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

It is well known that meso-scale microstructural features and 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 and 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 and 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 and 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 and the individual phase properties measured with in-situ high energy X-ray diffraction, and 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 and 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, and volume fraction are constructed based on the experimentally characterized defect descriptors and their statistics. The modeling framework is then validated by comparing the predicted ductility and failure modes with experimental measurements.

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 multiphase advanced high strength steels, Mg castings, aluminum alloys and microstructure based manufacturing process simulations. 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.