On the design of polycrystalline materials with an integration of multiscale modeling and statistical learning

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Abstract: A sophisticated though efficient and accurate multiscale stochastic framework for uncertainty quantification has been developed to investigate the mechanical property variability of polycrystalline materials due to diverse sources of uncertainties. Crystal plasticity constitutive model is employed as the point simulator to capture the mechanical response of polycrystalline microstructures under deformation in the mesoscale. Homogenization techniques are introduced to link the meso- and macro-scales. Stochastic partial differential equations are solved via an adaptive sparse grid collocation method with the assistance of model reduction techniques for the input space. The probabilistic distribution of the macroscale properties/responses of the material subjected to a specific process induced by the uncertainty in initial microstructure is studied based on the current framework. A statistical learning approach is also developed for the design of polycrystalline materials. Support vector machine and x-means clustering are introduced as the classifier of microstructural features. Sensitivity-based optimization method is utilized for the design of processes.

1. Motivation and work summary. The effect of diverse sources of uncertainties and the intrinsically multiscale nature of physical systems poses a considerable challenge in their analysis. Such phenomena are particularly critical in material systems where the microstructural variability and randomness at different scales have a significant impact on the macroscopic behavior of the system. Our goal is to develop a novel, high-fidelity multiscale stochastic framework to study mechanical response/properties variability of materials/structures due to uncertainties in microstructural features, processing parameters, etc. The design of processes which can produce desired microstructure and properties is also of interest. Mathematical tools for both simulating material deformation and probabilistic learning are developed. The major achievements are listed below:

- Development of crystal plasticity constitutive model to evaluate mechanical responses of polycrystalline microstructures subjected to deformation.
- Development of multiscaling strategy linking mesoscale features to macroscale properties through homogenization techniques.
- Development of a non-linear model reduction strategy to construct stochastic input models of mesoscale topology variations based on limited data (emphasis on polycrystalline materials).
- Development of an adaptive hierarchical sparse grid collocation algorithm for solving stochastic partial differential equations.
- Development of stochastic paradigms to investigate mechanical properties/response of polycrystalline microstructures due to uncertainties in microstructural features.
- Development of a stochastic multiscale paradigm to address simultaneously the effects of randomness and multiscale nature of physical systems.
- Development of a stochastic optimization technique for robust design of deformation processes of polycrystalline metals based on statistical learning.

2. Crystal plasticity constitutive model. Plastic deformation of FCC crystals is primarily controlled by slips of atoms constrained on certain slip systems. In order to study mechanical behavior of crystalline materials subjected to deformation, continuum slip theory is taken into the constitutive model. A total Lagrangian scheme developed in [1] is implemented with Newton-Raphson linearization of the principle of virtual work to solve the governing equations due to the non-linear nature of the large deformation problem. The complete procedure is detailed in [1,2]. In recent work, we extended the single phase FCC constitutive model to two-phase ( γ and γ' phase) nickel-based superalloys. The large size primary γ' phase is explicitly modeled as individual grains distributed among homogenized γ grains which contain small secondary and tertiary γ' precipitates. Comparing with our original single-phase model, two main changes are made. First, two separate constitutive models are explicitly programmed. Distinct material parameters are calibrated for γ' grain and homogenized γ matrix. Secondly, cube slip systems
\{110\}\{001\} are introduced to take cross slip mechanism at high temperatures into consideration. The nickel-based superalloy constitutive equations [3] are summarized below. The model can be easily extended to more general two-phase crystalline materials.

For both phases, the total deformation gradient \( F \) is decomposed into elastic and plastic parts, i.e., \( F = F^e F^p \). The plastic deformation, produced by collective motion of dislocations on slip planes, leaves the crystal lattice undeformed, whereas the elastic deform leads to stretch and rigid body rotation of the lattice. The resolved shear stress on the \( \alpha \) th slip system is given as

\[
\tau^{(\alpha)} = \mathbf{T} : S^{(\alpha)} = \mathbf{T} : (\mathbf{m}_s^{(\alpha)} \otimes \mathbf{n}_s^{(\alpha)})
\]

where \( \mathbf{T} \) is the local PK-II stress and \( \mathbf{m}_s^{(\alpha)} \) and \( \mathbf{n}_s^{(\alpha)} \) are vectors in the slip direction and normal to the slip plane, respectively, in the initial configuration. When the resolved shear stress is larger than the slip resistance \( \kappa_0^{(\alpha)} \), dislocations start to slide on the plane. \( \mathbf{T} \) is related to elastic deformation gradient \( F^e \) by

\[
\mathbf{T} = \mathbf{C}^e \mathbf{E} = \frac{1}{2} \mathbf{C}^e (F^e F^e - \mathbf{I})
\]

The homogenized \( \gamma \) matrix with dispersion of secondary and tertiary \( \gamma \) follows the flow rule:

\[
\gamma^{(\alpha)} = \dot{\gamma}_0 \Theta(T) \left[ \frac{\tau^{(\alpha)} - \kappa_0^{(\alpha)} - \rho^{(\alpha)}}{D^{(\alpha)}} \right] \exp \left( B_0 \left[ \frac{\tau^{(\alpha)} - \kappa_0^{(\alpha)} - \rho^{(\alpha)}}{D^{(\alpha)}} \right] \right) \text{sgn}\left( \tau^{(\alpha)} - \kappa_0^{(\alpha)} \right)
\]

where \( \dot{\gamma}_0 \) is the initial shearing rate, \( \chi^{(\alpha)} \) is a back force term, which model the Baushinger effect arising principally from matrix dislocation interaction with primary \( \gamma \), \( D^{(\alpha)} \) is the drag stress assumed to be constant, and \( \Theta(T) \) is the diffusivity parameter dependent on temperature \( T \).

The evolution of the slip resistance \( \kappa_0^{(\alpha)} \) (\( \lambda = \text{cub, oct} \)) follows strain hardening law determined by dislocation density \( \rho^{(\alpha)} \)

\[
\dot{\kappa}_0^{(\alpha)} = k_0^{(\alpha)} + \alpha u_b \sqrt{\rho^{(\alpha)}}
\]

and

\[
\dot{\rho}_s^{(\alpha)} = \sum_\beta k^{(\alpha \beta)} \left\{ Z_0 + k_{1,\beta} \sqrt{\rho_s^{(\alpha)}} - k_{2,\beta} \rho_s^{(\beta)} \right\} \dot{\gamma}^{(\beta)}
\]

The evolution of the back stress \( \chi^{(\alpha)} \) is also based on dislocation density and shearing rate

\[
\chi^{(\alpha)} = \{ \eta ub \sqrt{\rho^{(\alpha)}} \text{sgn} \left( \tau^{(\alpha)} - \kappa_0^{(\alpha)} \right) \} |\gamma^{(\alpha)}|,
\]

where \( \eta = \frac{n_0 Z_0}{Z_0 + k_{1,\alpha} \sqrt{\rho^{(\alpha)}}} \). In \( Z_0 \), \( d \) represents spacing of large precipitate that introduces length-scale effects. A material point of the solid solution matrix phase situated very close to a primary \( \gamma \) grain has higher dislocation density due to geometrically necessary dislocations (GNDs). Hence, each point in the matrix has a different spacing term (\( d \)) corresponding to the distance to the nearest primary \( \gamma \) grain boundary in the slip direction [3]. It can be seen that this constitutive model is a system of nonlinear equations; functions are correlated with each other through shared parameters. To solve for the quantities, we developed an implicit iterative algorithm.

For primary \( \gamma \) grains, we explicitly developed a constitutive model. The flow rule does not have the back force term

\[
\gamma^{(\alpha)} = \dot{\gamma}_0 \Theta(T) \left[ \frac{\tau^{(\alpha)} - \kappa_0^{(\alpha)} - \rho^{(\alpha)}}{D^{(\alpha)}} \right] \exp \left( B_0 \left[ \frac{\tau^{(\alpha)} - \kappa_0^{(\alpha)} - \rho^{(\alpha)}}{D^{(\alpha)}} \right] \right) \text{sgn}\left( \tau^{(\alpha)} \right)
\]

The hardening law is also a modified Taylor strain hardening model but the octahedral slip systems differ from cube slip systems.

\[
k_0^{(\alpha)} = k_0^{(\alpha)} + \alpha u_b \sqrt{\rho^{(\alpha)}}
\]

and

\[
\dot{\rho}_s^{(\alpha)} = \sum_\beta \{ h^{(\alpha \beta)} \left\{ Z_0 + k_{1,\beta} \sqrt{\rho_s^{(\alpha)}} - k_{2,\beta} \rho_s^{(\beta)} \right\} \dot{\gamma}^{(\beta)}
\]

\[
- h_0 \Theta(T) \{ \rho_s^{(\alpha)} - \rho_s^{(\alpha)} \}
\]

The evolution of the back stress \( \chi_0^{(\alpha)} \) is also based on dislocation density and shearing rate
\[ \rho_{\text{el}}^{(a)} = \sum_{\rho} h^{(a)} \left[ k_{\text{el}} \sqrt{\rho_{\text{el}}^{(b)}} - k_{\text{el}} \rho_{\text{el}}^{(b)} + k_{\text{el}} \right] \]
\[ k_{\text{el}} \frac{1}{h_{\text{el}}} \exp \left( -\frac{H_{\text{el}}}{RT} \right) - k_{\text{el}} \Theta \left( \rho - \rho_{\text{el}}^{(b)} \right) \]

The constitutive parameters can be calibrated by either the experimental data [3] or the results from lower scale simulations, such as dislocation dynamics.

The plastic deformation gradient is then updated by
\[ F^p = \left( I + \sum_{\rho} \Delta \epsilon^{(a)} S_{\rho} \text{sgn}(\epsilon^{(a)}) \right) F^p \]

Grain orientations are changed by elastic deformation gradient as
\[ m^a = F^e m_0^a \]
\[ n^a = F^e n_0^a \]

2. Multiscaling strategy. The mechanical response of single grains are evaluated using the crystal plasticity constitutive introduced above, while the deformation of the microstructure is coupled with the local deformation at a typical material point of the macro-continuum in a multiscale simulation. In a deformation driven process, this coupling can be defined by three alternative constraints of the microstructure deformation: (1) Zero fluctuation in the domain (Taylor assumption); (2) zero fluctuation on the boundary (homogenization assumption); or (3) periodic fluctuations on the boundary [4]. The macroscopic responses, such as stress and strain, are investigated as the volume-average of the microscopic values. For example, the macroscopic Cauchy stress \( \hat{T} \) and average plastic rate of deformation \( \bar{D} \) are calculated from the micro quantities. They are the bridging variables linking microscale to macroscale.
\[ \hat{T} = \left\langle \nabla \right\rangle = \frac{1}{V_{\Omega(\text{B})}} \int_{\Omega(\text{B})} T dV \]
\[ \bar{D} = \left\langle \nabla \right\rangle = \frac{1}{V_{\Omega(\text{B})}} \int_{\Omega(\text{B})} D dV \]

While the zero and periodic fluctuation on boundary lend more accurate estimation to the microstructure response, Taylor assumption is computationally more efficient. Applying current constitutive model and zero fluctuation on boundary to realistic 3D single phase polycrystalline copper microstructures (Fig.1(a)) with random orientation distribution, the effective stress-strain response is captured using a in-house finite element solver and compared with literature [1].

The texture (orientation distribution) after compression is described in pole figures and also compared with [1].

A two-phase nickel-base superalloy example is also conducted. Constitutive parameters are obtained from [3] that were calibrated from the experimental data. A macroscopic hysteresis loop is depicted in Fig.3. The current model will be extended to the study of strain based fatigue crack formation.

![Fig.1](image1.png) (a) A realistic microstructure realization generated by phase field method. (b) Effective stress-strain curve of compression of the microstructure.

![Fig.2](image2.png) Texture pole figures of a polycrystalline microstructure subjected to uniaxial compression.

![Fig.3](image3.png) Macroscopic hysteresis loop of nickel-base superalloy microstructure. (a) Current work; (b) simulation and experimental results from [3].
We also embedded our point simulator into an in-house Lagrangian simulator. A necking test of a polycrystalline nickel strip is presented. We trigger the necking by assigning microstructures with different mean grain sizes. Since grains with large size tend to present lower strength, they are attached to the Gauss points in the middle part of the strip. To the contrary, small grains are assigned to the top and bottom of the strip. Taylor homogenization is employed to reduce the computation cost of the multiscale simulation. The effective strain fields of the strip at different stages are plotted below.

![Multiscale simulation of necking of a strip.](image)

**Fig.4** Multiscale simulation of necking of a strip. (a) Discretization of the strip. Microstructures with large grain size are assigned to the middle of the strip, while small grains are assigned to the top and bottom. (b) Deformation and equivalent strain when the tensile force reaches the peak value. (c) Deformation and equivalent strain when obvious necking is observed.

3. **Data-driven methodology to construct stochastic input models of mesoscale topological/orientational variations.** Properties of the products depend on underlying microstructures, which, in essence, is a high dimensional random field. Study of the variability of mechanical properties/response due to uncertainties in microstructures is essential for microstructure-sensitive design applications in industry. The importance of performing stochastic analysis on heterogeneous media necessitates the development of realistic input models of the microstructural features. The thermal, mechanical and chemical behavior of microstructures is highly anisotropic and heterogeneous, depending on the randomness of features of importance. For instance, orientation of the crystals as well as the nature of the grain size represents sources of randomness in polycrystalline materials. Knowledge about the feature/property variation of a polycrystalline material is usually only in a statistical sense (say, grain size distribution and the texture map). To provide reliable failure criteria for critical applications involving such materials, it becomes imperative to access this variability in properties, quantify it and predict its effect on the performance of the system. Stochastic analysis of random heterogeneous media provides information of significance only if realistic input models of the topology and material property variations are used. We have introduced a framework to construct such stochastic input models for the mechanical properties/response variations in polycrystalline microstructures using a data-driven strategy. Given a set of microstructure realizations (input samples) generated from given statistical information about the medium topology, the framework constructs a reduced-order stochastic representation of the topology and material properties. This problem of constructing a low-dimensional stochastic representation of microstructural variations is analogous to the problem of manifold learning and parametric fitting of hyper-surfaces encountered in image processing and psychology.

### 3.1 Manifold learning on grain size:

The grain sizes of microstructure samples resulted from similar processes usually satisfy the same statistics such as mean grain size, standard deviation, and some higher order moments. With these constraints, the grain size representation (grain size vector or histogram) can be treated as ‘points’ lying on a manifold \( \Omega \in \mathbb{R}^d \) embedded in high dimensional space. The model reduction strategy is based on the so-called principle of “manifold learning” [5]. The mathematical framework is to “unravel and smooth the” (Fig.5) this manifold and represent it as a smooth low-dimensional curve \( \Gamma \in \mathbb{R}^d \). The key notion is that by keeping specific geometrical features of the embedded manifold invariant one can construct a low-dimensional representation that is equivalent to the manifold. A natural choice of a geometric feature is the distance metric. This results in an isometric mapping to transform \( \Omega \) into \( \Gamma \). The important idea is that the distance encodes the geometric information about the non-linear manifold in the geodesic distance. The geodesic distance reflects the true geometry of the manifold embedded in the high-dimensional space.

![Unraveling and smoothing the 3D spiral into a 2D sheet.](image)

**Fig.5** Unraveling and smoothing the 3D spiral into a 2D sheet.

Construction of \( \Gamma \) reduces to finding a low-dimensional representation \( \{y_i, i = 1, \ldots, M\} \) of the given data points (e.g. grain size histograms) \( \{y_{i,}^0, i = 1, \ldots, M\} \)
such that \( \{ y_i \} \) is isometric to \( \{ Y^d_i \} \) based on the geodesic distances between points. The principle of multi-dimensional scaling (MDS) can subsequently be used to compute the set of low-dimensional points that best represent the high-dimensional points. The MDS procedure essentially computes the eigen-decomposition of the geodesic matrix and sets the low-dimensional points as linear combinations of the nearest \( N \) eigenvectors of the geodesic matrix. The convex hull \( \Gamma \) of the low-dimensional points \( \{ y_i, i = 1, \ldots, M \} \) defines the surrogate low-dimensional space all possible microstructures that belong in the initial high-dimensional manifold.

3.2 Karhunen-Loeve expansion on texture. The texture of a microstructure is preferred orientation distribution of the grain components. This distribution is usually described by an orientation distribution function (ODF) defined in Rodrigues space for cubic crystals. It can be defined as a function of Rodrigues parameter \( r \) and random field \( w \), having the form of \( \Lambda = A(r, w) \). Assume we are given a set of texture samples and we want to compute the underlying random texture process (to be used as our input model in e.g. stochastic forging analysis). The unbiased estimation of covariance matrix of the initial texture samples \( \{ A(r, w), i = 1, \ldots, N \} \) is constructed at first,

\[
C = \frac{1}{N-1} \sum_{i=1}^{N} (A_i - \bar{A})^t (A_i - \bar{A}), \quad \bar{A} = \frac{1}{N} \sum_{i=1}^{N} A_i \quad (16)
\]

The KL expansion of the random vector \( \hat{A} \) is

\[
\hat{A}(r, w) = \bar{A}(r, w) + \sum_{i} \sqrt{\lambda_i} \phi_i(r) \eta_i(w)
\]

(17)

where \( \phi_i, \lambda_i \) are the ith eigenvector and eigenvalues of \( C \). Uncorrelated random variables \( \eta_i(w) \), having the same dimensionality \( n \) with \( \Phi \), satisfy the following properties

\[
E(\eta_i(w)) = 0, \quad E(\eta_i(w)\eta_j(w)) = \delta_{ij}, \quad i, j = 1, \ldots, n
\]

(18)

\( \eta(w) \) can be truncated to lower dimension \( d \) guaranteeing that the first \( d \) principle eigenvalues can capture most energy. In this manner, the high dimensional random space is reduced to a low dimensional space \( \eta \in \mathbb{R}^d \). Using Maximum Entropy Estimation (MaxEnt) [6,7], we can construct the least biased distribution for \( \eta \) as multi-variant Gaussian distribution with the satisfaction of the two constraints. Adopting Rosenblatt transformation [8], the multi-variant Gaussian distribution of \( \eta \) will be mapped to a unit hypercube, which is the sample space for the sparse grid collocation method (to be discussed later on).

Utilizing the above model reduction methodology, the dimensionality (i.e. the number of independent random variables) of the microstructure representation can be significantly reduced. Combining the reduced representation of microstructure features we can investigate the variability of the resulting microstructures and properties at one point of the macro-continuum at a given deformation process. The collocation method that we propose to use for this purpose is based on sparse grids.


The above generated low-dimensional representation of the stochastic fine-scale material property is utilized as an input stochastic model for the solution of SPDEs. We utilize an adaptive sparse grid collocation (ASGC) strategy for constructing the stochastic solution. The basic idea of ASGC is briefly describe in this paper. More details are given in our recent work in [9,10]. This technique is general as it can be applied for creating a high-dimensional interpolant (in the stochastic space) to the solution of any stochastic PDE physical system using only the deterministic solver as a black box simulator.

The sparse grid collocation is to approximate the multi-dimensional stochastic space \( L \) using interpolating functions on a set of collocation points \( \{ \xi_{i,j}^l \}_i \in L \). The collocation method collapses the multidimensional problem (based on the Smolyak algorithm) to solving \( M \) (\( M \) is the number of collocation points) deterministic problems. One computes the deterministic solution at various points in the stochastic space and then builds an interpolated function that best approximates the required solution. Notice, during the process, the mapping \( F^{-1} \) from low-dimensional surrogate \( L \) to high-dimensional microstructural space \( H \) needs to be implemented, so that the deterministic solver can work. In the context of incorporating adaptivity, Newton-Cotes grid is utilized with equidistant support nodes. Hierarchical basis is used in constructing the interpolant. The interested function \( u(t, \xi) \) can be approximated by

\[
\hat{u}_{d,q}(t, \xi) = \sum_{H_{d,q}} \sum_{k=1}^{B_{d,q}} w_i^j(t) \cdot a_i^j(\xi) \quad (19)
\]

The mean of the random solution is evaluated as

\[
E(\hat{u}_{d,q}(t, \xi)) = \sum_{H_{d,q}} \sum_{k=1}^{B_{d,q}} w_i^j(t) \cdot \int_{L} a_i^j(\xi) d\xi \quad (20)
\]

where \( q \) is the depth (level) of sparse grid interpolation and \( d \) is the dimensionality of stochastic space. \( B_{d,q} \) is a multi-index set. \( w_i^j \) is the hierarchical surplus, which is the difference between the function value \( u(t, \xi) \) at the
current point $\xi$ and interpolation value $\hat{u}_{d,i}(t,\xi)$ from the coarser grid in the previous level. $a^j_i$ is the $d$-dimensional multi-linear basis functions defined by tensor product. With increasing level of interpolation, new support nodes are added to the hypercube if the error indicator

$$
\gamma^j_i = \frac{\left\| w^j_i \int_{I^n} a^j_i(\xi) d\xi \right\|_{L^2}}{\left\| E_{\mathbf{H}_{d-1}} \right\|_{L^2}}
$$

(21)

is larger than a threshold $\gamma$. The error indicator $\gamma^j_i$ measures the contribution of each term in Eq. (20) to the integration value (mean of the interpolated function) relative to the overall integration value computed from the previous interpolation level. After the ASGC has been performed, solutions of the SPDEs have been computed as an interpolant in the stochastic support space that defines the microstructure variability. Using this high-dimensional interpolant of the mechanical response, one can compute statistical quantities of interest such as realizations, moments and the probability density function (PDF) using kernel density estimation.

5. Variability of mechanical properties/response due to uncertainties in microstructural features. With the development of the techniques above, we are able to investigate the variability of mechanical properties/response of microstructures due the uncertainties in their features (grain size and texture). Two examples are presented below to demonstrate the variability of mechanical properties/response of polycrystalline microstructures due to uncertainties in microstructural features (emphasis is on grain size and texture) and process parameters (deformation mode).

5.1 Variability of mechanical response due to grain size and texture uncertainties. Grain size samples are first generated satisfying certain statistical constraints (the mean size, standard deviation, and/or third order moment). Each sample contains 54 grains resulting in a 54-dimensional vector. Texture samples are also generated from a sequence of random deformation processes (e.g. by taking the forging rate to vary). Since each orientation has 3 components, a texture vector has 162 components. Non-linear model reduction and Karhunen-Loeve Expansion schemes are employed to reduce the dimensionality of grain size and texture vectors, respectively. With the reduced representation of microstructural features as random input, ASGC is applied to solve the stochastic partial differential equations (kinematics and constitutive equations) and estimate the variability of mechanical response of random microstructures subjected to uniaxial compression. The deterministic solver adopted is the single phase crystal plasticity constitutive model along with Taylor homogenization hypothesis (all grains have the same deformation gradient). The effects of grain size and texture on mechanical response of FCC nickel microstructures are examined. The material parameters are chosen from [2,11]. Only a few results are shown in this report. More information is provided in [12].

The distributions of macroscopic equivalent stresses at 0.2 strain of microstructures satisfying different grain size and/or texture constraints are plotted in Fig. 6. It is observed that equivalent stress distribution is narrowed when higher order moments of grain size are constrained. The texture generated from a process with higher randomness leads to wide distribution of mechanical response.

5.2. Mechanical property variability due to texture and process parameter uncertainties. The quantification and propagation of uncertainty in process conditions and initial microstructure on the final product properties in a deformation process are also interested. In this section, we will demonstrate a complete example that investigates the mechanical property (Youngs modulus, shear modulus, and bulk modulus) variability of single phase polycrystalline microstructures using the methods we have developed [13]. The stochastic deformation problem was modeled using the sparse grid collocation approach. The ability of the method in estimating the statistics of the macro-scale microstructure-sensitive properties and constructing the convex hull of these properties is shown through the example featuring randomness in initial texture and process parameters. In modeling the
texture evolution, the random initial texture was represented as a random field. The Karhunen-Loeve expansion together with a maximum entropy approach is used for reducing randomness in initial texture in a low-dimensional surrogate space.

The crystal plasticity constitutive model with Taylor hypothesis is adopted to evaluate the properties of a microstructure under deformation. A Lagrangian scheme for updating orientation distribution function (ODF) is used to capture the texture evolution by assuming a continuous random field of ODF. The ODF conservation equation and is given as follows

\[
\frac{\partial A(s,t)}{\partial t} + A(s,t)\nabla \cdot v(s,t) = 0 \tag{22}
\]

where \(v(s,t)\) is the re-orientation velocity of the crystals and the ODF, \(A(s)\), is subjected to \(A(s,0) = A_0(s)\) as the initial condition.

The uncertainty in the problem we consider comes from: (a) variation in the initial texture: \(A(s, \omega), s \in \Omega, \omega \in \Omega\) and (b) variation in the velocity gradient representing the variation in process parameters: \(L(\omega), \omega \in \Omega\). The velocity gradient is written in terms of various deformation modes such as tension, compression, plain strain compression, shear and rotation. The coefficients of these terms \(\beta_1, \ldots, \beta_6\) can be assumed as random variables to represent variation in process conditions.

\[
L = \begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_1 \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_2 \begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_3 \begin{bmatrix}
-1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_4 \begin{bmatrix}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_5 \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 0 & 0 \\
\end{bmatrix} + \beta_6 \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0 \\
\end{bmatrix} \tag{23}
\]

The incompressibility condition is assumed here and only eight component of \(L\) are independent and hence \(\beta\) consists of eight components, as well. We use a random field, \(A_0(s, \omega): s \in \Omega, \omega \in \Omega\) to represent the variability of the initial texture. The stochastic partial differential equation for the evolution of texture, \(A(s,t,\omega): \Omega \times [0,T] \times \Omega \rightarrow \mathbb{R}^+ \cup \{0\}\), can be written by modifying Eq. (22):

\[
\frac{\partial A(s,t,\omega)}{\partial t} + A(s,t,\omega)\nabla \cdot v(s,t,\omega) = 0 \tag{24}
\]

Maximum entropy (MaxEnt) principle is employed to seek a joint probability distribution of the low-dimensional random texture representation. Applying ASGC method, the SPDEs are solved. The convex hull of properties was obtained from a material subjected to uncertain process parameters and initial texture. This can be important in providing us with the means to quantify how well process conditions and microstructure need to be known to attain desired properties but also to identify risks (e.g. failure probabilities) affiliated with critical values of the material properties. To the best of our knowledge this is the first time these concepts have been explored in the analysis and design of polycrystalline materials. Figure 7 shows the convex hull of Bulk modulus, shear modulus and Young modulus for copper in a given deformation process.

![Convex hull of Bulk modulus, shear modulus and Young modulus for copper](image)

**Fig.7** The convex hull of bulk modulus, shear modulus and Young modulus for polycrystalline copper obtained in tension for random initial texture (uncertainty driven by data). Extreme properties can be identified together with the affiliated probabilities. These unique ideas are very important not only for design under uncertainty but also for failure prediction from extreme scenarios.

6. Microstructure model reduction and uncertainty quantification in multiscale deformation processes. When the stochastic problem comes into multiscale, the uncertainty in microstructures becomes a function of spatial location. The dimensionality of the random field increases dramatically. We developed what we think is the first framework for stochastic multiscale deformation processes [14]. Including the underlying microstructure and its evolution for every integration point on macroscale is essential in quantifying the effect of deformation process on macroscale properties. A reduced-order model for representing the data-driven stochastic microstructure input is developed. The multiscale random field representing the random microstructure is decomposed into few modes in different scales (the Rodrigues space for representing texture on mesoscale and the continuum macroscale space). Realizations from a stochastic simulation are used to obtain a small number of modes approximating
the stochastic field. Then a bi-orthogonal expansion is used to describe the variability of the initial microstructure. The coefficients of the polynomial chaos terms in this expansion are obtained using projections of the random modes on the chaos polynomials.

Each integration point on the macro scale is associated with a random microstructure. We consider simultaneously model reduction on both scales. To reduce the stochastic dimensionality, we use all microstructure data at all points in the continuum in a bio-orthogonal KL expansion that allows us to reduce the number of random variables that drive the multiscale simulation. In essence the model accounts for the microstructure correlation from point to point in the continuum and at the same time produces spatial eigenfunctions.

Assume an $L^2$ random field $\tilde{a}(x,s,\omega)$ defined on a probability space $(\Omega, F, P)$.

$$\tilde{a}(x,s,\omega): D \times \Re \times \Omega \rightarrow \Re$$

(25)

where $D$ is the spatial domain, $\Re$ is the fundamental part of Rodriguez space, $\Omega$ is the set of elementary events and $\omega \in \Omega$ is the vector of random inputs. One can use KL expansion to express this field by a bi-orthogonal representation in the form

$$\tilde{a}(x,s,\omega) = \overline{a}(x,s) + \hat{a}(x,s,\omega)$$

(26)

where $\overline{a}$ is defined as $\overline{a}(x,s) = \{\tilde{a}(x,s,\omega)\}$ and $\{\cdot\}$ is the averaging operation; $\rho_i$ are eigenvalues of the eigenvalue problem defined later, the $\psi_i$ are modes strongly orthogonal in Rodrigues space, $\Phi_i$ are spatial modes weakly orthogonal in space with respect to an inner product defined as

$$\langle f, g \rangle = \int_{D} \langle f, g \rangle \, dx$$

(27)

$$\langle f, g \rangle = \int \langle f(\omega), g(\omega) \rangle p(\omega) \, d\omega$$

(28)

where $p(\omega)$ is the probability distribution. The strong orthogonality of $\psi_i$ modes in Rodrigues space can be written as

$$\langle \psi_i, \psi_j \rangle = \int_{\Omega} \psi_i(\omega) \psi_j(\omega) \, d\omega = \delta_{ij}$$

(29)

and the weak orthogonality of spatial modes can be written as

$$\langle \Phi_i, \Phi_j \rangle = \delta_{ij}$$

(30)

By minimizing the distance (based on the norm defined in Eq. (27) between the KL expansion and the random field, one ends up with

$$\psi_i(s) = \frac{1}{\sqrt{\rho_i}} \langle \hat{a}, \Phi_i \rangle$$

(31)

and from the orthogonality condition

$$\Phi_i(x,\omega) = \frac{1}{\sqrt{\rho_i}} \int_{\Omega} \langle \hat{a}(x,s,\omega) \psi_i(s) \rangle \, ds$$

(32)

Eqs. (30) and (32) lead to the following eigenvalue problem

$$\rho_i \psi_i(s) = \int_{\Omega} C(s,s') \psi_i(s') \, ds'$$

(33)

where the covariance $C$ is defined as

$$C(s,s') = \frac{1}{n_r} \sum_{i=1}^{n_r} \sum_{l=1}^{n_r} \hat{a}(x_{i,l}) \hat{a}^T(x_{i,l}) \hat{J}_{\omega} |J_{\omega}|$$

(34)

where $|J_{\omega}|$ is the Jacobian determinant of the element $i_{\omega}$, $\hat{J}_{\omega}$ is the integration weight associated with the integration point $i_{\omega}$, $n_{r}$ is the number of integration points in each element, $n_{r}$ is the number of realizations, $n_{a}$ is the number of elements in macro scale and $\hat{a}$ is a column vector with elements corresponding to integration points in Rodrigues space and $x_{i_{\omega}}$ represents global coordinate of the integration point $i_{\omega}$ in macro scale. The ODF representing the texture takes positive values. Hence, the KL expansion should provide us with positive values. To obtain a positive random field, one can use the KL expansion for $\tilde{a}(x,s,\omega) = \log \left( \hat{A}(x,s,\omega) - A_{min} \right)$ assuming $\hat{A}(x,s,\omega) > A_{min} > 0$ almost surely. The process $\hat{A}$ can be reconstructed as

$$A_{min} + \exp(\tilde{a}(x,s,\omega))$$

(35)

In practice, $\tilde{a}(x,s,\omega) = \tilde{a}(x,s,\xi_1(\omega),...\xi_{n_{a}}(\omega))$, where $\xi_1,...,\xi_{n_{a}}$ are a set of finite number of random variables and $n_{a}$ refers to the number of random variables considered in the problem.

Next, the polynomial chaos decomposition of $\Phi_i(x,\omega)$ can be written as

$$\Phi_i(x,\omega) := \Phi_i(x,\xi_1(\omega),...\xi_{n_{a}}(\omega))$$

(36)

$$= \sum_{j} \phi_j(x) \eta_j(\omega)$$

where $\eta_j(\omega) = \eta_j(\xi(\omega))$ are in a one-to-one correspondence with the Hermite polynomials in Gaussian variables, $\xi(\omega)$ is the vector consisting of $n_{a}$
independent Gaussian random variables \( \{ \xi_1, \ldots, \xi_n \} \) and the coefficients \( \phi_j(x) \) can be obtained from
\[
\phi_j(x) = \frac{\Phi_j(x, \xi)}{\eta_j^2}
\]
(37)
After obtaining the reduced model on the two scales simultaneously, ASGC can be used to solve the resulted SPDEs. This is the first time to introduce a new framework that makes the otherwise intractable task of quantifying the effect of random initial texture in a multiscale problem feasible. Figure 8 shows a representative result of this method of FCC copper forging.

![Fig.8](image)

**Fig.8** (a) Schematic view of the multiscale problem. Each point on this underlying coarse grid corresponds to a different crystal orientation \( R \). The Rodrigues axis-angle parameterization is used as a convenient scheme to represent \( R \). Model reduction is conducted simultaneously on the Rodrigues space and the coarse grid. (b) Mean and variance of the shear modulus obtained from the reduced-order representation of texture. This reduced order representation is then used in a stochastic multiscale simulation to compute the variability of properties in the final product (e.g. forged product) induced from the uncertainty in the initial microstructure [14].

7. A statistical learning approach for the design of polycrystalline materials. Important physical properties such as yield strength, elastic modulus, and thermal conductivity depend on the material microstructure. Realizations of optimal microstructures is important for hardware components in industrial applications. Microstructures can be tailored through controlled deformation or heat treatment. However, identification of the optimal processing path is a non-trivial (and non-unique) problem. We developed a data-mining technique for process design based on the fact that optimal processing paths can be selected by available information from a large database-relating processes, properties, and microstructures [15].

The microstructures of metallic materials are composed of an aggregate of miniscule grains of various shapes and sizes. The large variety of microstructure arrangements can be classified according to either topological descriptor such as grain sizes and shapes, or through orientation descriptors such as ODF. We first developed a microstructure classification approach to create an organized database of microstructural information from which relationships between materials process and microstructures can be identified. The classification of microstructures is based on both topology features (e.g. grain size or correlation function) and orientation features (e.g. ODF).

7.1 Topology feature classification. For topology features, a hierarchical Support Vector Machine (SVM) classifier is employed [16]. The initial SVM is restricted to a two-class problem \( (p=2) \). Its basic idea is to determine a classifier which minimizes the empirical risk (the graining error). Let the \( n \) sets training features (e.g. grain size descriptor extracted from the microstructure samples) given as \( \{ y_i, x_i \}, i = 1, \ldots, n \), where \( y_i \in \{-1,1\} \) are the class labels of the \( i \)th data \( x_i = \{ x_{ij} \}, x_i \in \mathbb{R}^m \). Support Vector Machine finds the optimal separating hyperplane between microstructural features in the \( m \)-dimensional space such that the error for unseen test image features is minimized. The hyperplane is of the form
\[
y = w \cdot x + b
\]
(38)
where \( w = \{ w_1, \ldots, w_m \} \) is the weight vector and \( b \) is a scalar. If the data is nonlinear separable, we can map the them into a feature space which can be linear separated by \( z = \phi(x) \). To allow the possibility of the soft boundary, the hyperplane can be found by maximizing the margin \( \xi \) and minimize the training error simultaneously. The cost function to be minimized is
\[
F(w, \xi) = \frac{1}{2} \| w \|^2 + C \sum \xi_i
\]
(39)
where the purpose of \( C \) is to control the number of misclassified points.
7.2 Orientation Feature Classification. As for the classification of texture, a non-supervised $x$-means clustering algorithm is implemented [17]. The $x$-means is a variant of the traditional $k$-means clustering by treating the number of classes $k$ as unknown. The goal of the clustering is to find the cluster centers \{C_1, ..., C_k\} that the cost function $J$ is minimized,

$$J(C_1, ..., C_k) = \sum_{i=1}^{k} \min_{a \in \{1, ..., n\}} \left( \frac{1}{2} \| x_i - C_a \|^2 \right)$$

(41)

Given the data set $D$, the model chosen should maximize the Bayesian information criterion (BIC) defined as

$$\text{BIC} = \hat{I}(D) - \frac{p}{2} \log(n)$$

(42)

where $\hat{I}(D)$ is the log-likelihood of the data taken at the maximum likelihood point, $p$ is the number of free parameters in the model, and $\text{BIC}$ is the Bayesian information criterion. The maximum of $\text{BIC}$ is then chosen.

In our classifier, lower order features of the ODF are determined in the form of probability density functions of important orientation fibers in the fundamental region of Rodrigues space and are used to create the class hierarchy. These features are extracted from a given desired ODF and pattern recognition is employed to propagate the information over the existing class hierarchy to identify the required texture class and process parameters. Each set in the database is associated with a particular process sequence and corresponding processing parameters and ODF basis for the process that it represents. The final ODF in each data set is used in the classification scheme to identify classes of textures.

Fig.10 The classification hierarchy on topological descriptors.

Fig.11 Results of the $x$-means and $k$-means algorithm on a 2D feature set. The squares represent the cluster centers. (a) Clustering using $k$-means ($k=4$), (b) clustering using $k$-means ($k=6$), (c) clustering using $x$-means.

In our classifier, lower order features of the ODF are determined in the form of probability density functions of important orientation fibers in the fundamental region of Rodrigues space and are used to create the class hierarchy. These features are extracted from a given desired ODF and pattern recognition is employed to propagate the information over the existing class hierarchy to identify the required texture class and process parameters. Each set in the database is associated with a particular process sequence and corresponding processing parameters and ODF basis for the process that it represents. The final ODF in each data set is used in the classification scheme to identify classes of textures.

Fig.12 The classification hierarchy for ODFs.
local optimum within a few iterations. Intelligent choice of initial guesses can be made using prior information available in the form of a database through classification. In the process design problem, the class of desired texture or property distribution is first identified. Required processing parameters and process sequences are then found from the data sets in the identified class. Given the initial processing sequence and parameters, a sensitivity-based optimization scheme identifies the processing parameters can lead to the desired texture or property. Proper orthogonal decomposition (POD) is applied to build a reduced-order optimization process based on reduced ODF basis to simply the design problem.

An example of texture design is demonstrated in Fig. 13. The desired texture is first classified and initial guess would be identified by the classifier. Then, the reduced-order optimization is performed to produce the final texture which is close to the target.

![Fig.13 Control of material texture: (a) the desired texture, (b) the initial guess identified by the classifier and (c) reduced-order optimized ODF.](image)

Another example is given in Fig.14 for the design of processes to match the desired Youngs Modulus.

![Fig.14 Optimization of Youngs modulus distribution: (a) comparison of the desired distribution and optimized distribution and (b) variation of the objective function with iterations.](image)

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9. References:


