Modeling Energetic Materials That Change From Solid to Liquid to Gas to Burnt Vapor

D. Scott Stewart
Theoretical and Applied Mechanics, University of Illinois, Urbana

The ignition of energetic materials, such as explosives and propellants, when subjected to low speed impacts at velocities on the order of 100-200 m/sec, requires the study of models that fully take into account the solid nature of the materials. Unlike the hydrodynamic models that describe shock-to-detonation transition and are appropriate for higher impact speeds, the models for lower speed impact exhibit a much greater degree of complexity due to the large number of mechanisms available within the material by which energy can be transformed and localized. The simplest hydrodynamic models have energy advection, potential energy storage in the pressure, and energy release by virtue of chemical reaction. In contrast, a model for an energetic material that begins as a solid must account for the same mechanisms and for dissipative processes associated with more complex stress distributions, phase transformations, heat conduction, and other localized processes. Such a model is intrinsically more complex with many more distinct length and time scales than its simple hydrodynamic counterpart.

In a recent effort with G. A. Ruderman and Eliot Fried we have applied the tools of continuum thermomechanics to develop a thermodynamically consistent model of an energetic material like HMX, that has three states, solid, liquid and gas and can undergo chemical reaction. This model describes the phase transitions with phase-field modeling in the sense of Gurtin and Fried’s prior works. Thermomechanically consistent rate laws are obtained for chemical reaction and phase transitions and these evolution equations are solved simultaneously with the standard balance laws.

In work with Ruderman and J. Yoh, we have started to explore the behavior of this model in various limiting cases when the equations of motion can be reduced to time dependent equations with one space dimension. This includes one-dimensional shear loading (representative of shear bands), and one-dimensional longitudinal compression loading (piston impact), and spherical geometries as well such as the ignition of HMX by expanding hot inert gases from initiating center. We will also talk briefly about issues associated with the numerical simulation of multi-material interactions in the context of studies of igniton.