An atomistic study of shock front evolution in a nanocrystalline Al

R. VALISETTY, U.S. Army Research Laboratory - APG, A. RAJENDRAN, University of Mississippi, G. AGARWAL, A. DONGARE, University of Connecticut, J. IANNI, Lockheed-Martin, ARL DOD Supercomputing Resource Center, R. NAMBURU, U.S. Army Research Laboratory - APG — The precursor decay phenomenon in solids was investigated using large scale atomistic molecular dynamics simulations. The main objective was to study the strain rate effects on the evolution of stress wave profiles at the elastic-plastic transition point (Hugoniot Elastic Limit – HEL). The simulations employed a multi-billion nanocrystalline aluminum atom system with an average grain size of 100nm for five impact velocities ranging 0.7 km/s to 1.5 km/s. The results comprised of the histories of stress, strain rate, and precursor decay with respect to time and distance from 100s of terabytes of data were analyzed towards evaluating the transient shock fronts. The stress amplitude (HEL) at all strain rates exhibited high strain rate dependency and as one would expect the steady state value was never reached. The HEL data from computational results at nanoscales when extrapolated reasonably matched with the experimental data across maso to macro scales. Finally using a crystal analysis algorithm and a twin dislocation identification method, dislocation densities were reduced and reported in terms of type of dislocation vs. axial stress. The analyses also showed that certain types of dislocations seemed to strongly influence the elastic-plastic transition response of the aluminum atom system.

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