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GRAIN-SCALE SIMULATIONS OF HOT-SPOT INITIATION FOR SHOCKED TATB

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Abstract. High-explosive (HE) material consists of large-sized grains with micron-sized embedded impurities and pores. Under various mechanical/thermal insults, these pores collapse generating high-temperature regions leading to ignition. A computational study has been performed to investigate the mechanisms of pore collapse and hot spot initiation in TATB crystals, employing the thermo-hydrodynamics arbitrary-Lagrange-Eulerian code ALE3D. This initial study includes non-reactive dynamics to isolate the thermal and hydrodynamical effects. Two-dimensional high-resolution large-scale meso-scale simulations have been undertaken. We study an axisymmetric configuration for pore radii ranging from 0.5 to 2μm, with initial shock pressures in the range from 3 to 11 GPa. A Mie-Gruneisen Equation of State (EOS) model is used for TATB, and includes a constant yield strength and shear modulus; while the air in the pore invokes a Livermore Equation of State (LEOS) model. The parameter space is systematically studied by considering various shock strengths, pore diameters and material properties. We find that thermal diffusion from the collapsed pores has an important effect in generating high-temperature hot spots in the TATB.

Keywords: Hydrodynamics, thermal transport, shocked TATB, pore collapse, ALE3D.
PACS: 44.35.+c, 62.50.Ef, 95.30.Lz.

INTRODUCTION

Solid plastic-bonded high-explosive (HE) materials consist of crystals that are usually between 10 and 100 microns, with micron-sized impurities and pores embedded inside the crystals. These voids increase the ease of shock initiation by generating high-temperature regions during their collapse that might lead to ignition. Understanding the mechanisms of hot-spot initiation in HE materials has had significant research interest in the literature due to safety, reliability and development of new insensitive munitions. Bowden & Yoffe [1] systematically studied the role of void collapse. The main mechanisms of hot spot formation identified consist of adiabatic compression of small entrapped bubbles of gas, friction due to confining surfaces or extraneous grit particles, and intercrystalline friction of the explosive particles, and viscous heating of rapidly flowing explosive material. Frey [2] reviewed the theoretical effects concerning the role of voids in explosive initiation and ignition. Mader [3] studied numerically the shock initiation of detonation in nitromethane, liquid TNT and single-crystal PETN**.** Lee & Tarver [4] proposed a phenomenological model for ignition and growth to compute shock initiation of heterogeneous HE materials. They compared their results of pressure and particle velocity gauges to experimental measurements of various HE materials.

The objectives of the current study are to investigate using the multiphysics computational framework, ALE3D, the mechanisms of pore

collapse and hot spot initiation in simulated TATB crystals. TATB explosives are known their resistance to such external insults, referred to as HE "insensitivity". Results obtained with hydro-thermal processes for various pore sizes and different shock pressures will be discussed.

COMPUTATIONAL APPROACH

The multiphysics software, ALE3D [5], is used to perform these simulations and consists of several physics modules including hydrodynamics and thermal transport. The mathematical formulation is based on an Operator-Split method and invokes an arbitrary Lagrangian-Eulerian (ALE) approach in two and three-dimensional (3-D/2-D) Cartesian configuration as well as 2-D axisymmetric one.

The current configuration is represented by a continuum material of an insensitive HE material, TATB, where an embedded defect consisting of a spherical air-filled pore is present with an initial radius, r_p. The cylindrical computational domain consists of a rectangular grid with length and radius, L = 15 μm, and R = 8 μm, respectively. The dynamics of pore collapse have been verified to be independent of the computational length and radius (L and R) used. The following boundary conditions are imposed: a velocity loading on the left boundary, and non-reflective outflow condition on the right boundary, with symmetric conditions on the top and bottom boundaries. The initial field is set to zero-velocity components, with atmospheric conditions for the pressure field and temperature (p=1atm and T=298K).

Constitutive relations for TATB and air are based on a Mie-Gruneisen model and a Quotidian EOS (QEOS) [6], respectively. The 2-D simulations invoked a two-way coupling solver, including the hydrodynamic and thermal transport modules in ALE3D. In the future, the thermo-chemistry solver, Cheetah [7], will be included with appropriate kinetic reaction mechanisms.

The simulation matrix consists of several pore radii including 0.5, 1 and 2 μm and for various shock strength of 3, 6, and 11 GPa. A mesh resolution of 1.875M is used to properly capture all the relevant hydro and thermal scales. Table 1 provides a summary of the properties for TATB and Air at the initial state. Temperature-dependent heat capacity and thermal conductivity have been invoked as part of the material model.

TABLE 1. Summary of TATB and Air properties at Standard Conditions

Properties	TATB	Air
Density (g/cm^3)	1.90	1.129 x10^{-3}
Heat Capacity (J/K-kg)	0.837	1.04
Thermal Conductivity (W/m/K)	0.799	0.08
Yield Strength (Kbar)	1.0	-
Shear Modulus (GPa)	7	-
Melt Temperature (K)	623	8.76
Ignition Temperature (K)	~2500	

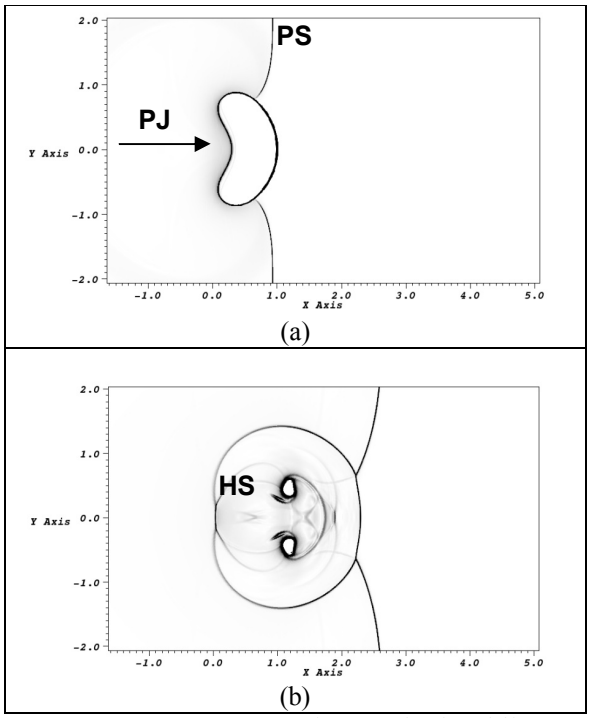

FIGURE 1. Contours of numerical Schlieren (corresponding to the magnitude of the density gradient) at representative time instances for a spherical pore with a radius of 1μm and a shock strength of 6GPa: (a) creation of primary jet (PJ), also shown in Primary shock (PS); (b) pore collapse, lifting from axis of symmetry transforming into a toroidal shape and formation of hot spots (HS).

RESULTS AND DISCUSSION

Fig. 1 presents contours of numerical Schlieren at two representative time instances. The

shock moves from left direction (negative/small x) to right one (positive/large x); while the pore is centered at the origin. As the shock propagates through the HE material in the computational domain, HE melting occurs due to the thermal heating on the back side of the shock. Once the primary shock (referred to as PS since secondary shocks will form at the pore collapse) impinges on the pore, a primary jet (PJ) is generated in the softened HE material upstream of the shock (see Fig. 1a). That primary jet pushes on the front wall of the pore, moving it towards the back wall. Once the front wall merges with the back wall, the pore collapses and lifts from the centerline, becoming a torus. In Fig. 1(a), the pore is convecting in the positive streamwise direction while rotating. An interesting feature captured is the formation of a hot spot (HS in the figure) in the HE material. The mechanisms of the hot spot creation will be described in detail later on. Further details are discussed in [8].

Fig. 2 presents contours of the instantaneous temperature fields at various time instances following the pore collapse and lifting from the centerline. The formation of the Secondary Jet (referred to as SJ) is clearly captured as the melted HE is accelerating close to the collapsed pore. It is clearly seen in Fig. 2a, the secondary jet in the HE material extracts heat from the collapsing pore (now having a toroidal shape). Eventually, these dynamics will lead to the creation of a heated concentrated HE region, which we refer to as "hot spot" (we define a hot spot as a concentrated HE region with a temperature of at least 2500K. At this temperature, TATB is expected to ignite on the nanosecond timescale). The hot spot is highlighted in Fig. 2b during its initial formation phase. The hot spot is found to occupy an HE region approximately 1/4th the size of the collapsed pore. It should be noted that when the thermal transport module is not active, the SJ formation is captured; however, a region of temperature above 2500K is not observed. Hence, the hot spot is not created under these conditions.

The time evolution of the temperature is summarized in Figure 3 for the simulations performed with the hydrodynamics module and hydro-thermal modules. It is seen that the PJ evolves in similar manner for both simulations and is maintained around 2500K. The hot spot temperature (dashed line) increases significantly to nearly 6000K when the thermal solver is active; while it stays quite low without the thermal solver peaking at 1500K.

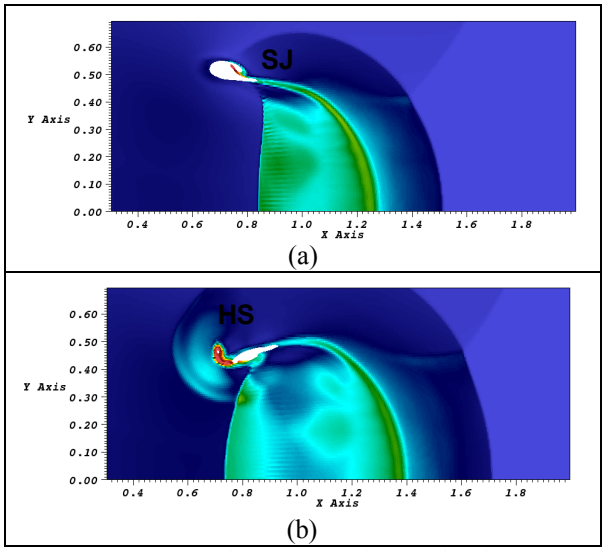

Figure 2. Contours of temperature for two time instances for a spherical pore with a radius of 1μm and for a shock strength of 6GPa. Contour levels extend in the range of [300K, 5000K].

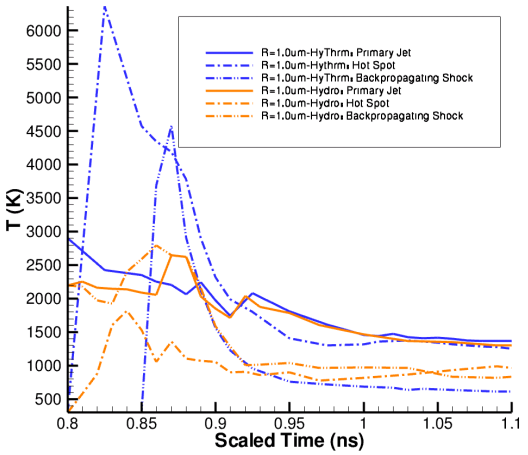

Figure 3. Time variation of the maximum temperature field for key features, including PJ (solid line), HS (dash-dot line) and the secondary shock (dash-dot-dot line). Blue (orange) lines correspond to results obtained with hydrodynamic (coupled hydrodynamic-thermal) analysis.

Hence, its evolution will have minimal effect on HE ignition for simulations performed with

hydrodynamic module. The peak temperature in the triple-shock (dashed-dotted line) is enhanced to 4500K, although not quite as high as the temperature achieved in the hot spot.

Finally, contours of the temperature field in the TATB material are shown in Fig. 4 as obtained for two pore radii of 1 and 2μm. The coupled Hydrodynamic-Thermal analysis is used. The hot spot temperature is observed to increase with larger pore radius, highlighting that the thermal transport mechanism is not scale invariant, as opposed to the hydrodynamic phenomena.

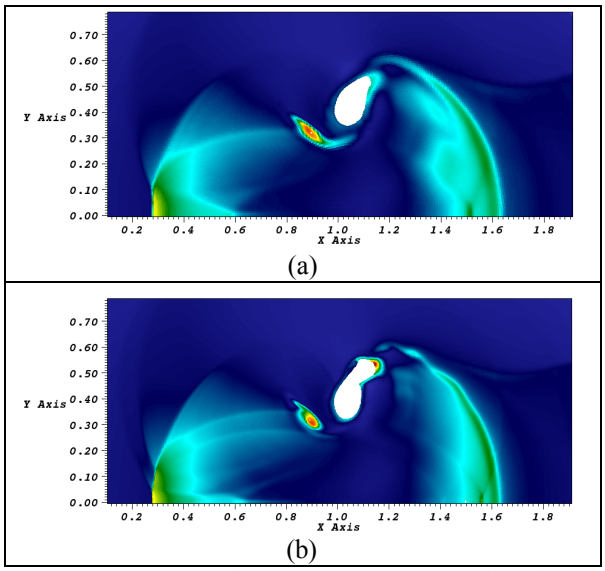

Figure 4. Contours of temperature at representative time instances showing the effects of pore radius for a shock strength of 6GPa: (a) r=1μm, (b) r=2μm. Contour levels extend in the range of [300K, 5000K].

CONCLUSIONS

Two-dimensional high-resolution meso-scale simulations are performed on an axisymmetric pore configuration in a shocked TATB material using the multiphysics software, ALE3D. ALE3D is a massively parallel hydrodynamics framework and coupling of the hydrodynamics with the thermal transport has been used. Results have been described for various pore sizes and different shock pressures. It is seen that a secondary jet forms leads to a hot spot. The similar assumption at various pore radii obtained with hydrodynamic assumption breaks once the thermal transport is activate. Future research will focus on a three-way coupling process including chemistry using Cheetah, with refined three-step reactive model obtained from Ab-initio MD computations.

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