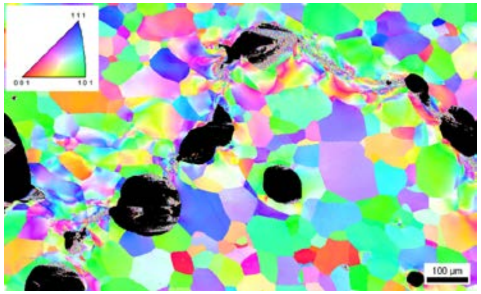
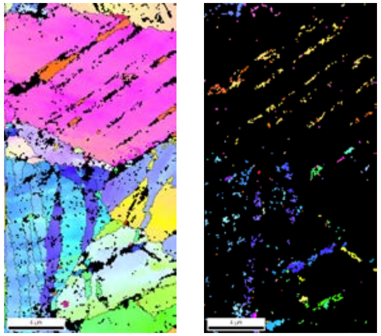
Mesoscale Priority Research Direction

Microstructure Based Heterogeneity Evolution Leading to Phase Transformation and Damage/Failure Events

Dynamic damage/failure & phase transformation processes are believed to occur by a series of nucleation, growth, and coalescence events. The linkage of these events to the details of the material chemistry and microstructure are poorly understood.



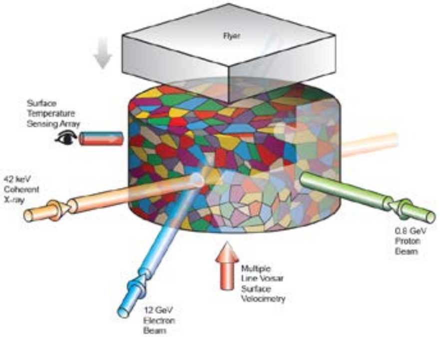
Pores and pore coalescence in dynamically loaded Tantalum



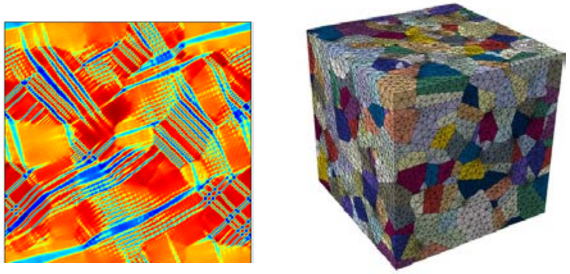
Retained high pressure ω phase (left) and parent α phase (right) in dynamically loaded Zirconium

Much more study of these physical events at the length scales at which they occur are required.

Meso-Scale Experiment and Data Analysis



+



Meso-Scale Theory and Simulation

Escobedo, J. P., Cerreta, E. K., Dennis-Koller, D., et al. , 2011. *Effects of Grain Size and Boundary Structure on the Dynamic Tensile Response of Copper*, J. Appl. Phys. 110, 033513.

Lebensohn R.A., et al., 2011. *Dilatational Viscoplasticity of Polycrystalline Solids with Intergranular Cavities*. Philosophical Magazine 91, 3038.

Addessio, F. L., et al., 2003. *Model for High Strain-Rate Deformation of Unranium-Niobium Alloys*, J. Appl. Phys. 93(12), 9644.

Lookman, T. et al., 2008. *Phonon Mechanisms and Transformation Paths in Pu*, Phys. Rev. Let. 100, 145504.

Bronkhorst, C. A., 2011. *Accounting for Microstructure in Large Deformation Models of Polycrystalline Metallic Materials*, in Computational Methods for Microstructure-Property Relationships, S. Ghosh and D. Dimiduk eds., Springer Science, New York.

Mesoscale Priority Research Direction

Microstructure Based Heterogeneity Evolution Leading to Phase Transformation and Damage/Failure Events

Opportunity

A predictive understanding of microstructure-based heterogeneity evolution and its consequences for material damage / failure and phase transformation is presently lacking. This lack of understanding prevents us from predicting material response under severe loading conditions.

Meso Challenge

This challenge is an evolving length scale problem, beginning with nucleation events at the atomic scale and ending with failure or percolation at the grain scale. We lack the experimental and theoretical capability to adequately address this class of problem. These length scales are too large for MD and too small for macro-scale theories to properly represent.

Approach

New experimental capabilities must be developed to observe the evolution of 3D physical events in-situ with micron scale resolution while the material is exposed to severe loading conditions. New theory and simulation capability must be fostered at the length scale of these nucleation and growth events in order to best extract insight from the experiments and tangibly test our hypotheses.

Impact

This work will provide the proper statistical perspective, information and tools at the length scales at which these physical events occur and interact. This understanding and new capability will allow us to predict these statistical events under the extreme loading conditions of strategic importance and allow us to design new materials for improved performance.

Contact: C. A. Bronkhorst, cabronk@lanl.gov