are needed in the analysis for comparable level of accuracy.
5.3.4 Investigation of grain size effect using conforming grids

In conforming grids, the mean grain size is computed from equivalent mean grain volume, which is simply defined as \( V_{\text{grain}} = V_{\text{total}} / N_{\text{grain}} \), where \( V_{\text{grain}} \) is the equivalent mean grain volume, \( V_{\text{total}} \) is the volume of the whole region and \( N_{\text{grain}} \) is the number of grains in the region. The grain is approximated as a sphere with the same volume. The mean grain size \( D_{\text{grain}} \) of the microstructure is defined to be the diameter of that sphere.

A 3D microstructure of 50 grains (Fig. 15(a)) is generated and meshed. The average grain size, according to the formula above, is 0.337mm, which can be classified to be large grain size. In experiments, it is relatively easy to obtain large grains in a microstructure because the required processing technique is less strict than that of acquiring smaller grain sizes. Some related research reported large grains in Nickel up to 0.5mm by annealing and cold rolling [29]. Other works showed some micrographs of Nickel grains with mean sizes up to 0.3 – 0.4 mm [30–32].

The configurations of the microstructure before and after the deformation (up to the strain of 0.2) are shown in Fig. 15. A full Lagrangian algorithm is adopted and the reference configuration of deformation is always the initial configuration. No remeshing is used during the simulations. The surface of the

Fig. 14. A comparison of conforming grids with 87416 elements with that of non-conforming grids using 91125 and 343000 elements (converged result).
Fig. 15. The deformation of an arbitrary microstructure with 50 grains: (a) The initial configuration of the 50-grain microstructure, $\epsilon = 0.0$; (b) The deformed configuration at $\epsilon = 0.2$.

Microstructure is deformed homogeneously. On the $y$-plane, all the points are compressed at the rate of 0.001/s while on the $x$ and $z$ planes, all the points are stretched at 0.0005/s. With conforming grids, the deformation of an arbitrary 3D microstructure can be simulated without any approximation of geometric information. Fig. 16(b) also shows the mechanical response (equivalent stress) obtained using conforming and non-conforming grids. The conforming grid results are consistent with the configuration of the microstructure shown in Fig. 15(b). The distribution of the high and low stress regions matches the geometry of the grains in the microstructure. For example, the red triangle high stress region at $x = 1$ in Fig. 16(a) corresponds to the purple triangle grain in Fig. 15(b), the blue low stress region at $x = 1, z = 1$ in Fig. 16(a) corresponds to the orange grain in the same position in Fig. 15(b), etc. This proves that the distribution of the stress field is highly dependent on the geometry of the microstructure.

The inside of the deformed microstructure is shown in Fig. 17. The results are obtained from the cross sections at $x = 0.5, y = 0.5$ and $z = 0.5$, respectively. The plots in (b), (d) and (f) show the displacement field on the three cross sections (a), (c) and (e), respectively. Since the cubic microstructure is compressed in the $y$-direction and stretched in the $x$- and $z$-directions, the cutting sections of the grains deform consistently. In (a), the grains are squeezed in the $y$-direction but stretched in the $z$-direction. The situation in (e) is similar except that the grains are stretched in the $x$-direction. In (c), the grains are stretched in both $x$ and $z$ directions. The distribution of the equivalent stress field also matches the geometry of the grains in this case. For example, comparing (a) and (b), the blue low stress regions in the lower and upper left parts of (b) fit well with the grains with similar shapes in the corresponding
Fig. 16. Equivalent stress field of a 3D microstructure: (a) The equivalent stress field of the deformed 50-grain microstructure at $\epsilon = 0.2$; (b) A comparison of the mechanical response up to the strain of 0.3 using both conforming and nonconforming grids methods.

positions in (a). This proves that the stress field can be fully captured no matter how complex the geometry of the microstructure is.

To investigate the grain size effect on more microstructures with different mean grain sizes, two more microstructures with 20 and 100 grains are generated. The three available random microstructures up to now are presented in Fig. 18. According to the definition above, the mean grain sizes are 0.457\( mm \), 0.337\( mm \) and 0.267\( mm \), respectively. As discussed previously, these are all realistic grain sizes. Some details about the three microstructures and elements utilized to generate the meshes are presented in Table 1. With the number of grains increased, the number of elements grows up roughly proportionally.

Table 1
A comparison of the parameters used when generating and meshing microstructures with 100, 50 and 20 grains.

<table>
<thead>
<tr>
<th>Number of grains</th>
<th>100 grains</th>
<th>50 grains</th>
<th>20 grains</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean grain size (mm)</td>
<td>0.267</td>
<td>0.337</td>
<td>0.457</td>
</tr>
<tr>
<td>Elements</td>
<td>382,212</td>
<td>169,200</td>
<td>73,348</td>
</tr>
<tr>
<td>Nodes</td>
<td>423,261</td>
<td>188,323</td>
<td>82,381</td>
</tr>
</tbody>
</table>

Fig. 19 shows the stress-strain curves for the grain sizes of 0.457\( mm \), 0.337\( mm \) and 0.267\( mm \). In comparison with Fig. 6, the difference between the stress at distinct strains is smaller. This is expected because of the grain sizes that we consider here. Recall from the experimental data in Fig. 7 that the stress at a
certain strain depends linearly on the inverse of grain size $\frac{1}{D}$. The difference in the three stress responses for a given strain is small here as the variability
Fig. 18. Generate microstructures with (a) 100 grains; (b) 50 grains; and (c) 20 grains.

on the inverse of the grain sizes is also small.

Fig. 19. Stress-strain curves for grain sizes of 0.267 mm, 0.337 mm and 0.457 mm.

Table 2 provides the calculated stress at the strains of 0.5, 1.0, 1.5 and 2.0 in the three cases considered. The experimental results obtained are also presented [21]. The two groups of data fit well with each other. This not only proves the validity of our present work, but also shows the feasibility to capture the features of real microstructures. Once the microstructure of a certain material is given, the mechanical response can be obtained through the procedures introduced in this paper.
Table 2
Comparison of calculated results and experimental results for the three grain sizes of 0.457mm, 0.337mm and 0.267mm.

<table>
<thead>
<tr>
<th>Grain size</th>
<th>Strain</th>
<th>0.05</th>
<th>0.10</th>
<th>0.15</th>
<th>0.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.457mm</td>
<td>This work (MPa)</td>
<td>197.718</td>
<td>312.597</td>
<td>404.163</td>
<td>479.101</td>
</tr>
<tr>
<td></td>
<td>Experiment</td>
<td>190.728</td>
<td>311.584</td>
<td>409.474</td>
<td>491.597</td>
</tr>
<tr>
<td>0.337mm</td>
<td>This work (MPa)</td>
<td>200.250</td>
<td>316.467</td>
<td>408.618</td>
<td>483.886</td>
</tr>
<tr>
<td></td>
<td>Experiment</td>
<td>191.608</td>
<td>312.525</td>
<td>410.564</td>
<td>492.705</td>
</tr>
<tr>
<td>0.267mm</td>
<td>This work (MPa)</td>
<td>202.160</td>
<td>321.207</td>
<td>414.754</td>
<td>491.144</td>
</tr>
<tr>
<td></td>
<td>Experiment</td>
<td>192.486</td>
<td>313.465</td>
<td>411.652</td>
<td>493.811</td>
</tr>
</tbody>
</table>

6 Summary

This paper presented a comprehensive model for interrogating properties of 3D microstructures of FCC polycrystals. A series of simulated results have been obtained using both non-conforming and conforming grids. Comparison with experimental observations in the literature and other numerical results have proved the validity of the present work. The following conclusions have been obtained:

(1) A finite element analysis of large deformation of 3D polycrystals is presented using cubic elements as well as elements conforming with grain boundaries. Rate-independent constitutive model using homogenization method is constructed. The effect of grain size distribution is included by considering a physically motivated measure of lattice incompatibility which provides an updated shearing resistance on the slip directions.

(2) A domain decomposition method is adopted for decomposing a whole region into sub-regions processed independently by individual processors in parallel computation. The Voronoi tessellation method is adopted to generate arbitrary microstructures with any shape and any number of grains. Conforming grids generation technique is developed to mesh the grains in the microstructure.

(3) The calculated mechanical properties of polycrystals are shown to be consistent with experimental results for different grain sizes. The strengthening effect on mechanical response has been captured. The stress at different strains below 0.2 has a linear relation with the inverse of grain size $D$. For the grain sizes of $1/6mm$ and $1/24mm$, the stress increases about 4% at different strains.

(4) The conforming grids method is adopted to investigate the strengthening effect of grain sizes. The convergence and validity of the calculated results
are verified using the results obtained with pixel based grids. The grain size effect was captured for different microstructures with variant mean grain sizes. Further work is expected to further speed up the calculation for properties of more complicated microstructures.

References


