OPPORTUNITIES IN MESOSCALE SIMULATION: INTEGRATION OF PHYSICS BASED CONSTITUTIVE THEORIES WITH MICROSTRUCTURE EVOLUTION

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ABSTRACT Many time-dependent deformation processes, particularly those occurring at elevated temperatures produce significant concurrent microstructural changes that could alter mechanical response in a profound manner. Such microstructure changes are usually missing in crystal plasticity or other purely mechanical modeling. Although efforts have been made on developing microstructure-aware crystal plasticity models, the microstructure evolution is essentially still an auxiliary local constitutive law. Here we present an integrated full-field modeling scheme that couples the mechanical response with the underlying microstructure evolution.

Based on the seminal work of Moulinec and Suquet and recent extension by Lebensohn and colleagues, fast Fourier transform based methods have become a popular approach for the computation of the complete micromechanical fields in heterogeneous materials. On the other hand, the phase-field method is a well-known methodology for the simulation of the evolution of microstructural fields under a thermodynamic driving force. Here we present a fully coupled simulation framework for thermal-mechanical processing which simultaneously updates the local mechanical (stress/strain rate) fields and evolves the local microstructure (grain growth, phase separation etc). The algorithm is formulated in such a way that the Green’s function integrals can be cast as convolution with kernel operators that can be efficiently solved by spectral approaches. Since both methods are image-based and use an identical spectral formulation, datasets generated by one method can be used directly by the other as simulation RVEs, eliminating the difficult and time consuming meshing step that would be required for coupling via finite element.

In this talk two case studies will be explored: 1) The management of shear banding in bulk metallic glass composites with dendrite reinforcements and 2) The relationship between dynamic recovery and dynamic recrystallization in f.c.c metals. The focus of the talk will be on the development of physics based constitutive theories (dislocation based crystal plasticity, and free-volume dependent flow for the glass) and what new materials knowledge can be learned form the simulations, rather than on the numerics and computational advances.
**Biosketch:** Stephen Niezgoda is an Assistant Professor in the departments of Materials Science & Engineering and in Mechanical & Aerospace Engineering at OSU. Prior to his engineering studies Dr. Niezgoda worked as an industrial mechanic and machinist, and as an F.A.A. certified aircraft mechanic (A&P ratings). He obtained his Ph.D. from Drexel University in 2010 where his research was focused on Microstructure Sensitive Design. For his thesis work, he received the Drexel Thesis Award “Most Promise to Enhance Drexel’s Reputation in the Mathematical and Physical Science.” Niezgoda then went on to postdoctoral research appointments at Los Alamos National Laboratory in the Materials Science in Radiation and Dynamic Extremes group and at the Lujan Neutron Scattering Center (LANSCE). Stephen R. Niezgoda is the leader of Micro- & Mesoscale Mechanics and Structures Laboratory at The Ohio State University. His research interests include micromechanical modeling and simulation, constitutive model development, crystal plasticity, experiment and simulation co-design, computational materials design tools and materials data sciences.