Department of Materials Science and Engineering,

PhD Defense

October 19th at 11am
Curtis 162 (MEM Seminar Room)

Damage Tolerance and Mechanics of Interfaces in Nanostructured Metals

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The concept of interface driven properties in crystalline metals has been one of the most intensely discussed topics in materials science for decades. Since the 1980s researchers have been exploring the concept of grain boundary engineering as route for tuning properties such as fracture toughness and irradiation resistance. This is especially true in ultra-fine grained and nanocrystalline materials where grain boundary mediated properties become dominant. More recently, materials composed of hierarchical nanostructures, such as amorphous-crystalline nanolaminates, have attracted considerable attention due to their favorable properties, ease of manufacture and highly tunable microstructure. While both grain boundary engineering and hierarchical nanostructures have shown promise there are still questions remaining regarding the role of specific attributes of the microstructure (such as grain boundaries, grain/layer size and inter/intralayer morphology) in determining material properties. This thesis will attempt to address these questions by leveraging atomistic simulations to perform deformation and damage loading studies on a series of nanolaminate and bicrystalline structures.

During the course of this thesis the roles of layer thickness, interlayer structure and interlayer chemistry on the mechanical properties of Ni-NiX amorphous-crystalline nanolaminates will be explored using atomistic simulations. This thesis found that layer thickness/thickness ratio and amorphous layer chemistry play a crucial role in yield strength and Young's modulus. Analysis of the deformation mechanisms at the atomic scale reveals that structures containing single crystalline, crystalline layers undergo plastic deformation when shear transformation zones

form in the amorphous layer and impinge on the amorphous-crystalline interface, leading to dislocation emission. However, structures containing nanocrystalline, crystalline layers (both equiaxed and columnar nanocrystalline) undergo plastic deformation through a combination of grain boundary sliding and grain boundary mediated dislocation nucleation. Since grain boundaries were found to play a critical role as sources and sinks for dislocations in amorphous-crystalline nanolaminates a follow-up study on the effect of grain boundary character on damage accumulation/accommodation in copper symmetric tilt grain boundaries was performed. This study found that grain boundaries will become saturated with damage, a state where grain boundary energy and grain boundary free volume oscillate about a plateau during continuous defect loading (vacancy, interstitial and frenkel pair loading were all considered). Further, grain boundary character (specifically equilibrium grain boundary energy) was strongly correlated to the damage accommodation behavior of grain boundaries in copper. Finally, a study that attempted to link grain boundary damage saturation behavior to variations in grain boundary mechanical properties was performed. This study found no direct relationships between grain boundary damage saturation behavior and variations in grain boundary properties.

The results of this thesis provide researchers with several strategies for tuning the properties of amorphous-crystalline nanolaminates. These strategies include manipulated bulk attributes such as layer thickness and morphology as well as manipulation of microscale attributes such as grain boundary engineering. Finally, this thesis provides valuable insight into the damage loading/accommodation behavior of FCC symmetric tilt grain boundaries.