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An atomistic study of the effect of micro-structure on the HEL evolution in a nanocrystalline aluminum R. VALISETTY, Comp., and Info., Sci., Directorate, U.S. Army Research Lab., A. RAJENDRAN, University of Mississippi, A. DONGARE, University of Connecticut, R. NAMBURU, Comp., and Info., Sci., Directorate, U.S. Army Research Lab. — This study focuses on the shock precursor decay phenomena in pure aluminum crystals and nanocrystalline aluminum (nc-Al) systems under one dimensional strain condition using large scale molecular dynamics (MD) simulations. For this purpose, two different atom systems are modeled for the nc-Al: 1) 900 Å thick (~20 million atoms) with grain sizes (Å): 60, 100, 140 and 180, and 2) 5000 Å thick (~2 billion atoms) with grain sizes (Å): 180, 500, and 1000. The MD simulations considered a plate-on-plate configuration at five impact velocities between 0.7 km/s to 1.5 km/s. The very large MD results (~100s of terabytes) are modeled using a material conserving atom slicing method, based on averaged stress distributions along the shock fronts. The effects of grain sizes on dislocation evolutions at the HEL are analyzed in terms of precursor decay profiles at various distances along the shock front. The results indicate that the effect of impact velocity on the HEL amplitudes becomes insignificant after the wave propagates certain characteristic distances. However, the grain size significantly influences the material shock strength. By combining HELs determined from MD results with plate impact experimental data reported in literature for pure aluminum, the precursor decay for nc-Al systems was constructed across nano to macro length scales. The construct is based on the assumption that the plasticity is a result of accumulations of defects or dislocations from a very small scale to a large scale of the material.

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