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Using Simulation to Quantify the Sensitivity of Mechanical Property Distributions to Features of the Microstructural State in Engineering Alloys

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Patrick F. Taylor Hall 1502
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Abstract:

Thermomechanical processing is commonly used to alter the microstructural state of engineering alloys to achieve desirable mechanical properties. Historically, the processing routes that deliver superior properties have been determined by costly trial-and-error experimentation and codified as empiricisms between processing conditions and bulk properties (like strength) or between processing conditions and an important microstructural feature (such as grain size). A quantitative link between the microstructural state and particular mechanical properties largely has been missing, but is needed to allow a more direct prediction of the mechanical performance of new alloys or existing alloys processed by new methods. As a consequence, a long-standing goal of computational mechanics is to estimate an alloy's aggregate properties from knowledge of its microstructural state, the local properties of its constituent phases, and the type of loading being applied.

A combination of experimental and modeling capabilities have emerged over the past decade that provide practical tools to reach this goal. From the experimental side, these include electron and x-ray diffraction methods for quantifying microstructures of polyphase, polycrystalline alloys and for measuring mechanical behaviors at the scale of individual grains. From the simulation side, these include tools to instantiate virtual samples that adequately replicate measured microstructures, parallel finite element formulations capable of dealing with the kinematic and material nonlinearities of large strain deformations. Considerable work lies before us, however, to determine how to apply the tools ways that assure accurate and reliable estimates of mechanical properties.

In this presentation, I will discuss how we are coordinating the use of these capabilities to estimate distributions of strength and ductility in a two-phase titanium alloy (Ti-6Al-4V) that has been processed to achieve distinctly different microstructures. Corresponding strength and ductility data were measured by conventional testing for comparison. I will use this system to discuss several challenges associated with computing the sensitivity of the strength and ductility to microstructure. The particular challenges are discussed in the context of titanium, but arise in other fields that employ micromechanical modeling as well. First, I'll address the instantiation of virtual samples the adequately replicate the different microstructures using different types of tessellation together with 2D and 3D electron back-scattered diffraction data. Second, I'll address the quantification of phase (local) properties using a novel method to compare crystal-scale elastic strains measured by high-energy x-ray diffraction and computed via finite element simulation. Third, I'll address the issue of how large must a representative volume element be to be representative in the context of elastic moduli and yield strength. Finally, I'll discuss a few challenges that persist and offer interesting opportunities for continued research.

Speaker's Bio:

Professor Dawson received a BS from Montana State University and MS and PhD degrees from Colorado State University. Prior to his graduate studies, Professor Dawson worked for one year as an Associate Engineer at the Advanced Reactors Division of Westinghouse. Following his graduate students, he worked for three years as a Member of the Technical Staff in the Computational Physics and Mechanics Division of Sandia National Laboratories. Professor Dawson joined the Cornell faculty in 1979 as an Assistant Professor in the Sibley School of Mechanical and Aerospace Engineering. In 2013 he was elected the Joseph C. Ford Professor of Engineering at Cornell. He is active in research at the interface of solid mechanics and materials science computational mechanical, with emphasis on computational mechanics applied to problems in mechanics of materials. He teaches courses related to stress analysis, metal forming, vehicle mechanics, solid mechanics and finite element methods.

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