ADVANCED COMPUTATIONAL TECHNIQUES FOR MATERIALS-BY-DESIGN

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ABSTRACT

Our AFOSR project activities (Comp. Math. program, AFOSR, grant FA9550-04-1-0070) are focused on the development of a multi-length scale and multi-stage deformation process design simulator for the control of microstructure-sensitive properties in critical aircraft manufacturing applications. As part of developing this robust design simulator, multiple technical developments need to be accomplished. One of the important steps to be addressed is the accurate modeling of microstructure evolution during materials processing. It is imperative that the process design solutions be developed by taking into account varying microstructural features and material properties. Furthermore, it is clear that the efficiency of the process design algorithm depends on our ability to guess the (initial) design solution with reasonable accuracy by exploiting the synergy between process sequence selection and classification of microstructural features. Second, we need to be able to represent the process of microstructure evolution through the use of a minimum number of microstructural degrees of freedom, for maximum computational efficiency. Third, uncertainty in process and material parameters, in initial conditions and in the microstructure need to be accounted. In particular, this presentation will address the following issues:

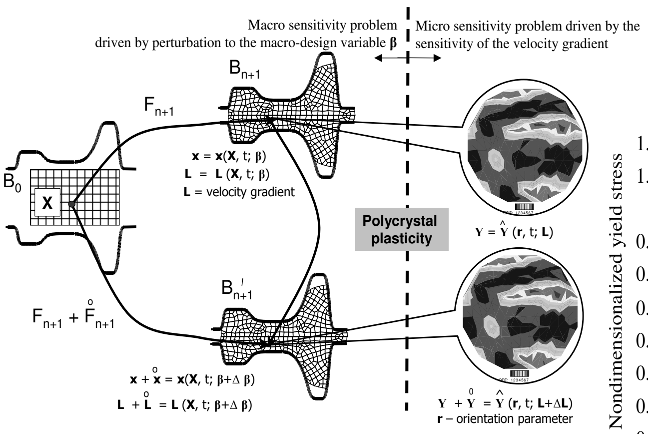

Figure 1: A continuum sensitivity framework for multi-length scale deformation process design. This framework actively couples the macro and micro scales. In a typical design problem, we compute the macro parameters needed for control of microstructure-sensitive properties.

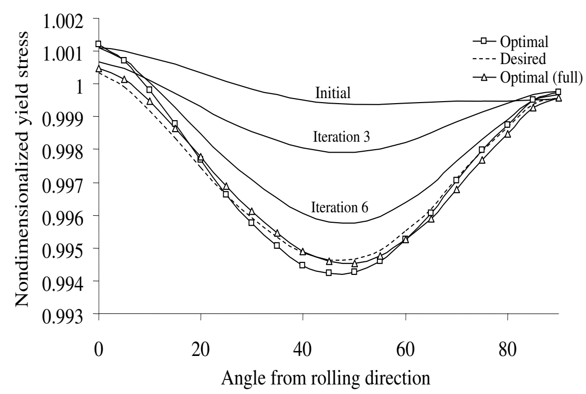

Figure 2: A sample material point design problem: a desired distribution of the yield stress (for f.c.c Cu) is obtained by designing an appropriate process velocity gradient (a macro process parameter).

- **Computational design**: The computational design algorithm proposed is based on a coupled length scale (polycrystal plasticity-based) direct and continuum sensitivity analysis (Fig. 1). This virtual simulator will not only accurately model the behavior of various industrially relevant materials, but also help in designing new materials for specific applications (refer to Fig. 2). It is envisioned that such an approach will assist in an accelerated insertion of new materials.

- **Reduced representation and classification of microstructures:** A multi-class support vector machine classification method is being developed in conjunction with principal component analysis to build a dynamic and evolving microstructure library that can be used to efficiently describe polyhedral microstructures. A framework of such an approach is schematically described in Figure 3. We

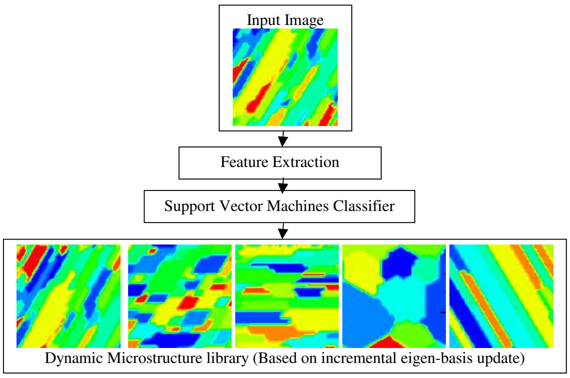

Figure 3: A framework for microstructure feature extraction, classification and reduced-model representation using a dynamic microstructural library.

  propose to apply the hierarchical classification framework for generating organized databases of 3D microstructures. In particular, pattern recognition techniques are utilized for generating real-time 3D realizations of microstructures from 2D features, thus accelerating prediction of material properties. Our earlier efforts have shown that reduced-order models of microstructure (texture in particular) are a simple approach towards the development of fast and reliable methodologies for control of microstructure-sensitive properties. We further propose to incorporate innovative statistical learning tools in our design algorithms. This has multi-fold benefits: accelerate the design of materials process paths that lead to a desired property, speed-up the prediction of material properties, and thus, contribute to the development of materials-by-design.

- **Uncertainty analysis and robust design**: In the development of a realistic process design simulator, one needs to be able to set variability limits in the desired properties in the final product and then compute the uncertainty or variability that can be allowed in the material and process data used in the simulator. As a first step, we are developing a method for quantifying uncertainty propagation in finite deformation elasto-plasticity using the spectral stochastic finite element method. These developments require a careful re-examination of continuum mechanics to allow extension of various fundamental quantities in large deformation analysis, such as deformation gradient, strain and stress measures to a stochastic framework. Further, a framework for robust design and control of processes in the presence of uncertainties will be discussed.

It is strongly believed that the use of advanced mechanics of materials along with innovative design technologies, realistic simulation algorithms, ability to statistically represent and model evolution of material microstructures, and technologies for studying the effects of uncertainties can drastically improve process and material predictions in critical components. These techniques can lead to material process design that is more efficient, more accessible and extremely accurate.