**Special Materials Seminar**

Department of Materials Science & Engineering

# Monday May 21, 2018

1:30–3:30 ~ 405 Ferris Hall

"Linking Materials Science & Materials Engineering -- Microstructure-based Performance Predictions for Advanced Multi-phase Materials"

**Speaker: Dr. Xin Sun** Director-Energy & Transportation Science Division Oak Ridge National Laboratory, Oak Ridge, TN

Abstract:

It is well known that meso-scale microstructural features & their stability and evolution under service condition control the macroscopic performance for most engineering materials. Even though the precise definition of meso-scale may be material specific, meso-scale typically serves as the critical linkage between the bottom-up materials science-based approach & the top-down materials engineering-based approach. In this talk, a suite of modeling capabilities will be discussed to predict the influences of microstructure features & their evolution kinetics on engineering properties of advanced multiphase materials. The key challenge addressed is the quantitative linkages between the lower length scale performance limiting factors & the macroscopic engineering properties. First, microstructure-based finite element method will be presented to predict the stress versus strain curves for multi-phase advanced high strength steels (AHSS) under different loading conditions. The methodology has been developed based on the actual microstructures & the individual phase properties measured with in-situ high energy X-ray diffraction, & it has been successfully demonstrated in predicting ductile failure of dual phase and TRIP steels without any prescribed failure criterion. In addition to property predictions, the microstructure-based finite element method has also demonstrated usage in computational materials design optimization for various design concepts for 3rd generation advanced high strength steels. Next, a hierarchical modeling methodology will be presented aimed at predicting the overall stress versus strain curves as well as ductility for thin-walled high pressure die cast (HPDC) Mg castings. At the lower length scale, a microstructure-based finite element model is used to predict the intrinsic deformation limits of the cell-type alpha-beta matrix of the Mg casting for various beta phase volume fractions & morphologies. Once the matrix deformation limit is predicted, various extrinsic casting defects will be introduced to the next length scale. Representative volume elements (RVEs) considering various porosity size, shape, & volume fraction are constructed based on the experimentally characterized defect descriptors & their statistics. The modeling framework is then validated by comparing the predicted ductility & failure modes with experimental measurements. In the second part of the seminar, Dr. Sun will discuss multi-physics manufacturing process simulations for advanced energy materials. The focus of the discussion will be the effects of various thermomechanical processes on the microstructures & the resulting mechanical performance of the engineering materials. The manufacturing processes include resistance spot welding, impact welding, friction stir scribe welding, self-piercing rivet, trimming/cutting & hole expansion for trimmed edges.

Biography:

Dr. Sun is currently the Division Director for the Energy and Transportation Science Division at Oak Ridge National Laboratory in Oak Ridge, Tennessee. Dr. Sun received her Ph.D. from the University of Michigan in 1995, and was a Laboratory Fellow and Technical Group Leader at Pacific Northwest National Laboratory prior to joining ORNL in May 2017. Over the past two decades, Dr. Sun has conducted cutting-edge multi-disciplinary research in the areas of microstructure-based performance predictions for multiphase advanced high strength steels, Mg castings, aluminum alloys, as well as manufacturing process simulations including welding, forming, trimming, etc. She is a national laboratory leading authority on integrated computational materials engineering (ICME) and has authored/co-authored 185 peer reviewed journal publications and 10 books/book chapters.