Fall 10-8-2015

Underpinning and benchmarking multi-scale models with micro- and nanoscale experiments

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Predictive models of materials behavior depend on: accurate databases of constitutive material properties, identification of underlying deformation mechanisms, and the availability of experimentally measured benchmarks with which to compare. Micro- and nano-scale experiments can be used to facilitate collection of salient mechanical properties of individual phases at appropriate temperatures, chemistries and microstructural states. Coupling with TEM observations allows one to identify underlying deformation mechanisms and to imbibe models with the requisite fundamental physics and materials science. Simulations must be benchmarked with experiments, conducted at scale with relevant material volumes and identifiable microstructures. This presentation will outline efforts to characterize the constitutive behavior of materials, to identify deformation mechanisms, and to benchmark crystal plasticity simulations at appropriate length scales.

Micro-scale experiments designed and conducted to complement crystal plasticity modeling of two different microstructural variants of Ni-base superalloys, polycrystalline Rene 88 and directionally solidified GTE 444, will be presented. If size-scale effect can be avoided, constitutive (single-crystalline) data may be obtained with micro-tensile tests at various orientations and temperatures. Moreover, preparing and testing specimens with reduced volumes and a finite number of grains allows for direct comparison with crystal plasticity simulations of stress-strain behavior as well as strain localization. With regard to the latter, digital image correlation (DIC) of spatially resolved surface displacements produces strain maps that provide a much more rigorous benchmark for crystal plasticity predictions than stress-strain curves. Using directionally solidified specimens allows for 2.5D microstructures (grains that extend through the thickness of the specimen) and greatly simplifies such comparisons. Moving beyond uniaxial tension, micro-bending resonance fatigue experiments provide an opportunity to measure the number of cycles, location, and microstructural features associated with slip, intragranular crack formation, and eventual transgranular crack growth. These experimental measures can in turn be used to inform and benchmark multi-scale fatigue simulations. Similarly, strain-controlled fracture experiments involving 2.5D unidirectional polymer matrix composites (PMC) have been developed and are being used to identify the microstructural features and fracture paths that govern delamination and fracture.

The availability of orientation mapping techniques (EBSD, PACOM, TKD) now allows for nano-scale characterization of underlying deformation mechanisms and their relation to crystallographic microstructures and surrounding neighborhoods. Studies investigating the role of grain growth, twinning and dislocation plasticity will be presented. Special attention will be placed on attempts to measure intragranular strains that can be related to the accumulation of geometrically necessary dislocations (GNDs) and compared with crystal plasticity simulations. Support for these projects has been provided through the AFOSR and AFRL funded Center of Excellence on Integrated Materials Modeling and the DOE office of Basic Energy Sciences.

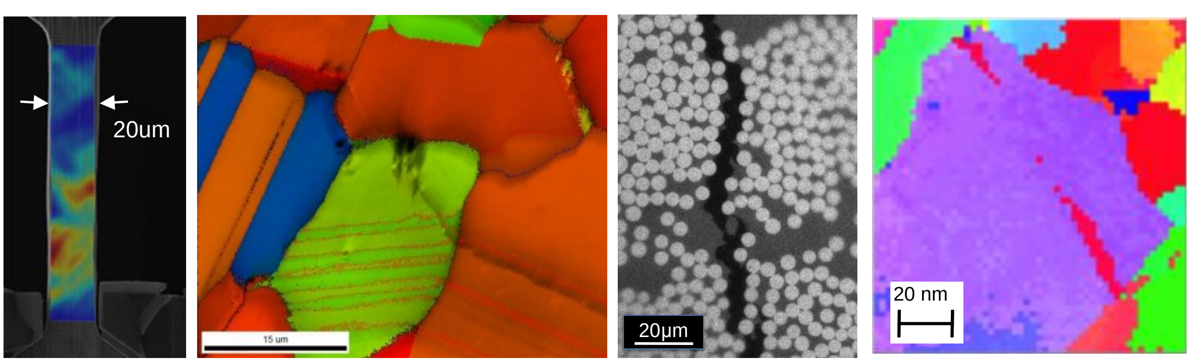

Figure 1: strain, stress and orientation maps of tensile, fatigue, fracture and twinning processes.