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Unraveling the Evolution of Microstructure during Shock Loading and Spall Failure at the Atomic Scales and the Mesoscales[1] AVINASH DONGARE, GARVIT AGARWAL, SERGEY GALITSKIY, University of Connecticut — The modeling of the spall failure of metals requires a fundamental understanding of the evolution of defects and the nucleation, growth and coalescence of voids under shock loading. Classical molecular dynamics (MD) simulations are used to investigate the links between the microstructure and the evolution of dislocation densities and damage (voids) during shock compression and spall failure of single crystal and nanocrystalline Al microstructures. However, this understanding of the onset of spallation at scales beyond the capability of MD simulations is still in an infancy. The "quasi-coarse-grained dynamics" (QCGD) method is able to scale up MD simulations to the mesoscales using scaling relationships for interatomic potentials and degrees of freedom for a reduced number of atoms. The spall failure behavior is investigated for polycrystalline Al systems with dimensions ranging from 0.1 microns to 10 microns for strain rates ranging from 10^7 s^{-1} to 10^{10} s^{-1}. The strain rate and grain size dependence on the evolution of dislocation densities and damage will be presented. The predicted atomic scale evolution of dislocation densities and void fraction at the mesoscales will be presented.

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