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MICROSTRUCTURE-PROPERTY-PROCESSING LINKAGES USING DISCRETE FOURIER TRANSFORMS

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ABSTRACT

Microstructure Sensitive Design (MSD) [1-4] embodies a rigorous mathematical framework for systematic design of material microstructure to meet the requirements of the designer in optimal ways. It is deeply rooted in the spectral representations of the first and second-order invertible linkages between a material's microstructure, its effective macroscale properties, and the processing history it has experienced. This methodology starts with the specification of microstructure hull defined as the set of all possible microstructures deemed relevant by the governing physics of the design problem. The microstructure hulls facilitate the delineation of the properties closures, depicting the complete set of all theoretically feasible combinations of anisotropic properties. Computationally efficient methodologies to build microstructure hulls and property closures, and to explore subspaces in these constructs that are readily accessible by available material processing routes, are at the core of the MSD framework. Some of the recent results from this effort from our research group will be presented and discussed in this paper. These include:

- *Quantification of Microstructures Using 2-Point Statistics:* It has been demonstrated that the important details of the microstructure can be described rigorously using *n*-point statistics. In fact, it was shown that it is possible to reconstruct the original microstructure, to within an arbitrary translation and/or an inversion, given a complete set of its 2-point statistics.
- *Property Closures:* In the MSD framework, the microstructure description is linked to its effective properties using generalized composite theories. Using highly efficient spectral representations, it is possible to delineate the complete space of all feasible property combinations for a given material system predicted using a selected composite theory. This construct is known as a property closure, and is the search space of most interest to the designer. For example, the complete range of combinations of the ultimate tensile strength (UTS) and the uniform ductility that are theoretically predicted using Taylor-type crystal plasticity models can be successfully delineated [5]. It is important to recognize that the range of properties predicted has hitherto never been realized in practice. This is because only a very small fraction of all physically realizable textures have been processed to date.
- *Localization Tensors*: The spectral framework of MSD facilitates formulation of computationally efficient scale-bridging laws in multi-phase materials that can be executed with minimal computational resources. As an example, the elastic localization tensor relating the macroscopic strain to the local strain can be expressed as a polynomial, in which the morphology independent coefficients are called influence coefficients. Figure 1 shows the distributions of local stress in two different microstructures of a 2-phase composite subjected to uniaxial macroscopic tensile strain, calculated using the spectral database of influence coefficients and compared against corresponding predictions from finite element models. As expected, the fiber arrangement leads to much narrower distributions, due to the reduction in richness of the local structure about each point. These local stress distributions are captured extremely well by the spectral method.

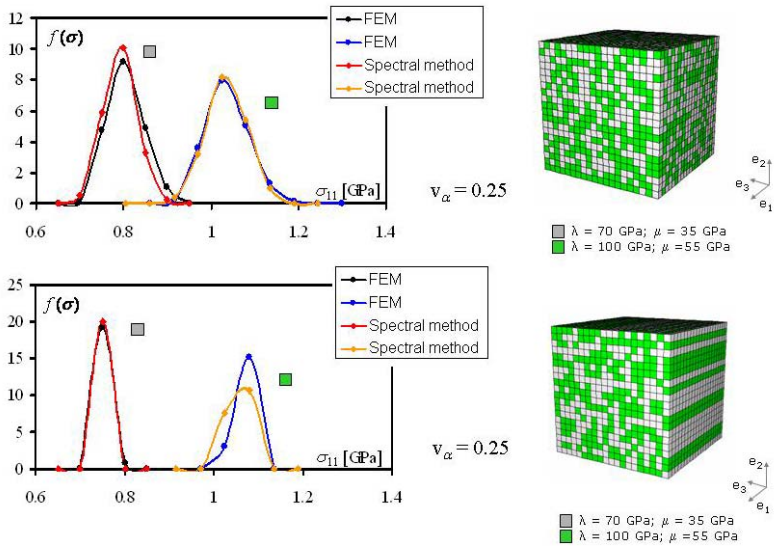

Figure 1. Stress distributions for each phase of a 2-phase microstructure due to an imposed average strain $\varepsilon^* = 0.005$ in direction e_1. The upper microstructure is random, and the lower has a fiber arrangement of the stiffer phase. Both have identical volume fractions of the two phases. Note that the distributions are narrower in the microstructure with fiber phase morphology.

- *Spectral Crystal Plasticity:* A new computationally efficient database approach to crystal plasticity calculations was developed. The underlying strategy involves pre-computing only once all of the needed variables in crystal plasticity calculations, storing them, and retrieving the values of interest according to the need in any specific simulation through local spectral interpolation using Discrete Fast Fourier Transform (DFFT) methods. The approach resulted in major improvements in the computational time over the conventional crystal plasticity calculations.

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