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Molecular Dynamics Simulation of the Shock Response of Nanocrystalline Cu-Ta Systems[1] JIE CHEN, Univ of Connecticut - Storrs, MARK TSCHOPP, US Army Research Laboratory, AVINASH DONGARE, Univ of Connecticut - Storrs — Nanocrystalline (nc) metal alloys comprising of second phase solutes show promise towards the design of high strength materials as compared to their coarse-grained counterparts. One such system is the high strength nc-Cu-Ta alloy. The improved deformation response is attributed to grain boundary pining due to the presence of Ta precipitates resulting in limited grain boundary sliding and rotation at high temperatures. A thorough understanding of the role of microstructure and chemistry on the nucleation and evolution of defects under shock loading conditions is crucial for the design and optimization of Cu-Ta alloys for dynamic loading environments. Large-scale molecular dynamics (MD) simulations are therefore performed to examine the deformation and failure behavior of Ta solute strengthened bulk nc-Cu systems under shock loading conditions. The dynamic evolution of defects (dislocations and twinning behavior) is investigated for variations in microstructure (grain size of nc-Cu and Ta distribution in the form of solute atoms as well as precipitates) during shock compression and spall failure. The MD simulations suggest that the spall strengths of the metal are largely influenced by the distribution of the Ta solute in the nc-Cu matrix. The effect of Ta distribution at the grain boundaries, grain interior and as precipitates on the evolution of dislocation densities and the spall strength of the alloy will be presented.

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