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Dynamic Evolution of Defects during Shock Loading and Spall Failure of Al Microstructures[1] GARVIT AGARWAL, AVINASH DONGARE, Univ of Connecticut - Storrs — Large scale molecular dynamics (MD) simulations are carried out to investigate the links between the microstructure and evolution of dislocations during shock loading and spall failure of Al microstructures. The MD simulations suggest that the variations in the spall strengths for the [001], [110] and [111] loading orientations of single crystal Al are influenced by the evolution of the densities of Shockley partials and twinning dislocations in the microstructure. In addition, the evolution of dislocation densities are investigated for nanocrystalline Al (grain size of 40 nm) to investigate the effect of distribution of grain boundaries on the defect evolution and spall failure behavior. While MD simulations are able to provide critical insights in the evolution of defects, the capabilities are limited to small system sizes. The newly developed quasi-coarse-grained dynamics (QCGD) method is able to scale up the capabilities of the MD simulations to model the shock loading and the spall failure behavior as predicted by MD simulations. The QCGD simulations are able to implicitly capture the nucleation, evolution and interaction of dislocations as well as the nucleation, growth and coalescence of voids as predicted by MD simulations by solving the equations of motion for a reduced number of representative atoms and show significant promise to model the materials behavior at the mesoscales. The evolution of dislocation densities as predicted by the MD and the QCGD simulations and the role of microstructure will be presented.

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