SHOCK11-2011-020020
Abstract for an Invited Paper
for the SHOCK11 Meeting of
the American Physical Society

The development and application of multi-scale materials modeling methods for the prediction of dynamic strength[1]

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It becomes more difficult to simply extract experimental information on the strength of materials under dynamic conditions simultaneously reaching high pressures, temperatures, and strain rates. The difficulty stems from the inability to independently control and extract the pressure, temperature and strain rate dependence under dynamic conditions, the inability to maintain those conditions, and the inability to probe into the volume of a material during an experiment. The observations that are made during dynamic materials experiments tend to be integrated measures of the equations of state and materials strength. As a result, materials experiments reaching dynamic extremes may be better suited to validate and constrain materials strength models and equations of state than they are for actually uniquely determining their forms and coefficients. Conversely, as the dynamic conditions become more extreme they may become more amenable to being investigated with the suite of materials modeling and simulation tools currently available. In studying the dynamic strength of simple ductile metals, molecular dynamics simulations are able to easily simulate the mobility of dislocations when their velocities are on the order of 0.1 m/s and above. The low velocity limit is controlled by the frequency of atomic vibrations, the spacing between atoms, and the limits of strong scaling of molecular dynamics simulations on massively parallel computers. For dislocation densities on the order of 10^{12}-10^{16} m^{-2}, and lattice spacings on the order of Angstroms, the mobility information becomes relevant for materials experiencing strain rates greater than 10^4 s^{-1}. The typical time scales of dislocation dynamics tools are controlled by the frequency of dislocation collisions, the natural frequencies of a dislocation line segment whose length scales with the spacing between dislocations, and the limits of strong scaling of dislocation dynamics simulations on massively parallel computers. These time scales practically limit dislocation simulations to strain rates greater than 10 s^{-1}. Furthermore, the efficiency of these simulations increases with increasing strain rate. When the mobility of the dislocations is obtained by molecular dynamics simulation the strain rate limit from the molecular dynamics simulations apply. The development of the constitutive models for dynamic straining conditions using a multiscale modeling methodology employing ab intitio, molecular dynamics, dislocation dynamics, and continuum finite element methods will be presented. Each modeling method is used to obtain information about material behavior that is sourced at its relevant length scale of applicability. The results obtained with the each simulation method are coarse grained and used as input for all of the simulations applicable at larger length scales. At the end of this chain, a final constitutive model for material strength is constructed for use in general engineering codes used to simulate the behavior of components under dynamic loading conditions. The final form of the model as well as all of its coefficients are determined by the supporting lower length scale simulations so that it can be considered a true numerical prediction of the material's dynamic strength. The predictive quality of the model is assessed by comparing the prediction of engineering simulations with the observations under a variety of loading conditions obtained with gas guns, explosive drives, and laser ramp loadings.