SAND2015-9020C

Experimental investigation and mesoscale modeling of irradiation-induced grain growth

Fadi Abdeljawad, Daniel C. Bufford, Stephen M. Foiles, and Khalid Hattar

Sandia National Laboratories, Albuquerque, NM 87185, USA

Nanocrystalline metals (NCs) exhibit a unique combination of properties that render them attractive materials of choice for many technological applications. Owing to the large fraction of grain boundaries (GBs) in NCs, these systems are unstable against grain growth and other homogenization processes even at low temperatures. Determining the role of grain orientation, and GB type and character is a key step in predicting material properties and ensuring long-term microstructural stability. Herein, we present a combined experimental and mesoscale modeling study in order to better understand the nature of radiation-induced grain growth and boundary migration in NC gold. With the aid of TEM precession-assisted electron diffraction orientation mapping, images and orientation maps were collected before and after *in situ* ion irradiation TEM with 10 MeV Si, where microstructural features, such as grain size, texture, and individual grain boundary character were quantified. The modeling framework on the other hand is capable of capturing the polycrystalline nature of gold and accounting for interface thermodynamics. Spatially localized regions with elevated temperatures are induced by irradiation and the model accounts for such effects by defining temperature-dependent GB mobilities. Experimentally collected orientation maps were used as initial inputs in the model and several GB properties were varied to better understand the effects of radiation on the microstructural evolution. On the whole, the combined experimental and modeling techniques provide future avenues to enhance quantification and prediction of the thermal and radiation stability of GBs in NC systems.