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Towards surrogate modeling of material microstructures through the processing variables

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ABSTRACT

In order to obtain high-performance materials, it is of significant importance to be able to depict the material microstructure corresponding to given values of processing variables in the manufacturing process. Conventional approaches require a knowledge of the internal mechanisms of the evolution in order to numerically simulate the microstructures. This work focuses instead on establishing a surrogate model in order to parameterize microstructures of Representative Volume Elements (RVE) using processing variables. The surrogate model requires a set of RVE microstructure snapshots generated experimentally *or* numerically. By using the Proper Orthogonal Decomposition (POD) method, the parametric space is developed using a series of approximated response surfaces of the POD projection coefficients. Thereafter, RVE microstructures may be parameterized for any given value of the processing variables. In addition, for the purpose of scaling down the storage requirement due to a high quality digital representation, the snapshots are given a bi-level reduced order epresentation in terms of the extracted common spatial and parametric bases. We showcase the approach by parameterizing Voronoi-simulated RVE microstructures under both uniaxial and biaxial conceptional compressions.

1. Introduction

In order to obtain higher performance materials, there is a growing demand for microscale models describing the evolution of microstructure and texture during material manufacturing processes, particularly thermomechanical processing [1]. Some early achievements have been made in the production of grain oriented silicon steels by controlling local inhomogeneities in texture and microstructure [2]. Conventional approaches require a knowledge of the internal mechanisms of the evolution in order to numerically simulate microstructures or textures [3–6]. Among the various numerical methods available, Voronoi tessellation has been considered as an efficient tool for the generation and simulation of material microstructures [e.g., 7,8,9,10]. As illustrated in Fig. 1, the unworked crystal Representative Volume Element (RVE) approximated using

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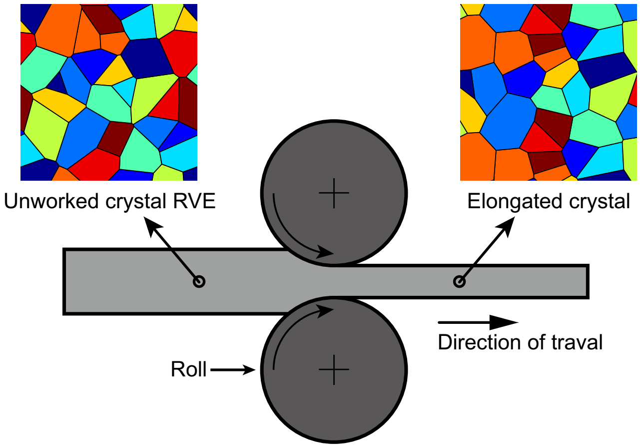

Fig. 1. Illustration of the crystal microstructure elongation during the rolling process.

Voronoi tessellation is elongated after the rolling process. The microscopic grain layout of the elongated crystal depends on the processing variables such as the compression ratio, rolling speed, temperature etc.

If we were to obtain material microstructures parameterized using the processing variables, numerical modeling approaches as in [11,12] could be avoided, and the numerical model may instead be directly generated using image-based reconstruction techniques [13–15]. In addition, we can automatically move on to other related subjects of research such as material property evaluation [16–18], multi-scale analysis [19,20], and optimization [21,22].

While model reduction techniques have found ever-increasing application in the field of Multidisciplinary Optimization [23,24], a survey of the existing literature reveals little investigation into developing parameterized material representations. In [25,26], Principal Component Analysis (PCA) has been applied to reduce the parametric space constructed by a large-dimensional data set using the so-called *method of snapshots* [27,28], where each snapshot may be represented as a combination of its eigen-images. For the purpose of reduction, fewer basis vectors selected in the order of decreasing importance may be used for the representation of the high-dimensional data set.

To the author's knowledge, no similar work in the existing literature has established a parameterization model using a surrogate modeling strategy that directly links processing variables and microstructures. In this work, a surrogate model based on Proper Orthogonal Decomposition (POD) is developed to map the processing variables to POD projection coefficients, i.e., the microstructure snapshots. By the *method of snapshots*, the parameter space spanned by the processing variables is then transformed into a series of approximated response surfaces of the POD projection coefficients with respect to the processing variables using *Diffuse Approximation* [29], a variant of the Moving Least Squares (MLS) approach. It is worth noting that the model is actually reduced to the order of the parametric space of processing variables, which is usually a much lower order in most cases. The surrogate model constructed in this work has similarities to what has been accomplished for multidisciplinary design optimization [30,31], where surrogate models were built by Kriging or Diffuse Approximation of the POD projection coefficients. Related idea has also been applied to reliability-based optimization of space truss structures [32], where the Polynomial Chaos Expansion coefficients were predicted using MLS response surfaces of the coefficients w.r.t. the input parameters.

Image-based microstructure analysis, especially when it involves a large number of micrographs, requires an increasingly higher memory storage requirement with the ever-increasing resolution provided by modern day image techniques such as computer tomography, magnetic resonance imaging, etc. [33]. Therefore, the considered data set, i.e., snapshots, can benefit from preprocessing in order to properly scale down this storage requirement. Considering the spatial and parametric similarities among the snapshots during the same manufacturing process, a bi-level reduction model is then proposed through the extraction of both common spatial bases and parametric basis.

The remainder of this paper is organized in the following manner: Section 2 presents the overall concept and formulations. The MLS-based parameterization methodology is presented in Section 3. The numerical implementations for the extraction of the common spatial and parametric bases is given in Section 4. We demonstrate this approach by parameterizing Voronoi-simulated microstructures in conceptional uniaxial as well as biaxial compression in Section 5. The paper ends with concluding comments and suggestions for future work.

2. Overall concept and formulations

2.1. Basic definitions

Without loss of generality, we consider a 2D real-valued continuous or discrete material phase indicator function $s = s(x, y, \mathbf{v})$ that depends on a set of processing variables $\mathbf{v}$, where x and y are the coordinates. Given an $N \times N$ grid of