Modeling the Effects of Quasistatic and Dynamic Stress on Extended Defects in FCC Al and Cu

ALISON KUBOTA, WILHELM WOLFER, Lawrence Livermore National Laboratory — There has been much interest in understanding the effect of extended defects on the static and dynamic responses of metals to applied stress. These aging effects, in the form of dislocation loops, voids, and He bubbles can possibly lead to changes in properties such as the equation-of-state of materials. In this work, we focus on the use of large-scale molecular dynamics simulations to model the loading response of voids and He bubbles in both low- and high-stacking-fault energy (Cu and Al) face-centered-cubic metals. In both quasistatic and dynamic loading conditions, both voids and He bubbles are found to initiate collapse by emission of stacking faults from the defect edge. However, we show the significant differences in the intermediate and end-state structures due to the presence of He. In addition, we discuss the effect of short-pulse shock waves on the unfaulting of dislocation loops and net change in Burgers vector through complex dislocation reaction pathways. These simulations using pulsed loading conditions are able to capture the details of these processes that would otherwise remain hidden from observation by electron microscopy. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.