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A hybrid mesoscale-continuum method to model laser shock loading and spall failure at the mesoscales SERGEY GALITSKIY, AVINASH DONGARE, University of Connecticut — A hybrid atomistic-continuum approach combining molecular dynamics (MD) simulations with a two-temperature model (TTM) is utilized to model spall behavior of single crystal and nanocrystalline (pc) Al systems induced by ultrafast laser irradiation. The TTM is combined with a mesoscale modeling method, to extend the capability of the MD/TTM simulations to the mesoscales while retaining atomic scale mechanisms that determine microstructure evolution. The mesoscale capability is obtained using a quasi-coarse-grained dynamics (QCGD). The QCGD/TTM simulations are able to model the laser energy absorption by conduction electrons, electron-phonon coupling, heat generation and transfer, melt dynamics, and defect nucleation and evolution behavior. The scaling relationships for QCGD/TTM simulations are developed for various levels of coarsening and enable the investigation of the evolution of microstructure (defects), temperature and pressure at the length and time scales of experiments. The capability of QCGD-TTM approach is demonstrated by modeling effect of system size on the laser shock loading of pc Al films with system sizes of up to 2 μm and an average grain size of 0.5μm. The results suggest that the shock wave propagation and spall failure is determined by the size of the system wherein phenomena such as no-spall, void nucleation and collapse and spall failure are observed. The pressure wave propagation, dislocation density evolution behavior and the mechanisms of void nucleation and growth will be presented.

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