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Uncertainty quantification of microstructural properties due to variability in measured pole figures

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ABSTRACT

Experimental pole figures are an important input for microstructure homogenization models. In this paper, we derive an exact analytical formulation to quantify the uncertainties in homogenized properties due to uncertainty in the experimentally measured pole figures. The pole figures are acquired from a set of Ti-7Al alloy samples. These samples were obtained from the same process: by compressing a beta forged ingot at room temperature followed by annealing. The samples were taken from different regions of the original ingot, and this created variability in the resulting pole figures. The joint multivariate probability distributions of the computed orientation distribution function (ODF) is then found using the method of characteristic functions based on a Gaussian model of the pole figures. Engineering properties such as elastic modulus can be obtained by volume averaging over the ODF. We also show that uncertainty in elastic properties can be analytically obtained using direct transformation of random variables in the homogenization approach.

1. Introduction

Integrated Computational Materials Engineering (ICME) (Allison et al. [1]) is an emerging paradigm for materials design that emphasizes integration of material models at multiple length scales with engineering analysis of products and processes. Critical inputs of these material models come from experiments, for example, initial orientation distribution function of the polycrystalline structure is a key input for multiscale crystal plasticity models. However, microstructures are inherently stochastic in nature. In other words, specimens made from the same manufacturing process have variations in microstructure both point-to-point in one specimen and across all specimens. One of the pillars of ICME is uncertainty quantification (UQ) and involves development of mathematical tools to quantify the effect of stochasticity of microstructure on the predicted engineering properties.

Current state of the art involves the use of expensive numerical simulations such as Monte Carlo simulations (MCS), collocation and spectral decomposition methods to quantify the uncertainties. Creuziger et al. [2] examined the uncertainties in the orientation distribution function (ODF) values of a microstructure due to the variations in the pole figure (PF) values by using Monte Carlo Simulation (MCS). Juan et al. [3] used MCS to study effects of sampling strategy on the determination of various characteristic microstructure parameters such as grain size distribution and grain topology distribution. Hiriyur et al. [4] studied an extended finite element method (XFEM) coupled with an MCS approach to quantify the uncertainties in the homogenized effective elastic properties of multiphase materials. The uncertain parameters were assumed to be aspect ratios, spatial distribution and orientation. They used a strain energy approach to analyze the uncertainties of in-plane Young's modulus and Poisson's ratio. Kouchmeshky and Zabaras [5] presented propagation of initial texture and deformation process uncertainties on the final product properties. They used a data-driven approach to identify the joint probability distributions of random variables with Maximum Entropy Method, and modeled the stochastic problem using a stochastic collocation approach. Madrid et al. [6] examined the variability and sensitivity of in-plane Young's modulus of thin nickel polycrystalline films due to uncertainties in microstructure geometry, crystallographic texture, and numerical values of single crystal elastic constants by using a numerical spectral technique. Niezgoda et al. [7] computed the variances of the microstructure properties by defining a stochastic process to represent the microstructure. They marked the sensitive regions in the convex hull generated with Principal Component Analysis (PCA), and calculated the probability

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distributions of stiffness and yield stress in case of low, medium and high variances.

These computational methods presented in literature involve using a numerical algorithm for uncertainty quantification and propagation. They represent the joint probability distributions of uncertain variables either using interpolation functions or sampling for random points. These techniques are not computationally efficient as the problem complexity or the number of variables increases since the number of interpolation terms or sampling points will also increase. This is especially true for orientation distribution functions that are discretized using finite element nodes or spectral basis and contain large number of free parameters whose joint distribution needs to be sampled. Another drawback is the difficulty of satisfying design constraints (such as volume fraction normalization) when using numerical approaches. Finally, these methods do not take advantage of the linear transformations involved in the conversion of pole figures to ODFs [8] that allow analytical representations of uncertainty under certain cases. All these disadvantages imply the necessity of developing analytical solutions as a first step in UQ.

In this work, we develop a set of analytical formulae to quantify uncertainty in the ODF due to variability in the measured pole figures. This uncertainty is 'aleatoric' [9] and arises from variations in texture across specimens subject to the same process. The measurements were taken across different beta forged Ti-Al samples that were subject to the same compression and annealing process. The measurements were also taken from different regions of these samples. The probability distributions of the PFs were computed from these scans and were found to be roughly Gaussian in nature. Then, the propagation of uncertainties on the ODFs are computed using an analytical formulation. Note that pole figure inversion is non-unique and several numerical methods have been developed for this purpose dating back to Bunge (1969) [10]. These different methods lead to a band of solutions for the true ODF. In the UQ community, the uncertainty that arises from lack of an exact solution is classified as 'epistemic' uncertainty [9], and such an uncertainty is not considered in this work. In this context, Randle and Engler [11] classified various inversion methods to categories of 'harmonic' or 'direct' methods and compared the methods against each other. While all methods were found to yield reproducible results, it was suggested to stay with a given method during a series of experiments. In this work, we stay within the least squares minimization method of Barton et al. [8] to compute the ODF. The secondary uncertainty that comes from the X-ray instrument itself is also not considered. Once the uncertainty in the ODF is quantified, we present an approach to identify the probability distributions of the material properties that are derived from the ODF such as Young's modulus and shear modulus using the random variable transformation method. The organization of this paper is as follows. Section 2 discusses the problem statement. In Section 3, the mathematical methods are described. Results and conclusions are addressed in Sections 4 and 5 respectively.

2. Mathematical background

The complete orientation space of a polycrystal can be reduced to a smaller subset, called the fundamental region, as a consequence of crystal symmetries. Within the fundamental region, each crystal orientation is represented uniquely by a coordinate $\boldsymbol{r}$, the parametrization for the rotation (eg. Euler angles, Rodrigues vector etc.). The ODF, represented by $\mathcal{A}(\boldsymbol{r})$, describes the volume density of crystals of orientation $\boldsymbol{r}$. The ODF representation in the Rodrigues fundamental region for Titanium (hcp) is shown in Fig. 1 and the locations of the k independent nodes are shown. The volume density of any other node in the fundamental region can be

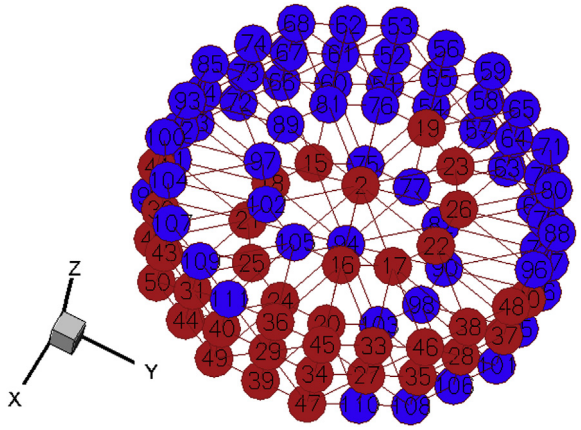

Fig. 1. ODF representation in the Rodrigues fundamental region for hexagonal crystal symmetry showing the location of the k = 50 independent nodes of the ODF in red color. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

obtained from these independent nodes through symmetry. The ODF also satisfies a normalization constraint, $\int \boldsymbol{A} dv = 1$, with the integral computed over the fundamental region. The normalization constraint can be written as a linear equation of the form $\sum_{i=1}^{k} q_i A_i = 1$ (see Appendix A), with A_i denoting the ODF value at node i.

The experimentally obtained pole figure for a particular diffraction plane unit normal $\boldsymbol{h}$ contains the pole density function $P(\boldsymbol{h},\boldsymbol{y_i})$ measured at locations $\boldsymbol{y_1},\boldsymbol{y_2}, \ldots,\boldsymbol{y_q}$ on a unit sphere. The value of $P(\boldsymbol{h},\boldsymbol{y_i})$ at location $\boldsymbol{y_i}$ can be computed from the ODF ($\boldsymbol{A}$) using a single linear equation based on the algorithm of Barton et al. [8]:

$$P(h, y_i) = \sum_{j=1}^{k} M_{ij} A_j \tag{1}$$

where M_{ij} are the values from a known system matrix $\boldsymbol{M}$. One such equation can be written for each of the m points in a pole figure. This set of equations can be combined with a similar set of equations for n other pole figures with different diffraction normals $\boldsymbol{h}$. This leads to a global system of equations $\boldsymbol{P} = \boldsymbol{MA}$. Here, $\boldsymbol{P}$ is a column vector of size $m \times n$, $\boldsymbol{M}$ is a matrix of size $(mn) \times (k)$ and the ODF $\boldsymbol{A}$ is a column vector of size k containing the volume densities of k independent nodes. In order to account for the normalization constraint $\sum_{i=1}^{k} q_i A_i = 1$, the overall system $\boldsymbol{P} = \boldsymbol{MA}$ is adjusted such that $M_{ij} = M_{ij} - \frac{M_{ik} q_j}{q_k}$ for $j = 1, \ldots, k-1$ and $P_i = P_i - \frac{M_{ik}}{q_k}$.

The system of equations is over–determined (ie. more pole figure data as compared to the unknown ODF values) and direct inversion is not possible. Instead following Barton et al. [8], the ODF is retrieved from the experimental pole figures using least squares minimization as follows:

$$\boldsymbol{A} = \boldsymbol{CP} \tag{2}$$

where the coefficient matrix, $\boldsymbol{C} = (\boldsymbol{M^T M})^{-1} \boldsymbol{M^T}$ is the pseudo–inverse.

If the orientation-dependent property for single crystals, $\boldsymbol{\chi}(\boldsymbol{r})$, are known, any polycrystal property can be expressed as an expected value, or average, over the ODF as follows:

$$< \boldsymbol{\chi} > = \int \boldsymbol{\chi}(\boldsymbol{r}) \boldsymbol{A}(\boldsymbol{r}) dv \,, \tag{3}$$