Design across length scales: A reduced-order model of polycrystal plasticity for the control of microstructure-sensitive material properties

Shankar Ganapathysubramanian, Nicholas Zabaras

Materials Process Design and Control Laboratory, Sibley School of Mechanical and Aerospace Engineering, 188 Frank H.T. Rhodes Hall, Cornell University, Ithaca, NY 14853-3801, USA

Abstract

Development of techniques for the control of material properties of polycrystal materials that are inherently dependent on preferred orientations (texture) is addressed. To account for the infinite degrees of freedom of microstructural features, a model reduction on the micro-scale is introduced. Reduced-order models are developed to model the evolution of microstructure described by an orientation distribution function using a finite element discretization of the orientation space. This reduced-order modeling approach is based on the technique of proper orthogonal decomposition (POD) and the method of snapshots. Furthermore, novel design problems are introduced for the control of microstructure based on realistic polycrystalline plasticity. Specifically, a gradient based optimization framework is introduced using a multi-length scale continuum sensitivity method (CSM). The model reduction is extended to the sensitivity analysis and is a key element for the success of computational design of deformation processes. Numerical examples that highlight the benefits of the continuum sensitivity method and model reduction are presented. In addition, the potential of the presented techniques towards process design for obtaining desired material properties is demonstrated with the control at a material point of the elastic modulus in f.c.c Copper. A desired distribution of the elastic modulus is achieved through an optimal selection of the velocity gradient.

Key words: Microstructure-sensitive design; Continuum sensitivity analysis; Reduced-order modeling; Polycrystal plasticity; Anisotropy; Gradient-based optimization; Viscoplasticity

1 Corresponding author: Fax: 607-255-9410
Email: zabaras@cornell.edu
URL: http://www.mae.cornell.edu/zabaras/

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1 INTRODUCTION

Most materials used in engineering applications are polycrystalline in nature. Their properties depend not only on the properties of the individual crystals but also on parameters, like the crystallographic orientation, that characterize the polycrystal. During a deformation process, crystallographic slip and reorientation of crystals (lattice rotation) can be assumed to be the primary mechanisms of plastic deformation in a limited regime of processing conditions. These occur in an ordered manner so that a preferential orientation or texture develops. The developed texture characterizes the mechanical, optical and magnetic behavior of the material. For example, earing during deep drawing of cups/cans along with variations in thickness of the cups/cans is attributed to anisotropy [1]. Anisotropy has its advantages too, as appropriate textures block the propagation of cracks or make a material magnetically/optically superior in particular directions. The vastness of fields wherein texture affects properties makes it an interesting, challenging and industrially important problem [2,3].

The state of art in simulation of texture evolution is based on the analysis of a discrete aggregate of crystals [4]. This approach combines single crystal responses with a macro-micro linking hypothesis. An alternate approach is based on describing texture through an orientation distribution function (ODF) which expresses the density of crystal orientations over the space of orientation parameters [5]. Common methods of ODF representation include series expansion using generalized spherical harmonics, infinite polynomial series or tensorial Fourier series [6,7]. In [7], the authors discuss the design of a compliant beam so as to maximize the deflection without plastically deforming the beam. Analysis was performed using spectral methods which, are complex and have global support thus providing no local control of the quality of the ODF. This tends to create problems in the context of sharp textures and requires significant number of terms in the series to obtain an accurate texture representation. Alternately, Dawson et al. in [8,9] proposed the idea of representing the ODF with finite element polynomial functions defined over an explicit discretization of the orientation space (angle-axis parametrization).

In [5], different finite element solution schemes - Eulerian, Lagrangian and updated Lagrangian ODF schemes - have been described for texturing over the cubic fundamental region of the Rodrigues’ space [10,11]. In this paper, the neo-Eulerian angle-axis spaces described in [8,12] are used. All of the above mentioned methods are characterized by a large number of degrees of freedom which, in the context of design, require enormous computational resources. The emphasis of this paper is to introduce a mathematically rigorous reduced-order model for the evolution of the microstructure and extend its use to design. A reduced set of basis functions are generated for Galerkin representation of partial differential equations. Other publications on microstructure model reduction include the work of Adams et al. [7] on microstructure-sensitive design (MSD) that is carried out in a common Fourier space.

The plan of this paper is as follows. A brief introduction on modeling mi-
Fig. 1. A framework for the association of a crystal $p$ with unique parameters $r$, drawn from the fundamental region. Also shown are the reorientation vector $\hat{r}$ and the texture maps $\chi$ and $\chi_t$.

A comprehensive set of applications and design examples are considered in Section 6. Finally, Section 7 concludes with a discussion of several open issues related to the simulation and control of microstructural properties.

2 Overview of microstructure in polycrystalline materials

Consider a macroscopic material point associated with microstructure $\mathcal{M}$. The response of any crystal comprising this microstructure is determined by the orientation $R$, which is the rotation relating the crystal lattice frame, $\hat{e}_i$, to the reference sample frame $e_i$ as $e_i = R \hat{e}_i$. The rotation $R \in O^+$ ($O^+$ is the set of all proper orthogonal tensors) is not unique due to the presence of crystal and sample symmetries. This non-uniqueness is resolved by restricting the choice of orientations to an appropriate fundamental region of $O^+$ [8]. Thus for a particular choice of the fundamental region $\mathcal{R}$, the orientation of the crystal is uniquely represented by $r \in \mathcal{R}$ where $R = Q(r)$ and $Q$ maps the fundamental region to the set of all proper orthogonal tensors. Texture can be described as a map that takes individual crystals, $p$, to orientations within the fundamental region. Let $\Xi$ be a collection of such maps, then each map $\chi \in \Xi$ is a one-one map of the microstructure $\mathcal{M}$ onto the fundamental region $\mathcal{R}$. The orientation of a crystal $r$, described above, is developed as $r = \chi(p)$. A graphical representation of this framework is shown in Fig. 1.

Observe that every $r$ in the fundamental region is associated with a crystal
\( \chi^{-1}(r) \in \mathcal{M} \). Thus microstructure is treated as a continuum of crystals, that under the map \( \chi \) occupies the fundamental region. An ODF, represented by \( \mathcal{A} \), describes the crystal density over the fundamental region. In the context of time dependent texturing, \( \mathcal{M} \) is mapped onto the fundamental region, \( \mathcal{R}_t \), by a family of maps \( \chi_t \). The maps, \( \chi_t \), along with the reference map \( \chi \) determine a family of mappings \( \hat{r}(\bullet, t) : \mathcal{R} \rightarrow \mathcal{R}_t \) referred to as the reorientation. The reorientation vector, \( \hat{r} \), is associated with the one-parameter family of ODF’s, \( \mathcal{A}(r, t) = \mathcal{A}_\chi(r) \) and this representation is Eulerian. The Eulerian rate form of the conservation equation can be obtained as [8]:

\[
\frac{\partial \mathcal{A}(r, t)}{\partial t} + \nabla \mathcal{A}(r, t) \cdot \mathbf{v}(r, t) + \mathcal{A}(r, t) \nabla \cdot \mathbf{v}(r, t) = 0 \quad (2.1)
\]

where \( \mathbf{v}(r, t) \) is the Eulerian reorientation velocity. The polycrystal average of a property, \( \Upsilon(r, t) \), is determined as:

\[
\langle \Upsilon \rangle = \int_{\mathcal{R}} \Upsilon(r, t) \mathcal{A}(r, t) \, dv \quad (2.2)
\]

Angle-axis parameterizations, which define an alternative to Euler angles, are used to represent an orientation. These are derived from the natural invariants of a rotation: the rotation axis, \( \mathbf{n} \) and the rotation angle, \( \theta \). The orientation, \( r \), is obtained by scaling \( \mathbf{n} \) through some function of \( \theta \) as,

\[
r = \mathbf{n} f(\theta) \quad (2.3)
\]

This paper utilizes the Rodrigues’ parametrization, with \( f(\theta) = \tan(\frac{\theta}{2}) \) [11]. This parametrization reduces the orientation space, under crystal symmetry, to between a pair of planes. Details regarding quaternion parametrization and the development of fundamental regions are available in [8]. The orientation space defined using the neo-Eulerian (angle-axis) parametrization is Riemannian and the metrical properties need to be defined. The volumetric distortion associated with this Riemannian nature is given as \( dv = \sqrt{\det \mathbf{G}} \, dr_1 dr_2 dr_3 \) where \( \mathbf{G} \) represents the associated metric tensor and \( \det \mathbf{G} = \cos^4(\theta/2) \) for Rodrigues’ parametrization [11]. The other metrical quantity is the Riemannian connexion, \( \Gamma \). The connexion tensor describes the process of absolute differentiation associated with non-Euclidean spaces. In the case of Rodrigues’ parametrization, it is defined as [8]:

\[
\Gamma^i_{jk} = -\frac{1}{2} \sin(\theta) \left( n_j \delta^i_k + n_k \delta^i_j \right) \quad (2.4)
\]

In addition, the reorientation velocity can be evaluated as [13]:

\[
\mathbf{v} = \frac{1}{2} (\omega + (\omega \cdot r)r + \omega \times r) \quad (2.5)
\]
where \( \omega \) represents the spin vector, defined as \( \omega = \text{vect}(\dot{R}R^T) \). Further, the covariant derivative of the reorientation velocity can be evaluated as

\[
v^i_j = \frac{\partial v^i}{\partial r^j} + \Gamma^i_{kj} v^k
\]  

(2.6)

3 Constitutive relations for rate-dependent f.c.c crystals

The physical phenomena associated with the evolution of microstructure in f.c.c materials is addressed in this section. A polycrystal is composed of individual crystals and the macroscopic response of the polycrystal is coupled with those of the individual crystals using the extended Taylor hypothesis. This hypothesis assumes that the stretch and spin experienced by individual crystals are identical to the corresponding macroscopic values and the aggregate response is computed by averaging the individual responses (as defined in Equation (2.2)). The crystal kinematics are simulated using a viscoplastic constitutive model and elastic effects are considered negligible. The velocity gradient experienced by a crystal, with orientation \( r \), can be expressed as:

\[
L = \Omega + R \sum_\alpha \dot{\gamma}^\alpha \overline{T}^\alpha R^T
\]  

(3.1)

where \( \Omega \) is the lattice spin, \( \dot{\gamma}^\alpha \) is the shearing rate along the slip system \( \alpha \) and \( \overline{T}^\alpha = (\overline{m}^\alpha \otimes \overline{s}^\alpha) \) is the Schmid tensor for slip system \( \alpha \). \( \overline{m}^\alpha \) is the slip direction and \( \overline{s}^\alpha \) is the slip plane normal, both defined in the crystal reference frame. The shearing rate on the slip systems is given by a power law as:

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 |\frac{\tau^\alpha_s}{s}|^{1/m} \text{sign} \left( \frac{\tau^\alpha_s}{s} \right)
\]  

(3.2)

where \( s \) is the slip system hardness, \( m \) is the strain rate sensitivity, \( \dot{\gamma}_0 \) is a reference rate of shearing and \( \tau^\alpha_s \) is the resolved shear stress on slip system \( \alpha \). The resolved shear stress is related to the crystal Cauchy stress as \( \tau^\alpha = \overline{\sigma} \cdot \overline{P}^\alpha \). The expressions for the symmetric and spin parts are obtained, from Equation (3.1), as:

\[
\bar{D} = \sum_\alpha \dot{\gamma}^\alpha \bar{P}^\alpha
\]  

(3.3)

\[
\Omega = W - \sum_\alpha \dot{\gamma}^\alpha RQ^\alpha R^T
\]  

(3.4)

where \( \bar{P}^\alpha \) and \( Q^\alpha \) are the symmetric and skew parts of the Schmid tensor, respectively. Also, \( \bar{D} \) is the macroscopic deformation rate expressed in the lattice frame, i.e. \( \bar{D} = R^T D R \). By solving Equation (3.3), the crystal Cauchy
stress and shear rate can be evaluated. Using Equation (3.4), the lattice spin vector can be evaluated as:

$$\omega = \text{vect}(\Omega)$$ \hspace{1cm} (3.5)

The reorientation velocity can be computed using $\omega$ in Equation (2.5). The divergence of the reorientation velocity depends on $\frac{\partial \gamma^\alpha}{\partial r}$ which can be evaluated as

$$\frac{\partial \gamma^\alpha}{\partial r} = \frac{\partial \gamma^\alpha}{\partial \tau^\alpha} \left( \frac{\partial \sigma}{\partial r} \cdot \bar{P}^\alpha \right)$$ \hspace{1cm} (3.6)

$\frac{\partial \sigma}{\partial r}$ is obtained by differentiating Equation (3.3), resulting in the following linear system:

$$\frac{\partial \bar{D}}{\partial r} = \sum_{\alpha} \left( \frac{\partial \gamma^\alpha}{\partial \tau^\alpha} \bar{P}^\alpha \otimes \bar{P}^\alpha \right) \left[ \frac{\partial \sigma}{\partial r} \right]$$ \hspace{1cm} (3.7)

where the L.H.S. can be evaluated from $\bar{D} = R^T D R$.

The ODF, $A$, over the fundamental region, $R$, is evaluated from Equation (2.1). It has the form of the advective transport equation and may be subject to discontinuities in the divergence of the reorientation velocity. Therefore, a finite element implementation of this equation is based on the classical SUPG formulation with ‘shock capturing’ artificial diffusion and is given as follows [14]:

$$\int_{R} \left\{ \frac{\partial A}{\partial t} + \nabla \cdot A \cdot v + A \nabla \cdot v \right\} \eta \, dv + \int_{R} \nabla \cdot (\varepsilon \nabla A) \, \varphi \, dv = 0$$ \hspace{1cm} (3.8)

where $\eta$ and $\varphi$ are the Petrov-Galerkin and classical Galerkin weighting functions respectively, $\varepsilon$ is the shock capturing parameter and is a function of the residual of the system, $S(A) = |\frac{\partial A}{\partial t} + \nabla \cdot v \cdot A + \nabla A \cdot v|$.

4 Mathematical approach towards reduced-order modeling through proper orthogonal decomposition

In design and control of many complex continuum physical processes, standard simulation techniques using finite elements or spectral methods are not appropriate due to the large number of degrees-of-freedom needed for the analysis and the associated mathematical and computational complexity. It is in this context that reduced-order models play a significant role. These models help reduce the computational complexity by capturing the dynamics.
of the associated process through smaller number of degrees-of-freedom. The techniques of reduced modeling have been in use for sometime for the control of fluid dynamical systems (see [15]-[19] for applications in turbulence). The proper orthogonal decomposition (POD) technique was first described in [15] and these techniques have been improved and expanded for mathematical and computational simplicity. Reduced-order modeling is based on the development of a reduced set of basis functions, \( \phi_i(\mathbf{r}) \), for the associated system (represented by partial differential equations). The ODF \( \mathcal{A}(\mathbf{r}, t) \) governed by Equation (2.1) is approximated here as follows:

\[
\mathcal{A}(\mathbf{r}, t) = \sum_{i=1}^{z} a_i(t) \phi_i(\mathbf{r}); \quad a_i(t) = \int_{\mathcal{R}} \mathcal{A}(\mathbf{r}, t) \phi_i(\mathbf{r}) \, dv \quad (4.1)
\]

The optimal basis functions \( \phi_i(\mathbf{r}) \) for the representation of the ODF are generated using the technique of POD (proper orthogonal decomposition) from an ensemble of ODF data, \( \{\mathcal{A}^i(\mathbf{r})\}_{i=1}^{N} \), obtained from different deformation modes. This requires maximizing the average projection of the ensemble data onto the basis. The resulting optimization problem can be stated as follows:

\[
\max_{\phi} \frac{\langle (\mathcal{A}, \phi) \rangle^2}{\| \phi \|^2} \quad (4.2)
\]

It has been shown [15] that the solution of the problem defined by Equation (4.2), leads to an eigenvalue problem, which can be computationally expensive for large ensembles of ODF data. To reduce the computational effort, the method of snapshots was introduced in which the basis, \( \phi \), is expressed as a linear combination of the original ensemble data as:

\[
\phi_j = \sum_{i=1}^{N} u_{ji} \mathcal{A}^i \quad (4.3)
\]

where \( u_{ji} \) is to be determined such that \( \phi \) satisfies Equation (4.2). The eigenvalue problem reduces to the following form:

\[
\mathbf{C} \mathbf{U} = \boldsymbol{\Lambda} \mathbf{U} \quad (4.4)
\]

where, \( \mathbf{C} \) is the spatial correlation matrix defined as:

\[
C_{ij} = \frac{1}{N} \int_{\mathcal{R}} \mathcal{A}^i(\mathbf{r}) \mathcal{A}^j(\mathbf{r}) \, dv \quad (4.5)
\]

and \( \boldsymbol{\Lambda} \) and \( \mathbf{U} \) are the complete eigen-description of the system. A suitable basis size \( z \) is computed by maximizing the energy contained by the eigenmodes. The energy contained by the eigenmodes is the sum of the corresponding eigenvalues. Once the modes have been evaluated, Equation (4.1) is used
in Equation (3.8) (without any need for the stabilizing term) to obtain the following ordinary differential equation (ODE):

\[
\dot{a} = Ba + b
\]  

(4.6)

where \(a\) is the time dependent coefficient that determine the ODF and

\[
B_{ij} = -\int_\mathcal{R} (\nabla \phi_j(r) \cdot \mathbf{v} \phi_i(r) + \phi_j(r) \phi_i(r) \nabla \cdot \mathbf{v}) \, dv
\]  

(4.7)

\[
b_i = 0
\]  

(4.8)

The initial value of \(a\) is determined from the initial texture as:

\[
a_i(0) = \int_\mathcal{R} A(r, t=0) \phi_i(r) \, dv
\]  

(4.9)

where \(A(r, t=0)\) is the initial texture of the polycrystal. Thus Equations (4.6) – (4.9) define the reduced-order model for the system governed by Equation (3.8). This is extremely helpful in defining optimal control problems to obtain desired orientation distribution function as only a smaller, finite number of degrees of freedom need to be controlled.

5 Computational design for desired microstructure-sensitive properties

The control of material properties through deformation process design (e.g. design of process sequence, design of dies and preforms and optimal process parameter selection) was addressed in [20]-[24]. Microstructure was modelled through state variables for which phenomenological evolution laws were prescribed [24]. The control process relied mainly on a gradient based optimization framework in which the gradients were evaluated from a continuum sensitivity analysis. Phenomenological techniques, do not allow for accurate modeling of microstructural evolution; hence a need for the development of multi-length scale computational process design techniques for control of microstructural features like texture. The next few sections address the development of an innovative continuum sensitivity analysis and the associated design problems.

5.1 A multi-length scale continuum sensitivity analysis

The design framework adopted here is based on a gradient optimization method. To calculate the gradients, the sensitivity of material properties with respect
Fig. 2. Pictorial of the two-length scale sensitivity analysis. On the left, the macro-sensitivity problem (following a Lagrangian approach) computes the sensitivities of continuum fields (e.g., of the velocity gradient) with respect to macro-design variables (here the die surface). On the right, the micro-sensitivity problem (following an Eulerian approach) computes the sensitivity of the ODF and properties related to the ODF.

To macro-design variables (like the preform, die shapes and process conditions) need to be evaluated. The process of evaluating the sensitivities of fields on the micro-scale due to perturbations on the macro-scale is shown schematically in Fig. 2. This requires a macro-sensitivity problem where the interest is to compute how perturbations on the macro-design variables $\beta$ affect the continuum fields including the velocity gradient $L$. The macro-sensitivity problem is examined in [20]-[24] and the reader is encouraged to consult these references for more details. The dependence of the field $L$ on $\beta$, in a total Lagrangian framework, can be expressed as $L = L(X, t; \beta)$. The parameter sensitivity $\overset{\circ}{L} = \overset{\circ}{L}(X, t; \beta, \Delta \beta)$ is defined as the total Gateaux differential of $L = L(X, t; \beta)$ in the direction $\Delta \beta$ computed at $\beta$:

$$\overset{\circ}{L}(X, t; \beta, \Delta \beta) = \frac{d}{d\lambda} L(X, t; \beta + \lambda \Delta \beta) \bigg|_{\lambda=0}$$ (5.1)

The micro-sensitivity problem, defined in Fig. 2, computes the resulting variation of the ODF and other microstructural properties from the perturbation $\Delta L$ of $L$. For the material point simulator developed here, a design vector $\alpha$ on the microscale is defined such that it has a one-to-one relation with $L$. The components of $\alpha$ are defined as coefficients of a unique decomposition of $L$. 

Polycrystal plasticity
into various deformation modes (while maintaining incompressibility):

\[
L = \alpha_1 \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & -0.5 & 0.0 \\ 0.0 & 0.0 & -0.5 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\
\alpha_4 \begin{bmatrix} 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \alpha_5 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix} + \alpha_6 \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\
\alpha_7 \begin{bmatrix} 0.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \alpha_8 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix}
\]

(5.2)

Even though this decomposition may not appear to be mathematically necessary, it will provide guidance for the selection of processes (rolling, shear, compression or tension) corresponding to a given vector \( \alpha \). Using the one-to-one dependence between the velocity gradient \( L \) and \( \alpha \), the parameter sensitivity of a micro-field (i.e. fields on the microscale), \( \hat{\Upsilon}(r, t; \alpha) \), is as follows:

\[
\hat{\Upsilon}(r, t; \alpha, \Delta \alpha) = \left. \frac{d}{d\lambda} \hat{\Upsilon}(r, t; \alpha + \lambda \Delta \alpha) \right|_{\lambda=0}
\]

(5.3)

The reader should note the explicit multiscale formulation of the sensitivity fields. The microscale perturbation \( \Delta \alpha \) is a result of a perturbation \( \Delta L \), which is linked across the length scales and is a result of the change in macro-design variables \( \beta \).

5.2 Polycrystal constitutive sensitivity analysis

The sensitivity problem, corresponding to the evolution of the ODF, is developed in this section. The sensitivity of the ODF is denoted by \( \hat{\mathcal{A}} = \hat{\mathcal{A}}(r, t; \alpha, \Delta \alpha) \). Using the earlier definition of parameter sensitivity, design differentiation of Equation (2.1) results in the following partial differential equation:

\[
\frac{\partial \hat{\mathcal{A}}}{\partial t} + \nabla \hat{\mathcal{A}} \cdot \dot{v} + \nabla \cdot \dot{\mathcal{A}} + \hat{\mathcal{A}} \nabla \cdot \dot{v} + \mathcal{A} \nabla \cdot \dot{v} = 0
\]

(5.4)
from which a finite element formulation over the fundamental region follows:

$$\int_{\mathcal{R}} \left( \frac{\partial \mathcal{A}}{\partial t} + \nabla \mathcal{A} \cdot \mathbf{v} + \nabla \mathcal{A} \cdot \mathbf{\dot{v}} + \mathcal{A} \nabla \cdot \mathbf{v} + \mathbf{A} \nabla \cdot \mathbf{\dot{v}} \right) \varphi dv = 0 \quad (5.5)$$

where $\varphi$ is an admissible test function. The equation defines the weak form of the sensitivity problem and can be solved to obtain the sensitivities of the ODF. The sensitivity of the reorientation velocity and its divergence are evaluated by design-differentiating the crystal constitutive relations. The design-differentiation of the macro-micro linking hypothesis (Equations (3.3) and (3.4)) results in:

$$\mathbf{\ddot{D}} = R^T \mathbf{\ddot{D}} R = \sum_{\alpha} \dot{\gamma}^\alpha \ddot{P}^\alpha = \sum_{\alpha} \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} \tau^\alpha \ddot{P}^\alpha \quad (5.6)$$

$$\mathbf{\ddot{W}} = \ddot{\Omega} + \sum_{\alpha} \ddot{\gamma}^\alpha \mathbf{Q}^\alpha \quad (5.7)$$

where $\mathbf{\ddot{D}} = \text{Sym}(\ddot{\mathbf{L}})$, $\mathbf{\ddot{W}} = \text{Skew}(\ddot{\mathbf{L}})$ and $\dot{\mathbf{L}}$ is a given perturbation in the velocity gradient. Incorporating $\tau^\alpha = \ddot{\sigma} \cdot \ddot{P}^\alpha$ into Equation (5.6) results in a linear system which is solved for $\ddot{\sigma}$. The sensitivity of the reorientation velocity is computed by design-differentiating Equations (2.5) as:

$$\mathbf{\ddot{v}} = \frac{1}{2} (\ddot{\omega} + (\ddot{\omega} \cdot \mathbf{r}) \mathbf{r} + \dddot{\omega} \times \mathbf{r}) \quad (5.8)$$

where $\ddot{\omega}$ represents the sensitivity of the spin vector and can be obtained from $\text{vect}(\ddot{\Omega}) = \text{vect}(\mathbf{\ddot{RR}^T})$. Further, the derivative of the sensitivity of the reorientation velocity is evaluated as

$$\dddot{v}^i_{,j} = \frac{\partial \dddot{v}^i}{\partial r^j} + \Gamma^i_{kj} \dddot{v}^k \quad (5.9)$$

5.3 Reduced-order modeling of the polycrystal continuum sensitivity analysis

Computational design of multi-length scale deformation problems can be simplified through the development of a reduced-order model for the sensitivity problem. The reduced-order model for the sensitivity problem is obtained from
the basis developed for the direct problem (ODF field). The sensitivity of the ODF field is approximated in terms of the basis functions as:

\[ \ddot{A}(r, t) = \sum_{i=1}^{z} c_i(t) \phi_i(r); \quad c_i(t) = \int_{R} \ddot{A}(r, t) \phi_i(r) dv \quad (5.10) \]

where \( c \) is the time dependent coefficient that determines the sensitivity ODF field. Performing an analysis similar to that in the direct problem, the reduced system is obtained as:

\[ \dot{c} = Gc + h \quad (5.11) \]

where

\[ G_{ij} = -\int_{R} (\nabla \phi_j \cdot v \phi_i + \phi_j \phi_i \nabla \cdot v) dv \quad (5.12) \]

\[ h_i = -\int_{R} (\nabla A \cdot \dot{\phi} + A \phi_i \nabla \cdot \dot{v}) dv \quad (5.13) \]

The initial value of \( c \), when \( \ddot{A}(r, t = 0) = 0 \) is assumed, is given by the following expression:

\[ c_i(0) = \int_{R} \ddot{A}(r, 0) \phi_i(r) dv = 0 \quad (5.14) \]

5.4 A gradient-based optimization approach to process design for microstructure-sensitive properties

The design problem requires the selection of the parameters, \( \alpha \), that lead to a desired distribution of a micro-field \( \Upsilon \). The objective function for the gradient optimization problem is stated as follows:

\[ \min_{\alpha} \mathcal{F}(\alpha) = \frac{1}{N_s} \sum_{i=1}^{N_s} (\Upsilon_i(\mathcal{A}(\alpha)) - \Upsilon_{\text{desired}})^2 \quad (5.15) \]

where \( N_s \) is the number of sampling points. The sampling points are specific angles of interest (for an angular distribution of a material property) or specific orientations in the fundamental region (for an ODF optimization problem). \( \Upsilon_{\text{desired}} \) is a discrete representation of the desired microstructural property and \( \alpha \) is the design parameter represented as:

\[ \alpha = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7, \alpha_8\} \quad (5.16) \]
The optimization process consists of computing the gradients of various Eulerian fields $\mathbf{Y}$ that are represented as: $\nabla \mathbf{Y} = \left( \frac{\partial \mathbf{Y}}{\partial \alpha_1}, \frac{\partial \mathbf{Y}}{\partial \alpha_2}, \ldots, \frac{\partial \mathbf{Y}}{\partial \alpha_n} \right)$ with $n = 8$.

These gradients are evaluated from continuum sensitivity fields $\check{\mathbf{Y}}$ (see Section 5.1) as follows:

$$\frac{\partial \mathbf{Y}}{\partial \alpha_i} = \frac{\check{\mathbf{Y}}(r, t; \alpha_1, \alpha_2, \ldots, \alpha_i, 0, \ldots, 0, \Delta \alpha_i, 0, \ldots, 0)}{\Delta \alpha_i} \quad (5.17)$$

The evaluation of the gradient requires $n = 8$ continuum sensitivity problems where the $i^{th}$ sensitivity problem is driven by $\Delta \alpha_i$ with $\Delta \alpha_j = 0$ for $j \neq i$. Thus, for computing the sensitivity fields one nonlinear direct problem and $n$ linear sensitivity problems are needed (a total of $n + 1$ problems). In comparison, the finite difference method (FDM) needs solution to $n + 1$ nonlinear direct problems to evaluate $\nabla \mathbf{Y}$. The problem definition considers the entire range of permissible control parameters (i.e. largest possible solution space) thus guaranteeing the existence of a solution. The gradient optimization methodology results in a local minimum and other heuristic optimization techniques need to be considered if interested in a global solution. Owing to the highly non-linear nature of the objective function, step size control must be exercised to achieve monotonic convergence. The next section highlights certain applications of the algorithms developed.

6 Numerical analysis

The initial microstructure, in all examples presented here, is assumed to be random. Further, the constants used in the power law (Equation (3.2)) are taken as $\dot{\gamma}_0 = 1.0 \text{ sec}^{-1}$, $m = 0.05$ and $s = 27.17 \text{ MPa} [8]$. The first example considers a hypothetical material with planar microstructure to simplify the computation and highlight the intricacies and effectiveness of the proposed algorithm. Following this, various examples address realistic microstructures associated with f.c.c Copper. Section 6.1 provides an accuracy study for the full-order and reduced-order models. Section 6.2 addresses design problems using the direct, sensitivity analysis and the gradient-based optimization approach highlighted in Section 5.4.

6.1 Evaluation of the direct full-order and reduced-order models and corresponding sensitivity analysis

An accuracy study is conducted by comparing the solutions obtained from the full-order and reduced-order models. In addition, the accuracy of the sensitivity fields computed through the full-order and reduced-order schemes is studied. Note that in all figures with sensitivity plots, the directional derivative is plotted and not the gradient of the field given in Equation (5.17).
6.1.1 Example 1: Modeling the ODF evolution in planar microstructure

This example considers the simulation of the evolution of the ODF, for a planar microstructure, through full-order and reduced-order models. The test velocity gradient was defined as \( \alpha = \{0, 0, 1, 0, 0, 0, 0, 0\} \). The test was conducted for 0.50 seconds at an increment of 0.01 seconds. The fundamental region was taken to be the simply connected region \([-\pi/2, \pi/2]\). The initial ODF is assumed to be uniform and is taken as \( \mathcal{A}(r, 0) = 1/\pi \). The plots describing the reorientation velocity and the divergence of the reorientation velocity are given in Fig. 3. These results are in good agreement to those obtained in [5].

![Fig. 3. The variation of the reorientation velocity and its divergence, respectively, for shear deformation at time t=0.50 seconds (Example 1 - Planar microstructure).](image)

As a first test of the applicability of the reduced-order model, a basis was generated using the data stored during the full-order modeling process. Six modes, that contained the most energy, were selected for the reduced basis. The reduced-order model, discussed in Section 4, was solved for the same deformation history. The ODF obtained by this approach is compared with the ODF obtained through the full-order model and is shown in Fig. 4. The \( L_2 \) norm of error between the ODF obtained from the reduced-order model and the ODF obtained from the full-order model was estimated at 1.1% of the random ODF. The maximum value of the ODF, at an orientation of 0.87 radians, was 5.64 for the full-order model and 5.02 for the reduced-order model.

6.1.2 Example 2: Polycrystal modeling of f.c.c Copper

A uniaxial tension test is conducted on a polycrystal made of f.c.c Copper crystals. The velocity gradient is defined through the design vector as

\[
\alpha = \{1, 0, 0, 0, 0, 0, 0, 0\} \quad (6.1)
\]

The ODF's developed using the full-order model and the reduced-order model, at a plastic strain of 0.2, are shown in Fig. 5. The reduced-order basis was
Fig. 4. Comparison of the ODF obtained using the full-order model and the reduced-order model at the final time for a pure shear test. The full-order model is represented by the dashed lines and the reduced-order model by the solid line. The two solutions are shown to be almost identical (Example 1 - Planar microstructure).

generated from the data of a different uniaxial deformation process, a process with strain rate defined by $\alpha_1 = 0.5$, $\alpha_j (j \neq 1) = 0$. Postprocessing indicates that the $L_2$ norm of the error was about 3.4% of the random ODF. The maximum value of the ODF’s from the full-order model was 7.4 and that from the reduced-order model was 7.2. Furthermore, the maxima and minima were observed at the same location. The reduced-order model consisted of only 3 modes and enormous savings in computational power were observed. The speed up was found to be around 6 without any appreciable loss of accuracy. In addition, this and other similar examples have shown that such reduced-order models work well not only in the interpolatory mode but also in the extrapolatory mode with only a few basis functions.

Fig. 5. The ODF obtained using the full-order and the reduced-order approach at the final strain for a uniaxial tension test (Example 2 - Modeling of f.c.c Copper).
6.1.3  Example 3: Continuum polycrystal sensitivity analysis

The objective of this example is to validate the parameter sensitivity analysis for a deformation process by comparison with the forward finite difference method (FDM). The continuum sensitivity analysis was performed on f.c.c Copper about a reference direct problem described in Example 2. The perturbation to the velocity gradient in terms of a perturbation of the design vector is given as:

\[ \alpha = \{10^{-2}, 0, 0, 0, 0, 0, 0\} \]  

(6.2)

The reference ODF's, obtained from the full-order and reduced-order models, at a strain of 0.2 are shown in Fig. 5. The sensitivity of the ODF is evaluated through 3 different methods: forward-based finite difference approximation (FDM), full-order model and reduced-order model (with the same basis as in Example 2). The sensitivity results obtained from these methods are compared in Fig. 6. It was observed that the \( L_2 \) norm of the error for the full-order model (with respect to the FDM solution) was 6% of the maximum FDM solution. Similar analysis performed on the reduced-order model resulted in an error of about 10%. Further, the maxima and minima of the sensitivity field were under-predicted by the reduced-order modeling approach even though the distributions were similar. It was also observed that as the number of basis functions increased, the quality of the solution approached the full-order model solution.

6.2  Optimization examples

Optimization problems are considered here to highlight the ability of the proposed reduced-order model in design algorithms. The initial guess for the examples are reported separately for each case. The first optimization problem deals with the design/control of the velocity gradient to obtain a desired orientation distribution function (ODF). The second problem is concerned with the design of the velocity gradient so that a particular distribution of the elastic modulus is obtained in the finished product.

6.2.1  Example 4: Design for a desired ODF in f.c.c Copper using full- and reduced-order models

The problem statement is as follows: given a desired ODF distribution - which translates to a desired property distribution - determine the velocity gradient to be imposed on this polycrystal so that the ODF obtained, at a particular plastic strain, resembles the desired ODF. The plastic strain, at which the ODF's are compared, was taken to be 0.2. The desired ODF was originally obtained through a velocity gradient represented as:

\[ \alpha = \{1, 0, 0.866, 0, 0, 0, 0\} \]  

(6.3)
Fig. 6. Comparison of the sensitivity of the ODF obtained using the full-order model, the corresponding reduced-order model and FDM solution at the final time (t = 0.20 seconds) for a uniaxial tension test (Example 3 - Polycrystal sensitivity analysis for f.c.c Copper).

The initial guess to the design problem was zero velocity gradient. The various ODFs - desired ODF, ODF generated from the initial guess and the ODF obtained through the optimal solution (full-order model) are shown in Fig. 7. The progress of the optimization problem is described by the objective function in Fig. 8. The converged (optimal) velocity gradient, obtained from the full-order model, was computed as:

$$\alpha = \{0.962, 0, 0.867, 0, 0, 0, 0, 0\}$$  \hspace{1cm} (6.4)

This design problem was also repeated using the reduced-order model. The reduced basis was selected, using the methodology discussed earlier, from snapshots taken during deformation problems consisting of shear, tension and plane strain compression. A total of 17 modes were used in this analysis. The desired and optimal ODF fields are seen in Fig. 9 together with the variation of the objective function. The optimal velocity gradient, obtained from the
Fig. 7. The ODF at various solution stages (desired, initial and optimal) in the optimization problem (Example 4 - ODF design using a full-order model for f.c.c Copper polycrystal).

Fig. 8. Variation of the objective function with optimization iterations for a problem with realistic polycrystal analysis (Example 4 - ODF design using a full-order model for FCC Cu polycrystal).

reduced-order model, was computed as:

\[ \alpha = \{0.93, 0, 0.862, 0, 0, 0, 0, 0\} \]  

(6.5)
6.2.2 Example 5: Control of microstructure-sensitive properties

An application of the control of microstructural properties is demonstrated through this example. The velocity gradient (through $\alpha$) is controlled/designed to obtain a specific distribution of the elastic modulus about the normal direction. The desired distribution is obtained through a uniaxial tension test with the velocity gradient expressed in terms of $\alpha$ as:

$$\alpha = \{0.6, 0, 0, 0, 0\}; \quad \alpha_6 = \alpha_7 = \alpha_8 = 0$$

(6.6)

The elastic modulus was evaluated through the following procedure:
• The stiffness in a crystal in the crystal lattice frame is taken to be:

\[
C = \begin{bmatrix}
168.0 & 121.4 & 121.4 & 0 & 0 & 0 \\
121.4 & 168.0 & 121.4 & 0 & 0 & 0 \\
121.4 & 121.4 & 168.0 & 0 & 0 & 0 \\
0 & 0 & 0 & 75.4 & 0 & 0 \\
0 & 0 & 0 & 0 & 75.4 & 0 \\
0 & 0 & 0 & 0 & 0 & 75.4 \\
\end{bmatrix} \text{ GPa} \quad (6.7)
\]

• The polycrystal stiffness, \( \bar{C} \), was computed through a weighted average of the stiffness of individual crystals expressed in the sample reference frame. The weighting factor is the ODF expressed over the fundamental region.

• The elastic modulus was then computed through this polycrystal stiffness by:

\[
E = \frac{1.0}{(\bar{C})^{-1}} \quad (6.8)
\]

Furthermore, the elastic modulus at an angle with the rolling direction (RD) can be evaluated through a coordinate transformation of \( \bar{C} \). The calculation of the elastic modulus is described in detail in [3].

The objective function is now defined as follows:

\[
\min_{\alpha} \mathcal{F}(\alpha) = \frac{1.0E + 05}{N_s} \sum_{i=1}^{N_s} \left( \log(E_i(\alpha)) - \log(E_{\text{desired}}^i) \right)^2 \quad (6.9)
\]

where \( N_s \) is the number of sampling points, taken here to be 19 ranging from 0° to 90° at 5° intervals, and the elastic moduli are expressed in GPa. The initial guess was chosen around the design solution as

\[
\alpha = \{0.4, 0.1, 0, 0, 0\} \quad (6.10)
\]

Fig. 10 compares the distribution of the elastic moduli (about different axis rotated around the RD) at different stages of the design process. Also shown in the Fig. 10 is the desired distribution (shown with dashed lines) and the distribution obtained from a random texture (i.e. isotropic material).

The optimum velocity gradient was obtained as:

\[
\alpha = \{0.674, 0.142, 0.082, -0.012, 0.029\} \quad (6.11)
\]
Fig. 10. Comparison of the distribution of the elastic modulus at different stages of the optimization process and the variation of the objective function with optimization iterations (Example 5 - Design for desired elastic modulus).

The variation of the objective function is also shown in Fig. 10. Though this solution (a local minimum) is not very close to the exact solution defined in Equation (6.6), the distribution obtained is very similar to the one desired.

7 CONCLUSIONS AND DISCUSSION

The paper presented a new direction towards explicit control of microstructure-sensitive properties using a virtual design laboratory. A reduced-order theory has been proposed for modeling the evolution of microstructure during deformation processing. In addition, an Eulerian continuum sensitivity problem was defined. It was then used in a gradient-based optimization framework for the design of deformation processes towards control of microstructure. Examples have been presented highlighting the potential benefits of this method. Complex material behavior and more realistic deformation mechanisms can easily be introduced in the present analysis including the effects of elastic stretching.

The sufficiency of a basis in the reduced-order modeling process needs to be examined. Adaptive selection of basis functions from a larger sample space may lead to optimal performance of the design algorithm. Many computational tools are available to address such problems. Recent research activities indicate that posing and solving classification problems can help in making an educated guess for the design problem. Such a classification algorithm would need to be a learning process where models are trained with data from different processes. In addition to direct high-fidelity numerical simulations, the use of experimental data is an alternative way to design low-order state models for the ODF evolution. Using experimentally obtained pole figures, the possibility exists of providing snapshots of the ODF that are true representations to the underlying physics and in addition cover a wide range of responses in the parameter space.
Finally, research is planned to integrate the present methodology with the computational process design algorithms developed earlier [20]-[24]. This integration may allow the development of a computational design laboratory for process selection that leads to products of desired microstructure-sensitive material properties.

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