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Technical Notes

Reduced-Order Modeling Approach for Materials Design with a Sequence of Processes

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I. Introduction

MICROSTRUCTURE design optimization is important for improving the performance of critical components in numerous aerospace applications. These critical components involve performance indices that are directly related to microstructures obtained during processing. This calls for direct control of microstructure evolution using well-designed processes. Recent developments in materials by design have allowed a more advanced systems approach that integrates the processing, structure, and property through multiscale computational material models [1]. The techniques that allow the tailoring of properties of polycrystalline alloys involve tailoring of the preferred orientation of crystals manifested as the crystallographic texture. During forming processes, mechanisms such as crystallographic slip and lattice rotation drive the formation of the texture and variability in property distributions in such materials. A useful method for designing materials is through the control of the deformation processes leading to the formation of textures that yield the desired property distributions.

The microstructure modeling of the present work is based on the quantification of the microstructure using the orientation distribution function (ODF). The ODF measures the volumes of single crystals in different orientations. The ODF is defined based on a parameterization of the crystal lattice rotation. In this work, the ODF values are parameterized using a Rodrigues representation. The computational microstructural modeling has been studied extensively in the earlier works of Acar and Sundararaghavan [2–6], Acar et al. [7,8], Acar and Sundararaghavan [9], Acar et al. [10], and other works in the literature [11–15] by using different computational techniques. The design of microstructures has also been exercised by Acar and Sundararaghavan [2–4] and Acar et al. [7,8] using the ODF model and a linear solution scheme to achieve optimum material properties. Multiple optimum microstructure designs were mathematically possible with the linear approach [2,3]. However, only a few of these optimum solutions was actually manufacturable. The texture evolution during deformation processing needed to be simulated to identify the optimum manufacturable design. The texture evolution in a deformation process was previously studied by Li et al. [16] by representing the processing paths as streamline functions in the space of the spectral coefficients. However, this model required a large number of spectral terms to capture sharp textural features and describe the processing paths. Instead, a reduced-order representation of the texture evolution was found to be a more powerful approach to solve the process optimization problem [4]. The reduced-order maps of different deformation processes were derived to identify the optimal process to achieve the predetermined material properties [4]. The present work is the extension of our recent work [4], in which the optimal single process was identified by using these reduced-order maps. It was observed that the number of manufacturable textures was limited when only one deformation process was studied and the variability in texture was higher when a sequence of deformation processes was applied. Therefore, the motivation of the present study is to find the optimal sequence of deformation processes that can produce the predetermined optimum material properties. The texture evolution is again represented by using reduced-order models in which the basis functions are derived with proper orthogonal decomposition (POD). The methodology is studied on the vibration tuning problem of a galfenol beam. The multiple optimum microstructure solutions of the same problem were computed in our recent works [2,3]. To determine the optimal processing sequence, the optimum solution directions are projected into the basis functions of different deformation processes. The sequence and strain rates of the deformation processes are optimized to achieve the closest material properties to the previously determined values. The remainder of this Note is organized as follows. Section II summarizes the mathematical background for microstructure modeling and proper orthogonal decomposition. Section III includes the problem definition for optimal sequential process property matching, and it reports the optimization results. A summary of the Note and the potential extensions are finally discussed in Sec. IV.

II. Mathematical Background

A. Microstructure Modeling with Orientation Distribution Function

The microstructure modeling approach employs a Taylor approximation [17] for averaged properties by assuming homogeneity of the deformation in a macroscale elementary volume. If the orientation-dependent property for single crystals $\chi(r)$ is known, any polycrystal property can be expressed as an expected value, or average, given by the following:

$$\langle \chi \rangle = \int_R \chi(r) A(r,t)\, \mathrm{d}v \tag{1}$$

where the ODF A is a function of orientation r. The averaged material properties are computed by integrating single crystal values within a representative volume element dv, which can be obtained by employing the crystallographic symmetries. Rodrigues parameterization is used to parameterize the orientation space [18]. Finite element discretization of the orientation space and associated integration schemes using Gauss quadrature allows the matrix representation of Eq. (1) [2–10]. The ODF is discretized into N independent nodes with N_{elem} finite elements and N_{int} integration points per element. Using this parametrization, any polycrystal property can be expressed in a linear form [19]. The readers are referred to recent works by the authors [2–6,9] and Acar et al. [7,8,10] for more information about microstructural modeling.

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B. Reduced-Order Modeling with Proper Orthogonal Decomposition

The reduced-order modeling approach used in this study follows the work in [4,20–22], in which the model reduction of crystal plasticity was first introduced using the technique of POD. Model reduction involves the generation of basis functions that are optimal for representing ODFs obtained from a process path. Using such basis functions and time-dependent coefficients of the POD method, any ODF (from the time history of ODF evolution in a given process) can be approximated. In this work, we use the "method of snapshots" to obtain the basis functions from an ensemble of ODF data. The reduced-order modeling of the ODFs is based on the same formulations that were previously presented in our recent work [4]. Each different sequence of deformation processes studied in the present work is represented by generating a unique basis function using the solution strategy in [4].

III. Identification of Optimal Sequence of Deformation Processes

The property process matching is posed as an optimization problem in which the goal is to identify the ODFs in the process plane that closely reproduce a desired set of properties. The objective function is defined as minimizing the maximum absolute error to achieve a set of desired properties. The material properties are selected as the optimum yield stress and nine independent orthotropic stiffness parameters, which were computed previously for the vibration tuning problem in [4]. The solution approach leads to an augmented system of linear equations, and it can be solved as a linear programming (LP) problem. The details on the formulation of this LP problem were explained in our recent work [4]. The optimization problem solves the sequence and strain rates of the deformation processes. Two cases are studied by assuming that the number of deformation processes is constant: 1) a sequence including two deformation processes, and 2) a sequence including three deformation processes. The basis functions are computed with a random initial texture assumption.

The solution for an optimal single deformation process to match a desired set of properties was presented before in our recent work [4], in which the basis used in the examples consisted of modes generated from an ensemble of data for tension, compression, and shear processes with a constant strain rate of 1 s^{-1}. In the present work, we generate a unique basis function that represents a whole sequence of processes (including either two or three deformation processes). To avoid the extrapolation of the basis functions, which may affect the accuracy of the reduced-order model representation, we define an additional design constraint to match the total strain rate of the sequence of the deformation processes to the strain rate of the single deformation process problem (1 s^{-1}). This constraint also gives an opportunity to make a direct comparison between the optimal results produced by the single and sequential processing approaches. The mathematical expression of the constraint is given as follows:

$$\dot{\epsilon}_{\text{single}} = \sum_{i=1}^{n=2,3} \dot{\epsilon}_i = 1\ \text{s}^{-1} \tag{2}$$

Here, $\dot{\epsilon}_{\text{single}}$ is the strain rate of any single deformation process used in our recent work [4], and it is equal to the total strain rate of the sequence of deformation processes, the sum of $\dot{\epsilon}_i$ values, (either two or three processes) in the present work. Tension, compression, *xy* shear, *xz* shear, *yz* shear, *xy* rotation, *xz* rotation, and *yz* rotation are considered as the different processes to generate the sequential processes database. All the rotation processes are constrained so that the first process can never be a rotation, or a rotation cannot be followed by a rotation. The order of the processes is determined with integer optimization by assigning an integer to each process. The individual strain rates are also optimized at the same time for each deformation process. The results are reported in Table 1 for both cases with two and three sequential processes. These results are also compared to the optimum solution when only a single process is considered. In Table 1, ξ denotes the maximum error in the stiffness parameters, and the optimum result on the last line is the predetermined solution for the vibration tuning problem.

Table 1 LP problem results for matching desired material properties

Process number	Order	ξ, GPa	σ_y, MPa
1	*xy* shear	1.9587	305.6497
2	*xz* shear–*xz* shear	1.9336	308.6296
3	*xy* shear–*yz* rotation–*xz* shear	1.9213	308.4964
Optimum result	— —	— —	308.4456

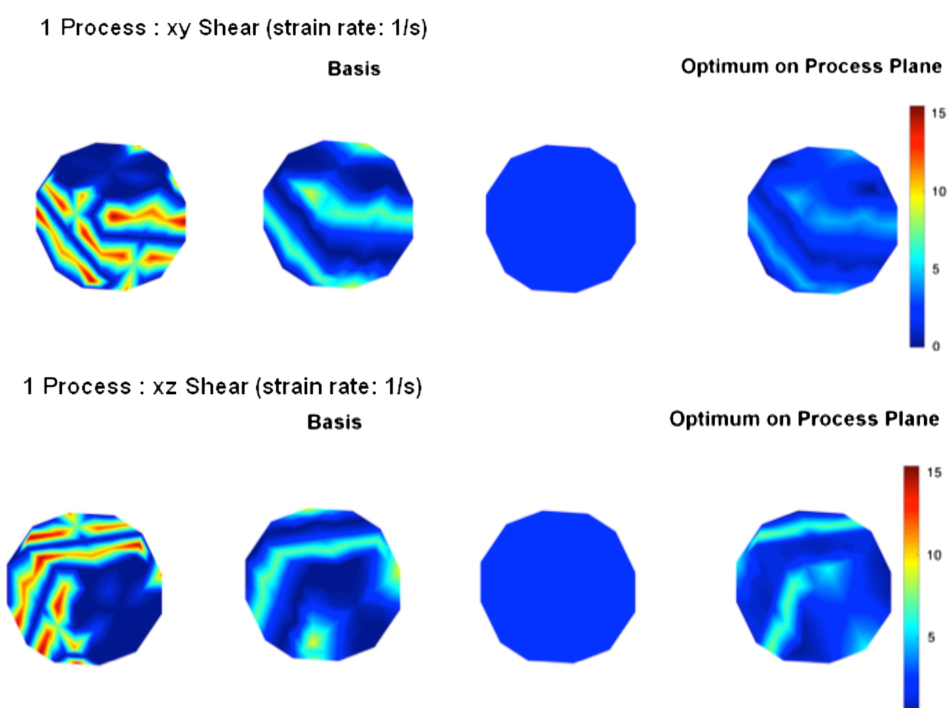

Fig. 1 Basis functions and optimal textures on the process plane (single deformation process).

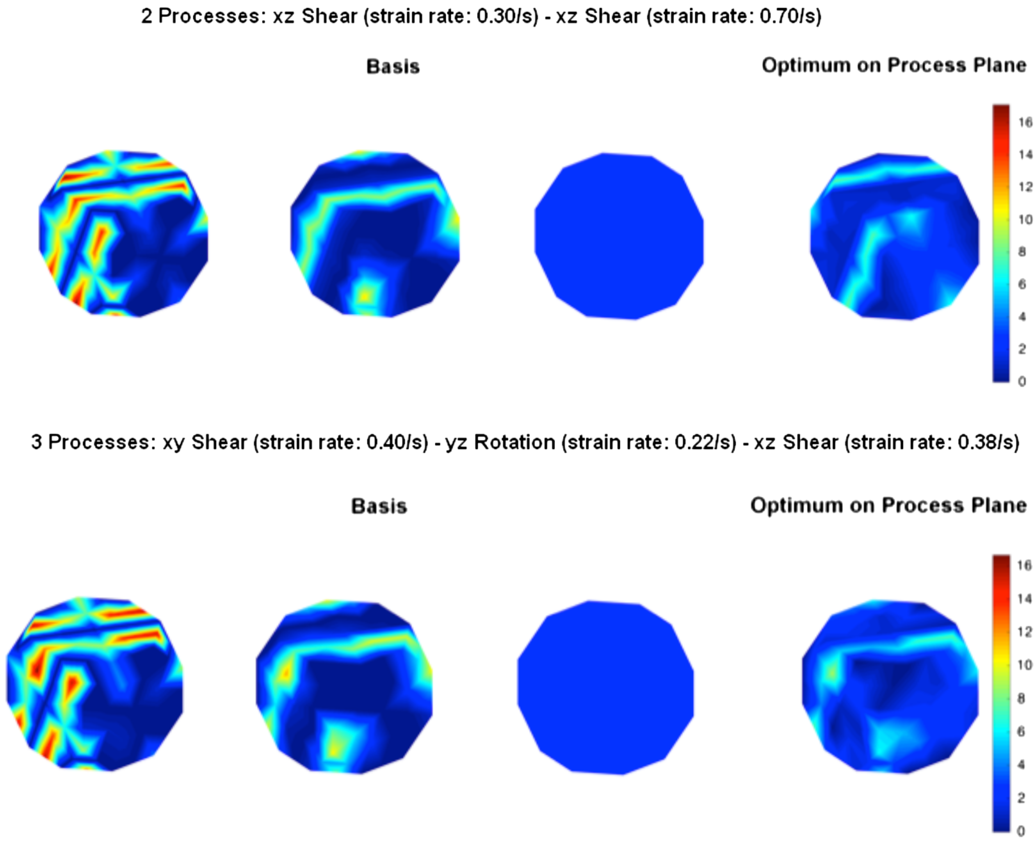

Fig. 2 Basis functions and optimal textures on process plane (sequential deformation processes).

The results in Table 1 indicate that, as the number of processes increases, the yield stress results match better with the optimum yield stress value (optimum result in Table 1) of the galfenol problem. The maximum error in stiffness values also tends to decrease as the number of processes increases. The reason is that the increasing number of deformation processes also increases the variability in texture. The optimization results show that there is only one optimal process (*xz* shear) when two sequential processes are considered. However, the processes vary in the case of three sequential processes. The optimal textures of all cases are shown together with the corresponding basis functions in Figs. 1 and 2. The optimal strain rate values are also shown in these figures. In Fig. 1, the basis functions and optimum texture representation of the single deformation processing problem are illustrated. The same is shown for the sequential deformation processing problem in Fig. 2. Because the reduced-order representations are generated for three modes, the corresponding three basis functions are represented in Figs. 1 and 2. The optimum texture on the process plane provides the best solution to the process property matching problem for the galfenol beam.

IV. Conclusions

This Note addresses an optimization methodology to find the optimal sequential processing route to satisfy the performance needs in materials design. A reduced-order modeling scheme is employed to represent the texture evolution in different deformation processes. The methodology is applied to a design problem for a galfenol beam under vibration tuning constraints. The optimum microstructure solution of this problem leads to multiple solutions. However, only a few of them can be manufacturable. The reduced-order maps are projected into the optimum solution directions to identify the optimal processing sequence to produce the predetermined material property values. The optimization with a sequence of deformation processes is shown to provide better results as compared to the optimization with a single process. Future work in this area may focus on analyzing the uncertainties in deformation processes and their effects to process design.

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