

SHOCK09-2009-020001

Abstract for an Invited Paper
for the SHOCK09 Meeting of
the American Physical Society

Beyond the Standard Model for High Explosives: Challenges & Obstacles to Surmount

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Plastic-bonded explosives (PBX) are heterogeneous materials. Nevertheless, current explosive models treat them as homogeneous materials. To compensate, an empirically determined effective burn rate is used in place of a chemical reaction rate. A limitation of these models is that different burn parameters are needed for the same PBX to describe shock initiation for different initial temperatures and initial densities. This is due to temperature fluctuations generated when a heterogeneous material is shock compressed. Localized regions of high temperatures are called hot spots. They dominate the reaction for shock initiation. The understanding of hot spot generation and their subsequent evolution has been limited by the inability to measure transients on small spatial ($\sim 1 \mu\text{m}$) and small temporal ($\sim 1 \text{ns}$) scales in the harsh environment of a detonation. With the advances in computing power, it is natural to try and gain an understanding of hot-spot initiation with numerical experiments based on meso-scale simulations that resolve material heterogeneities and utilize realistic chemical reaction rates. However, to capture the physics correctly, such high resolution simulations would require more accurate material properties than have been used for homogenized reactive models. Here we focus on the equation of state (EOS) of the solid reactants and the role shock wave studies have played in developing high pressure EOS. Simple solid EOS implemented in hydro codes assume that the specific heat is constant. While this is a good approximation for metals, it is not adequate for explosives. Explosives are large molecules with many internal vibrational degrees of freedom. These modes give rise to a significant temperature dependence to the specific heat in the region of interest for shock initiation. Due to the sensitivity of chemical reaction rates to temperature, thermal properties are critical for initiation simulations that resolve hot spots.