Structural Transitions and Local Deformation Processes at and Near Grain Boundaries

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At the Materials Science & Technology 2009 conference in October, a symposium with this title examined the heterogeneous structure, properties, and deformation characteristics near grain boundaries. These characteristics, when coupled with the anisotropic effects of different grain orientations, cause complex responses as the material is deformed, which affect the overall deformation behavior.

Grain boundaries are described by their character, which quantifies their structure and energy. The distribution of grain boundary character evolves with thermal activation to minimize system energy. Temperature and composition (minority elements) can dramatically affect grain boundary mobility or their ability to slide under the influence of stress. The structure also influences defect accumulation (e.g., low energy $\Sigma 3$ (twin) boundaries resist absorption of dislocations into the boundary, which affects the distribution of internal strain energy in the adjacent grains). Better understanding of grain-boundary composition and structure will improve our ability to optimize properties.

In both metals and ceramics, phases or “complexions” present in boundaries have important differences in structure and composition from the grains on either side. Complexions differ from phases in that they are not three-dimensional (3-D) like precipitates, so they can only be explored with advanced transmission electron microscopy techniques (TEM). The thermodynamics of complexions are intimately related but differ significantly from the grain interior, due to differences in structure and chemistry in the interface. These issues are explored in the following paper by Shen J. Dillon et al.

Deformation in metals is heteroge-

neous due to spatial variations in activated slip systems. Non-uniform interactions between slip systems within a grain lead to subgrains and orientation gradients. This substructure strongly affects subsequent changes via recovery and recrystallization during subsequent heat treatments.

With deformation, an initially smooth surface can develop significant topography near grain boundaries. This can be quantified using surface profilometry techniques. The influence of a neighboring grain on deformation near the boundary can also be characterized with nanoindentation experiments. Electron backscatter pattern mapping provides data sets that allow features of heterogeneous deformation to be characterized and quantified. Transmission electron microscopy continues to be an important tool to directly and visually examine defect structure near grain boundaries, as entangled dislocations remain pinned in place. However, the small size of TEM specimens does not allow examination of larger scale defect densities. New tools such as 3-D x-ray microdiffraction microscopy allow identification at the micrometer scale of local crystal orientation, orientation gradients, defect density, and internal strains. Observations of internal strain and defect distribution beneath the surface in loaded specimens are now possible. These experimental observations allow computational models to be evaluated against experimental observations that will lead to improvements in their predictive capability. An example of how several observation methods can be used synergistically to quantify heterogeneous deformation in order to provide a basis for comparison with crystal plasticity finite element modeling is presented in the paper by

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Emission of dislocations from grain boundaries under the influence of stress is an important mechanism of plastic deformation. The grain boundary structure, its inclination, and grain orientations affect the ability to emit dislocations, and can be modeled using molecular dynamics. Grain boundaries are also sites for nucleating bulk phase transformation by emission of partial dislocations that facilitate the sequential planar growth of new phases, or new orientations by mechanical twinning. The ability to nucleate new phases depends on the character of the grain boundary.

Damage nucleation at grain boundaries is common, and the mechanisms by which this occurs need to be identified. Solute atom segregation and precipitation in grain boundaries is a common cause of damage nucleation. Triaxial stress states arising from incompatible elastic or plastic deformation in adjacent grains also facilitate the opening of voids or cracks, and such stress states depend on the interaction between adjacent grains and the externally imposed stress state. Mechanical twins can impose large local shear displacements that can lead to damage nucleation. As defects are rare events, mechanisms that cause their nucleation need to be established. With such rules, processing paths that minimize conditions that facilitate damage nucleation can be identified. This understanding can then be used to examine how cyclic deformation in service leads to fatigue crack nucleation and growth, as illustrated in the paper by E-Wen Huang et al.

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