



## Materials Processing and Manufacturing Division Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Materials Design

*Sponsored by:* The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee, TMS/ASM: Mechanical Behavior of Materials Committee  
*Program Organizers:* Brent Adams, Brigham Young University; Hamid Garmestani, Georgia Institute of Technology

Tuesday PM                      Room: Northern A1  
February 27, 2007              Location: Dolphin Hotel

*Session Chairs:* David McDowell, Georgia Institute of Technology; Hamish Fraser, Ohio State University

### 2:00 PM

**Challenges and Prospects for Materials Design:** *David McDowell*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

Presently, a materials design revolution is underway in which classical materials selection is replaced by design of material microstructure to achieve certain performance requirements, subject to constraints on other properties. The materials design approach advocated here invokes the notion of robust design, i.e., insensitivity of the desired response to various sources of uncertainty. It utilizes decision theory and the notion of compromise decision support, leading to Pareto optimal solution sets. To this end we have developed notions of multilevel design and Type III robust design, addressing configuration of simulations/evaluations and uncertainty of models or database information. We close with an overview of Georgia Tech's AFOSR Multi-University Research Initiative (MURI) on Design of Multifunctional Energetic Structural Materials, a distributed collaborative materials design effort that employs modeling tools ranging from ab initio methods to molecular dynamics to mesoscopic and macroscopic continuum models.

### 2:25 PM

**Digital Material Frameworks for Material Design and Property Prediction:** *Matthew Miller*<sup>1</sup>; Paul Dawson<sup>1</sup>; <sup>1</sup>Cornell University

Dr. Hartley has been instrumental in emphasizing the need for accelerated material development formulations and for supporting the development of digital material representation frameworks. This talk summarizes our work conducted under Dr. Hartley's Materials Engineering for Affordable New Systems program, which we have continued to develop. Our "digital material" is centered on a relational database of material structure information in the form of distributions. There are tools for building (instantiating) and loading virtual samples drawn from the digital material, analogous to the processes used in a physical laboratory. Mechanical properties are derived from the predicted response; hence, designers are able to iterate on the material structure for optimal properties. New experimental techniques have enabled the measurement and storage of actual microstructures. A new material representation framework we are working on for titanium alloys that encompasses both the statistical structure of the digital material and measured microstructural volumes is also described.

### 2:50 PM

**Invertible Microstructure-Property-Processing Linkages Using Spectral Methods:** *Surya Kalidindi*<sup>1</sup>; Hari Kishore Duvvuru<sup>1</sup>; Marko Knezevic<sup>1</sup>; Massimiliano Binci<sup>1</sup>; <sup>1</sup>Drexel University

Effective properties of materials are derived from the details of the underlying microstructure spanning several hierarchical length scales. A complete description of the microstructure is experimentally impractical at the current time; it is also unwarranted in many engineering design applications. Instead, statistical descriptions of the microstructure are often employed in composite theories (or homogenization theories) to predict the effective overall properties of the material. Models also exist for accurate prediction of the evolution of these statistical descriptions of microstructure under certain prescribed

processing operations. This paper presents a new and highly efficient spectral framework, called Microstructure Sensitive Design, for building invertible microstructure-property-processing linkages.

### 3:15 PM

**On The Design and Control of Properties in Polycrystalline Materials Using Process-Texture-Property Maps:** Nicholas Zabaravski<sup>1</sup>; *Veera Sundararaghavan*<sup>1</sup>; <sup>1</sup>Cornell University

We put forth a methodology to generate graphical representations of texture-property relationships in polycrystalline materials during deformation processing. Graphical representations when combined with linear analysis techniques form a powerful method for property optimization. The orientation distribution function is represented using finite element interpolation techniques that allow matrix representation of the microstructure-property relationships using linear upper-bound relations. Computations of texture evolution based on model reduction are then used to derive texture-property-process maps for various deformation processes. Universe of textures realized from a deformation process is shown to be optimally visualized as simple polygons in the reduced texture space. Various optimization problems are solved in this representation using graphical cross-plots or linear programming. These include identification of textures with extremal properties and identification of processing paths for reaching a desired property. Statistical learning techniques that allow optimization of properties that depend on higher-order features of the microstructure are described.

### 3:40 PM

**Progress in Materials Modeling and Some Future Needs:** Hamish Fraser<sup>1</sup>; Somnath Ghosh<sup>1</sup>; Michael Mills<sup>1</sup>; *James Williams*<sup>1</sup>; <sup>1</sup>Ohio State University

At the end of the 20th century there was growing recognition of the need for high fidelity modeling tools to accelerate materials development. These tools could supplant multiple empirical iterations that were commonly used to develop new materials. In response to this need, there has been a renewed effort to develop a variety of material modeling tools that compliment newly available experimental capabilities. Included are phase field modeling methods for describing microstructure evolution, finite element and crystal plasticity models for analyzing mechanical behavior, improved thermodynamic computational methods for defining equilibrium and sophisticated statistical methods such as neural networks for dealing with complex alloys where first principle methods are not yet ready. This talk will review the progress made in materials modeling over the past ~5 years using examples. It will close with some suggestions regarding high impact materials modeling needs that will sustain progress in this vital area.

### 4:05 PM

**Application of Microstructure Sensitive Design in Fuel Cell Electrodes:** *Dongsheng Li*<sup>1</sup>; Hamid Garmestani<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

A statistical continuum mechanics formulation is presented by means of Green's function method to predict the electrical and mechanical properties of fuel cell electrodes. This model is applied within the framework of microstructure sensitive design (MSD) to guide the design of the microstructure in porous lanthanum strontium manganite (LSM) fuel cell electrode. To satisfy the property requirement and compatibility, porosity and its distribution can be adjusted under the guidance of MSD to achieve optimized microstructure. Processing parameters can be adjusted to tailor the microstructure to achieved desired properties.

### 4:30 PM

**Design and Control of Microstructure in Controlled Drug Release Systems:** *David Saylor*<sup>1</sup>; Chang-Soo Kim<sup>1</sup>; Dinesh Patwardhan<sup>1</sup>; James Warren<sup>2</sup>; <sup>1</sup>U.S. Food and Drug Administration; <sup>2</sup>National Institute of Standards and Technology

A popular method of controlling drug release is to incorporate the drug into a polymer matrix, which becomes a diffusion barrier, limiting the drug release rate. It has been demonstrated that the microstructure that evolves during manufacture significantly impacts the release kinetics. However, because the relationships between processing conditions, microstructure, and release kinetics are not well understood in these systems, the product development and approval processes are currently governed by limited, empirically derived correlations. We have, therefore, developed a phase-field theory for microstructure evolution in these systems. Calculations based on theory