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Materials-by-design: A multi-length scale approach

Nicholas Zabaras

Materials Process Design and Control Laboratory
Sibley School of Mechanical and Aerospace Engineering,
Cornell University, USA

Microstructural features such as texture, grain sizes, grain boundaries and second phase particles play an important role in determining the properties of a polycrystalline material and whether it is suitable for a particular application. Consideration of this `microstructure-sensitivity' is not only important in developing new materials but also in establishing the means of optimizing existing materials and extending the life of critical hardware components.

Even though significant experimental and modeling work is still needed to fully understand how different microstructural quantities affect material properties, this presentation will set forward a number of methodologies that can be used to obtain materials with desired microstructure-sensitive properties. This effort is of vital importance for developing materials-by-design and pointing to the corresponding required processes in the manufacture of critical hardware components.

Our work utilizes advanced mathematical and computational techniques to address issues in polycrystalline materials related to microstructure representation and classification, microstructure-model reduction and design for microstructure-sensitive properties through deformation and thermal process sequence selection and design. In this presentation, we will discuss the following ongoing research and development activities:

- Development of a mathematically rigorous and computationally efficient microstructure model-reduction that can allow representation of arbitrary microstructures in terms of a finite collection of experimentally or numerically obtained microstructure snapshots. The infinite microstructural degrees of freedom affiliated with the orientation distribution function representing texture are approximated with a finite collection of proper orthogonal decomposition modes that can be used adaptively for the analysis, classification or optimal design for desired material properties.

- Development of a virtual microstructure library which can be used for classification of arbitrary textures and for determining appropriate processing conditions to obtain desired microstructure-sensitive properties. Thus not only optimal microstructures leading to desired properties will be identified but also the required optimal process sequence (thermal and/or deformation). Moving beyond texture, we will also discuss extending this approach to a complete representation and classification of single phase microstructures using support vector machines and an incremental-principal component analysis.

- Integration of the virtual materials design simulator with the virtual robust design environment for deformation processes currently under development in our laboratory. This integrated multi-length scale environment will make it feasible to provide detailed design of manufacturing process sequence needed for an accelerated insertion of polycrystalline materials in the design of performance-critical hardware components in advanced applications.

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