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Anisotropic Modeling of Shocked Single Crystals with Application to Energetic Materials

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A continuum, anisotropic modeling framework has been developed for simulating shock wave propagation in single crystals of arbitrary orientation. Our modeling approach incorporates nonlinear elasticity and crystal plasticity in a thermodynamically consistent tensor formulation. Crystal plasticity is described using a model that considers dislocation motion along specified slip planes. Shear cracking along specified crystal planes is also considered. Numerical simulations, using a finite-difference code, for large amplitude wave propagation in single crystals are presented. From these simulations, issues related to pure mode propagation for nonlinear elastic waves are discussed. Also, the effects of plasticity on wave propagation in single crystals are explored by comparing simulations to wave profile data for copper (Jones and Mote, 1969) and for LiF (Asay, et al., 1972). For copper, a single dislocation model for slip on {111} planes provides good agreement with quartz gauge data for shocks along the [100], [110], and [111] directions. For LiF, slip occurs on {110} planes, and good agreement with data is obtained for shocks along the [100] direction. Using the same dislocation model, simulated shock wave propagation along the low symmetry [310] direction of LiF is also examined. In addition, simulations are compared to transmitted wave profiles (Dick and Ritchie, 1994; Dick, 1997) for various orientations of shocked pentaerythritol tetranitrate (PETN) single crystals. For shocks along the insensitive [100] orientation of PETN, dislocation slip is unhindered and a dislocation dynamics model provides good fits to the wave profile data. For shocks along the sensitive [110] orientation, in which steric hindrance impedes the motion of dislocations, evidence of strain-softening behavior is observed and a shear cracking model fits the data well. Work supported by DOE and ONR.