Abstract Submitted
for the DFD12 Meeting of
The American Physical Society

Developing Subgrid Models for Shock-to-Detonation Mesoscale Simulations THOMAS JACKSON, University of Illinois at Urbana-Champaign — Determining the thermal and mechanical sensitivity of new and existing energetic materials is important for transportation, safety and storage concerns. Initiation of an energetic material can occur when an impulse delivered to the material evolves into a self-sustaining detonation wave. The microstructure can lead to local regions of high temperature, so-called "hot spots." Temperatures in these hot spots can exceed the bulk temperature expected from shock heating, which in turn can trigger ignition even when a homogenized model might fail to predict it. If the chemical and mechanical energy release within hot spots exceeds cooling by diffusion and join up, a localized ignition can occur. Ignition spread due to evolution and growth of high-temperature regions, potentially with reinforcement from neighboring regions or preconditioning of the material, can then lead to detonation. Hot spots are thought to be formed due to shock interaction with microscale and molecular-scale material inhomogeneities through processes such as void collapse, shear banding, debonding, and grain sliding. The most important question at the device scale is whether or not the individual hot spots will coalesce to create a local ignition front, and whether the ignition front or fronts are in turn sufficient to initiate the entire device. Our approach has two principal steps. We first develop sub-grid models based on hot-spot dynamics, and then use the sub-grid model in our mesoscale simulations using our shock dynamics code. In this talk we present recent efforts into developing subgrid models that can be incorporated into mesoscale simulation codes.

Thomas Jackson
University of Illinois at Urbana-Champaign

Date submitted: 03 Aug 2012 Electronic form version 1.4