MESOSCALE PREDICTIONS FOR THE THERMOMECHANICS OF GRANULAR ENERGETIC COMPOSITES[1]

Michael W. Crochet[2] and Keith A. Gonthier[3]
Mechanical Engineering Department, Louisiana State University, Baton Rouge, LA, USA 70803

Summary A finite-element analysis is performed to characterize the impact induced multiscale thermomechanical response of explosively coated aluminum microspheres. Emphasis is placed on accurately describing the dependence of bulk uniaxial stress wave structure, including local stress and temperature fluctuations occurring near intergranular and material contact surfaces, on explosive mass fraction and impact speed. The time-dependent bulk wave structure is obtained by averaging the mesoscale response over representative elementary volumes. This analysis is a preliminary step in assessing the impact sensitivity of energetic composites.

Extended Summary

Energetic composites consisting of small explosively coated metal grains (diameter < 50 μm) can potentially provide higher energy release rates than conventional explosives by combining the high exothermicity of metal-oxides ($q_{rxn} \approx$ 14 MJ/kg) with the rapid combustion of high-explosives ($\dot{M}_b \approx 5 \times 10^9$ kg/m^3/s). An important unresolved problem is determining conditions for which the metal and explosive energy release rates can be suitably coupled for maximum power generation. In addition to combustion rate coupling, it is equally important to fundamentally understand their thermomechanical response (i.e., sensitivity) to impact if they are to find use in practice. Experiments and modeling have long demonstrated that confined granular explosives can be detonated by low amplitude shocks due to the formation and interaction of reactive hot-spots at the grain scale [1, 2]. Hot-spots are regions of intense localized heating induced by plastic deformation, intergranular friction, and fracture. In this study, we perform a numerical analysis on large grain ensembles to characterize both the grain and bulk scale response of explosively coated aluminum grains to constant speed piston impact. The high-explosive modeled in this work is RDX ($C_3H_6N_6O_6$). We are particularly interested in identifying the effect of RDX mass fraction, grain size, interface adhesion strength, and piston impact speed on bulk uniaxial stress wave structure and hot-spot formation within the material. Combustion is ignored for simplicity.

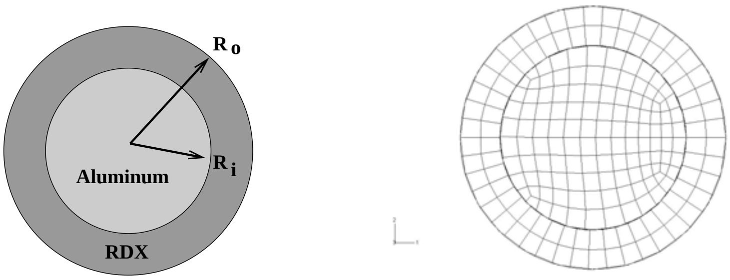
The simulations are performed on a 2.0 GHz Pentium IV Windows Workstation using the finite-element package ABAQUS/Explicit. The explicit algorithm incorporates an adaptive grid technique for increased accuracy and utilizes numerical damping to mitigate dispersive oscillations in the neighborhood of shocks; thus, it is well-suited for impact analysis. For tractability and computational expediency, we perform a 2-D stress analysis for the planar impact of a constant speed piston with a composite material consisting of a large number of identifiable grains ($50 \leq N \leq 500$). As shown in Fig. 1(a), each grain initially has an outer radius R_o and an inner radius R_i, the latter being the dimension of the Al core. An important parameter in this analysis is the nondimensional RDX thickness defined by $\eta \equiv (R_o - R_i)/R_o$, where $0 \leq \eta \leq 1$ (here, $\eta = 1$ corresponds to pure RDX). The RDX mass fraction is related to η by

$$\lambda(\eta) \equiv \frac{m_{RDX}}{m_{RDX} + m_{Al}} = \frac{(1-\eta)^2}{(1-\eta)^2(\frac{\rho_{Al}}{\rho_{RDX}} - 1) - 1},$$

where ρ_{Al} and ρ_{RDX} are the mass densities of aluminum and RDX, respectively. A random grain packing arrangement is numerically generated by an iterative 2-D Monte Carlo algorithm that minimizes the gravitational potential energy of the granular system [3]. We use simple constitutive theories to facilitate interpretation of the results. The material models describe isotropic, elastic-perfectly plastic behavior. Other material properties used for aluminum and RDX are taken from Refs. [4, 5, 6].

Representative predictions for the grain scale temperature field are shown in Fig. 2 at time $t = 0.7$ μs for (a) adiabatic plastic heating of the grains and (b) plastic heating with thermal energy transport by conduction. All grains were initially at an ambient temperature of 300 K. Only fifty grains were used in this simulation; for each grain $R_o = 25$ μm and $\eta = 0.3$. The computational grid within a single grain is shown in Fig. 1(b); it consists of approximately 56 quadrilateral elements within the RDX layer and 120 elements within the aluminum core. Here, the piston impacted the grains from above at a constant speed of 150 m/s. The dispersed waves within the granular material generated by the impact have just reached the rear boundary at the time shown. A comparison of the two cases indicates that lower peak temperatures are predicted within the RDX layer near intergranular contact surfaces for the simulation that includes thermal energy transport; a peak temperature of 398 K is predicted for case (a) whereas a value of 373 K is predicted for case (b). These temperature predictions, while well below that needed for RDX ignition ($T_{ig} \approx 550$ K), suggest that thermal conduction may have a significant effect on the evolution of grain-scale temperature for low impact speeds. Higher temperatures are

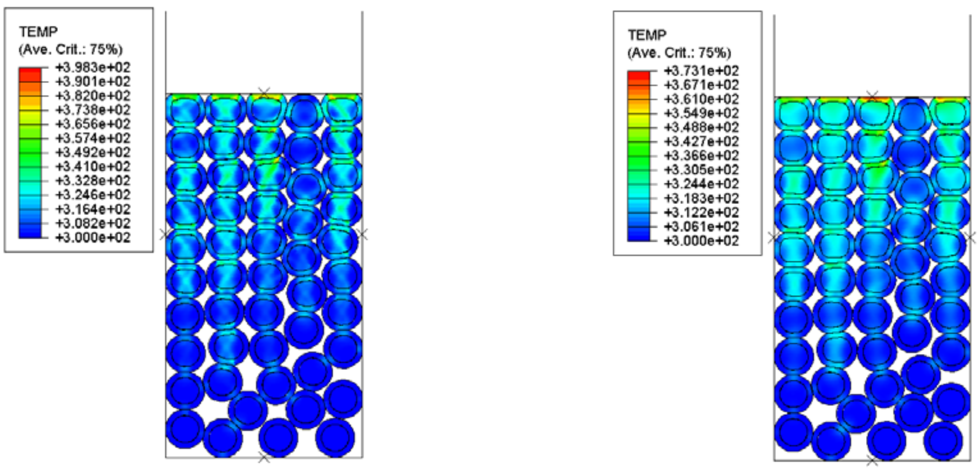
[1]This research is sponsored by the U.S. Air Force Research Laboratory, MNME, Eglin Air Force Base, FL, under agreement number F08630-02-1-0002. The contract monitor is Mr. Chad Rumchik.
[2]Graduate Research Assistant. Email: *mcroch2@lsu.edu*
[3]Assistant Professor. Corresponding author. Email: *gonthier@me.lsu.edu*



(a) (b)

Figure 1: Schematic of (a) an explosively coated aluminum grain and (b) the computational grid within a grain used for the representative simulation.

expected for larger grain ensembles having more internal degrees of freedom due to significant stress chain formation. As piston speed increases, plastic heating will become more pronounced resulting in higher peak temperatures. There likely exists a critical piston speed beyond which thermal diffusion is inconsequential. A key objective of this work, that will be explored in depth, is to determine if the cool aluminum core can suppress hot-spot formation in large grain ensembles due to its comparatively high thermal conductivity. As such, these composites may exhibit significantly lower impact sensitivity than conventional explosives.



(a) (b)

Figure 2: Predicted temperature field for explosively coated aluminum grains for a piston speed of 150 m/s: (a) without thermal conduction and (b) with thermal conduction.

References

[1] McAfee J. M., Asay B. W., Campbell W., and Ramsay J. B.: Deflagration to Detonation Transition in Granular HMX, Proceedings of the Ninth (International) Detonation Symposium, 265-278, 1989.
[2] Gonthier, K. A.: Modeling and Analysis for Reactive Compaction of Granular Energetic Solids, *Comb. Science Tech.*, **175**:1679-1709, 2003.
[3] Lin C. L., and Miller J. D.: Pore Structure and Network Analysis of Filter Cake. *Chem. Eng. J.* **80**:221-231, 2000.
[4] Callister W. D., Jr.: Materials Science and Engineering: An Introduction, 6th Edition. Wiley, NY 2000.
[5] Gibbs T. R., and Popolato A.: LASL Explosive Property Data, University of California Press, CA 1980.
[6] Armstrong R. W., Ammon H. L., Elban W. L., Tsai D. H.: Investigation of Hot Spot Characteristics in a Energetic Crystals. *Thermochimica Acta* **384**:303-313, 2002.