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Initiation of High Explosives

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Plastic-bonded explosives are heterogeneous materials. Initiation of a heterogeneous explosive is dominated by hot spots: localized regions of high temperature. Simulations of hot spots require resolving individual explosive grains. Computations on the grain scale are called mesoscale simulations. These are being used to understand the physical mechanisms that generate hot spots. This is a preliminary step towards following the evolution of hot spots leading to initiation of a detonation wave. The goal is to develop a better subgrid burn model based on the underlying physics.

At the grain level an explosive is crystalline and, by its very nature, anisotropic. Properties of the explosive HMX needed for mesoscale simulations have been examined. The available data and results of molecular dynamics simulations are reviewed. Data includes: (i) Hydrostatic measurements by Olinger, Roof & Cady (LANL) and recently extended by Yoo & Cynn (LLNL). (ii) Recent measurements of elastic constants by Joe Zaug (LLNL). In addition, Tommy Sewell (T-14), has employed molecular dynamics simulations to determine the elastic constants. (iii) Wave profiles in single crystal HMX by Jerry Dick (DX-1). Consistency among the different data sets is one of the issues being studied.

For weak compressive waves, plastic work and shear heatings are the dominant dissipative mechanisms for generating hot spots. The single crystal wave profiles can be fit with a rate dependent plasticity model. From the inferred value of the yield strength, 2.6 kb, the estimated plastic work does not lead to peak hot spot temperature sufficient for ignition. Shear heating depends on the value of viscosity. In the liquid phase, viscosity has been determined from molecular dynamics experiment. Sufficient heating for hot spots can only be generated by very narrow shear layers. For stronger stimuli the dominant dissipative mechanism is undoubtedly void collapse.

Thermal parameters are not well known. The most important one that we identified is the melt curve as a function of pressure and the specific heat in the liquid phase. Determining material properties is a necessary preliminary step for performing scientifically valid simulations. Work is continuing on determining material parameters along with the mesoscale simulations.

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