Dynamic 3-Dimensional Digital Structure: A Program Review

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The Office of Naval Research (ONR) hosted the fourth review of the Dynamic 3-Dimensional Digital Structure (D3DDS) program on 6–8 July 2009 in Arlington, Virginia. The focus of this project, initiated in 2005 and supported equally by ONR and the Defense Advanced Research Projects Agency, is to develop the characterization and computational tools necessary to enable the translation of micrographs (analog data sets) into digital data sets to more accurately include microstructure descriptions in design and prediction models for the affordable, accelerated insertion of materials into applications.

Three primary research teams are working to establish protocols for data and knowledge exchange, developing three-dimensional (3-D) characterization and modeling tools, and investigating the mechanisms that determine microstructural evolution and mechanical response. Their goals and progress were reported at this meeting.

The Naval-Research-Laboratory (NRL) (George Spanos) led team consists of NRL; Cornell, Northwestern, and Iowa State universities; Rensselaer Polytechnic Institute; and Risø National Laboratory researchers. Their work focused on serial sectioning; 3-D reconstruction, and quantitative analysis of grain curvature, topology, and crystallography leading to new understanding of grain growth; finite element modeling (FEM) of the elastic and plastic response of reconstructed 3-D β -titanium microstructures to mechanical loading; integrating FEM of deformation-induced microstructural evolution with micromechanical behavior and elastic moduli determined using in-situ synchrotron x-ray techniques; 3-D reconstructions of in-situ x-ray tomographic data; analytical tools for accurate and

computationally efficient 3-D descriptions of microstructure; and the initial direct comparisons of 3-D microstructures with phase field models that simulate microstructural evolution. Their on-line *3-D Materials Atlas* archives and makes accessible large microstructure data sets and relevant metadata. It is being used by all three teams, and will be demonstrated at the TMS 2010 Annual Meeting.

The Ohio-State-University-(Hamish Fraser) led team consists of Ohio State, Carnegie Mellon and Drexel universities, and University of Pennsylvania researchers. They presented work on 2-D and 3-D characterization and automated microstructure digitization tools; phase field modeling for microstructure evolution in titanium alloys; coupled phase field and atomistic modeling tools for analyzing deformation; image-based crystal plasticity FEM with multi-time scaling for cyclic deformation; two unifying tools based on microstructural sensitive design (for microstructure and properties); and neural network tools for predicting microstructure/property relationships. Notably, simulations in titanium alloys based on highly coupled phase field and atomistic modeling allow realistic predictions of microstructural evolution and deformation mechanisms as functions of thermal exposure (i.e., heat treatment) and applied stress. Atomistic simulations of key dislocation/microstructure interactions, such as slip transmission through α/β interfaces and the evolution of deformation twinning, in titanium alloys are critical to understanding and articulating these phenomena.

The team led by QuesTek Innovations, LLC (Greg Olson) consists of QuesTek, Northwestern and Georgia Tech universities, University of Michi-

gan, MIT, Scientific Forming Technologies Corporation, and Colorado School of Mines. They presented work on laser-assisted local-electrode atom-probe tomography applied to multiphase precipitation in damage-resistant steel (BA160); femtosecond laser serial sectioning for large representative volume element tomography; multiscale tomographic analysis of ultrahigh strength steels for toughness and fatigue strength; and tools to quantify spatial non-uniformity of precipitate dispersions. These microstructural descriptions in turn inform and guide topological analyses of 3-D charge density applied to interfacial de-cohesion, enabling predictive tools that capture the mechanics of microvoid shear softening and localization consistent with an experimentally observed dependence of critical shear instability strain on particle size and spacing. This work enables explicit 3-D fracture toughness prediction and development of ductile fracture simulation modules for incorporation into DEFORM. Of note, 3-D microstructure-sensitive hierarchical fatigue modeling has been successfully applied to martensitic gear steels.

These tools enable researchers to collaborate more effectively, to more accurately characterize 3-D microstructural features at appropriate length scales, to advance understanding of the mechanisms that determine microstructural evolution and mechanical behavior, and to capture this knowledge base in quantitative modeling and simulation tools. They are making tangible progress toward integrated computational materials science.

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