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UCRL-TR-221760

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June 1, 2006

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This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

NUMERICAL MODELING OF IMPACT INITIATION OF HIGH EXPLOSIVES

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ABSTRACT

We performed continuum mechanics simulations to examine the behavior of energetic materials in Ballistic Chamber Impact (BIC) experiments, using an Arbitrary Lagrangian-Eulerian code (ALE3D). Our simulations revealed that interface friction plays an important role in inducing the formation of shear bands, which result in "hot spots" for ignition. The temperature localization during BIC impact was found to be significant in materials with high yield strength. In those materials, there are multiple locations inside shear bands can achieve temperatures exceeding the threshold temperature for reaction. In addition, we investigated the relevant parameters influencing the pressure profile of a BIC test by numerical analysis from a simple phenomenological model. To our surprise, we found that the peaks of BIC pressure profiles not only can be a result of multi-center chemical reactions, but can also arise from factors associated apparatus configuration.

I. INTRODUCTION

Assessing explosive impact sensitivity has long been considered a challenging task. The microscopic processes involved in initiation by impact are complicated and not very well understood. In general, it is believed that ignition by impact starts from pockets of hot spots generated from energy localization as a result of shear band formation. [1-2] The initial set of shear-ignition reactions was observed to be fast, and followed by a relatively slow burning of high explosive.[1-2] The accurate modeling of explosives impact sensitivity requires an understanding of the mechanical, thermal and chemical responses of high explosives during the impact and subsequent chemical reactions.

One of the simplest and best-known small-scale safety tests is the drop-hammer test, which is routinely applied to many high explosives. [1-2] In general, a small amount of explosive is placed on an anvil. A heavy striker is dropped from various heights, and the height for 50% "go/no go" is recorded. Unfortunately, this 50% go/no go height is limited in assessing impact sensitivity. Since the drop-hammer test is not standardized, the heights recorded by different laboratories are not directly comparable. Its limitation is largely due to the fact that the 50% go/no go height does not correlate consistently with amount of plastic energy deposited onto a high explosive sample, since a large portion of the impact energy is stored elastically in apparatus, which cannot be easily quantified.[1] This made the 50% go/no go height an apparatus-dependent value. Therefore, results from drop hammer tests cannot be trusted beyond a rough ranking in categories of danger.

An alternative to the simple drop hammer test is the Ballistic Impact Chamber (BIC) apparatus developed in recent years.[1-3] In BIC tests, strikers and their height are chosen such that ignition is always guaranteed. The key data recorded in BIC is the pressure profile of gas produced from chemical reactions after impact. Furthermore, the velocity of a pellet accelerated by hot gas was measured and recorded as an energy output from explosives. BIC tests offer information on the growth and progression of initiation reactions that are not available from the drop hammer test mentioned above. It is hoped that pressure profiles of BIC correlate with explosive impact sensitivity and have little dependence on experimental apparatus. To our knowledge, there has not been a systematic modeling attempt based on BIC results. Previous published work on BIC has primarily been experimental results with limited computational analysis. We have also noticed that the pressure profiles from two experimental groups are qualitatively different in shape and figures.[1-3] There is clearly a need for theoretical modeling to understand what can be learned from BIC experiments, as well as its limitations.

II. COMPUTATIONAL DETAILS

In this paper, we investigated various processes that govern results of BIC tests. We have adopted two separated approaches in modeling of mechanical, thermal and chemical responses of high explosive. In one approach, we modeled the mechanical and thermal responses of high explosive by using a multi-physics hydrodynamic code of an arbitrary Lagrange/Eulerian [4] (ALE3D). The focus of this study is to determine the relevant mechanical properties that effects shear band formation and the consequent hot spots in explosives. In parallel, we used a phenomenological model to determine what are the relevant parameters in determining the pressure profiles of BIC tests through series of numerical analysis.

A. Continuum Mechanics ALE3D Simulations

Fig.1 shows our ALE3D simulation 3D domains with quarter symmetry used in our impact simulations. We generated meshes using both ALE3D's internal mesh generator and TrueGrid as needed. Explosive samples in disk shape (black) are crushed between a steel anvil (green) and a striker (blue). The mesh located on the bottom of anvil is constrained from motion during the simulations. In addition, the initial velocity of the striker is set to correspond to a free fall from a height of 1.5 m. We treated both anvil and the striker as 4340 steels. The two explosive samples were chosen to be HMX based high explosives with Viton plastic bonder in different percentages. We will refer the formulation one as HE_1 and the formulation two as HE_2 in this paper. They represent two high explosives with similar chemical properties, but HE_1 has higher yield strength than that of HE_2, since the plastic bonder Viton was treated with zero strength. HMX is treated as a Steinberg-Guinan material with the shear modulus and yield strength Y.

The equation of state (EOS) of unreacted HE is modeled as an isotropic elastic-plastic material with 7-term polynomial in the form of:

$$P(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + (b_0 + b_1\xi + b_2\xi^2)\rho_0 c_v (T - T_0)$$

The volume compression is defined as $\xi = \rho/\rho_0 - 1$. The parameters in this form were developed in modeling of cook-off STEX experiments.[5] Different computational mesh resolutions were tested to make sure that shear band formations were resolved adequately. A slide surface was implemented in between the sample and the anvil to represent the existence of the sand paper in BIC test. This allowed us to investigate the effect of interface friction on energy localization. However, decomposition chemistry is not included in ALE3D simulations.

B. Numerical Modeling of Pressure Profile of BIC

Fig. 2 shows the schematic drawing of experimental set up of BIC. The high explosive modeled in our calculation is JA2. We calculated the EOS of JA2 of burning in the pressure range of BIC experiments (up to 700psi) using a thermal equilibrium chemical code Cheetah. Over this pressure range, we found that the flame temperature of JA2 varies slightly (6%), and the relative concentrations of different gas products remains nearly unchanged. Therefore, in our numerical analysis, the system temperature *T* was set to be a constant of the average value of 3232K. The gas product concentrations $(C_{gas}^{species})$ were taken from the Cheetah result, with an ideal gas equation of state.

The pressure *P(t)* was computed as $P(t) = \dfrac{RT(\sum_{j=1}^{species} N_{gas})}{V(t)}$, where system volume is defined as $V(t) = V_{chamber}(t) + V_{gun}(t) + V_{leak}(t)$, and the mole function N_{gas} of gas products was determined by $C_{gas}^{species}$ and the mass of totally burned explosives (m_{burn}). $V_{chamber}$ and V_{gun} represent volumes occupied by gas products in the regions of BIC chamber and gun respectively. The value of $V_{chamber}$ was determined by the chamber geometry and the position of the striker, which follows Newtonian equation of motion subject to downward gravitational force and upward push from hot gas. The lead pellet is allowed to move when its pressure exceeds a certain friction threshold. The pellet's velocity is determined as: $U_{pellet}(t) = \frac{A_{gun}}{m_{pellet}} \int P(t)dt$, where A_{gun} and m_{pellet} are the area of the gun and the mass of gun pellet, respectively. The term V_{gun} was then computed by $V_{gun} = A_{gun} \int U_{pellet}(t)dt$. The value of V_{leak} was set to be non-zero only after pellet travels to the end of gun (30cm). After the pellet got captured at the end of the gun, we assumed that hot gases continue to leak to the outside of BIC apparatus at a constant rate, which value is varied in order to fit experimentally observed P(t).

The mass burned (m_{burn}) was computed under the following assumptions. Chemical reactions were assumed to occur at different "hot spots" (i), with distinct reaction rates k_i. Since k_i depends on the local temperature of hot spot $(Ae^{(-\Delta E_{act}/T_i)})$, variations in hot spots temperature (T_i) may give rise to different k_i. Reactions on different "hot spots" were allowed to ignite at different times $(t_o(i))$ as well. The burning after impact was assumed to be outward and spherical. Inward burning model from surface was also tested. However, it was dismissed based on its failure to reproduce experiments, and it is inconsistency with ALE3D results.

III. RESULTS AND DISCUSSIONS

A. ALE3D Simulations of Mechanical Deformation of Explosives By Impact

We have carried out ALE3D simulations applying several friction coefficients to the sliding surfaces between striker/sample and sample/anvil. For a friction free system, we observed that the deformation of explosive sample remains to be largely homogenous and hydrostatic up to time of 100 *ms*. No significant shear bands or hot spots were observed. In addition, the impact energy was largely absorbed elastically by both explosive sample and anvil.

Fig. 3 displays the maximum temperatures recorded inside the HE_1 sample as a function of time. The black line is for a friction free system, and is nearly flat. Clearly, the existence of friction plays an important role in generating temperature localization. We observed that the friction restricts the center motion of explosive sample near interfaces.

As we increased the friction coefficient of sample/anvil interface to above 0.3 (a reasonable lower bound value for explosives on sand papers), the center motion of the bottom of explosive remains stationary, while a large middle portion of explosive sample continues to be compressed. This induces shear deformation, which results in energy/temperature localizations. As shown in Fig. 4, our ALE3D simulations revealed that the shear localization upon impact is most significant around the bottom out rim of the explosive disk, and along a conical surface that extends to the center. During the impact, temperatures of many local regions can exceed the ignition temperature, which indicates that there are multiple centers for ignition. This is likely to be the case even we assume that explosive sample is fairly homogenous before impact.

The elevation of temperature in shear bands was found to rise faster and higher for materials with higher yield strength. Since plastic binder Viton has a low melting temperature, it is considered to have no strength in our ALE3D simulations. Increasing the percentage of binder lows the material's overall yield strength proportionally. Therefore, a larger increase in maximum temperature was observed for HE_1 in comparison to HE_2, which has higher binder concentration. This is consistent with the experimental observation that adding plastic binders improves high explosive safety.

B. Numerical Modeling of Pressure Profile of BIC

We have conducted series of calculations of P(t) using different numbers of reaction centers, ignition times, and reaction rates in order to reproduce the experimental pressure profile. We found that those factors play significant roles in determining pressure profiles. Using a five-center/inside burning model, we were able to obtain a remarkable fit to the experimental JA2 profile obtained by Woods and co-workers (see Fig. 5). The peaks in P(t) plot correspond to different hot spots burning at different rates and igniting at different times. This is consistent with the multi-shear band formations with temperature distributions observed in our ALE3D simulations. We also investigated the likelihood of outside-to-inside burning model. We found that the outside burn model is unlikely, since it resulted in a pressure profile that is much smaller in magnitude than the experimental data. This conclusion is supported by our ALE3D simulations that revealed maximum stress spots in localized shear bands were always found to be inside of a HE sample upon impact (see Fig. 4).

To our surprise, we have also discovered a factor related to apparatus setup which can give arise to features in the pressure profile. We found that the mass of sample can influence the shape of the pressure profile significantly given the length of gun is kept at 30cm. As shown in Fig. 6, a small sample size (< 50mg) results in a single peaked pressure profile, while a large sample mass (> 70mg) gives rise to a double peak in P(t). This finding explains why the typical P(t) profiles of BIC tests reported by Coffey and co-worker (using 45mg of sample) has one large background peak, while those recorded by Woods and co-workers typically have a double peak feature (using 72mg of sample).[1-3] In the case of small sample size, burning of the sample is complete before pellet travels to the end of gun. Therefore leakage of hot gases released after pellet capture won't be recorded in P(t). We concluded that one should use a small sample mass or increase the length of gun chamber, in order to avoid generating features in P(t) which are not relevant to ignition chemistry. We also examined the effect of the striker's gravitational motion on the pressure profile. We found that the downward gravitational force of the striker is not significant in comparison to the upward force generated by the gas product of HE.

IV. CONCLUSIONS

In summary, we have simulated the mechanical deformation of plastic explosives by impact. Initial shear band formation was observed near the bottom corners of explosive samples under the presence of friction on a sliding surface. Without friction, the deformation by impact is largely homogeneous elastic deformation, which produces little local heating. Under friction, the degree of local heating is found to be proportional to the explosive's yield strength. This is consistent with experimental observations that adding plastic binder decreases its yield strength and thus reduces the explosive's impact sensitivity.

Our modeling of the pressure profiles of BIC experiments has suggested that one needs to exercise caution in interpreting pressure profile peaks. Indeed, we found that localized hot spots do give rise to features in BIC pressure profiles. In fact, our five-center model gave an excellent pressure profiles in comparison to that of experiment for JA2. However, the twin peaks consistently observed over a number of explosives by the group at China Lake is also possible due to their apparatus configuration, rather than chemical reactions from crystal grains. We suggestion one should pay attention to the mass of explosive sample and length of gun in BIC setup. The mass of sample should be kept small enough to completely burn before the capture of the pellet at the end of gun. This will remove some experimental ambiguity and makes interpretation of pressure profile focus primarily on the explosive's chemical response.

V. ACKNOWLEDGEMENTS

This work was preformed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contact No. W-7504-Eng-48. Authors wish to thank Dr. Andy Anderson for providing his assistance and expertise on slide surface implementation of ALE3D.

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Figure 1. Simulation domains in our ALE3D impact simulations. Blue, black and green represent striker, sample and anvil.

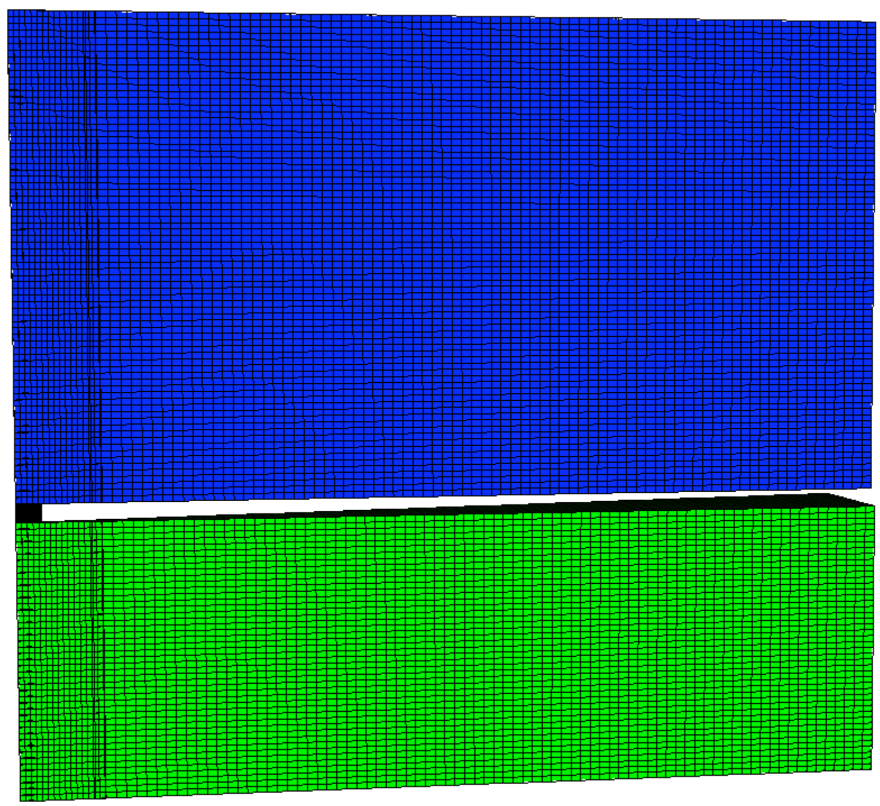

Figure 2. A schematic drawing of a BIC apparatus.

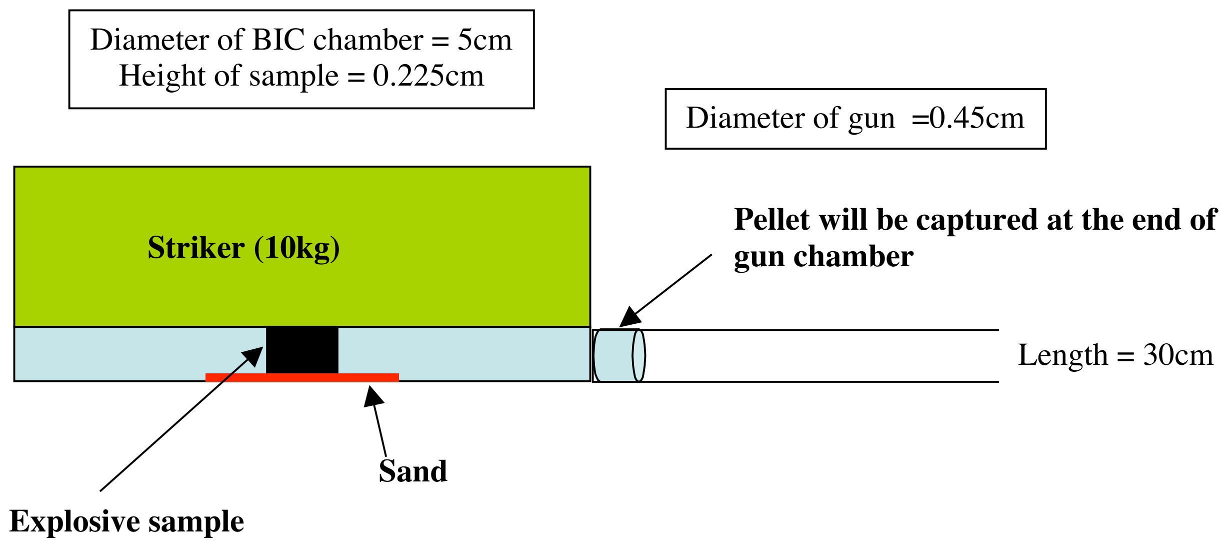

Figure 3. Maximum temperatures inside HE as a function of time. Different friction coefficients are used for surfaces of top (Fric_striker) and bottom (Fric_Anvil) of HE.

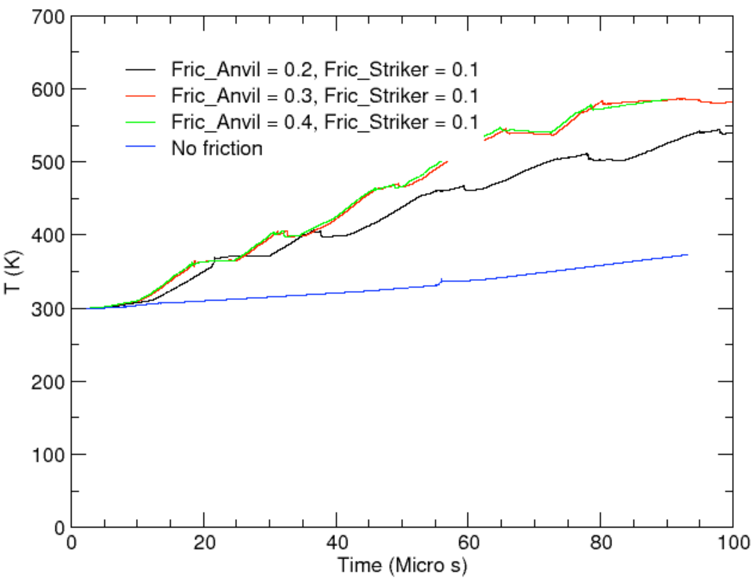

Figure 4. Temperature profile inside HE_1 sample at t = 80*ms* after impact (obtained from ALE3D simulation).

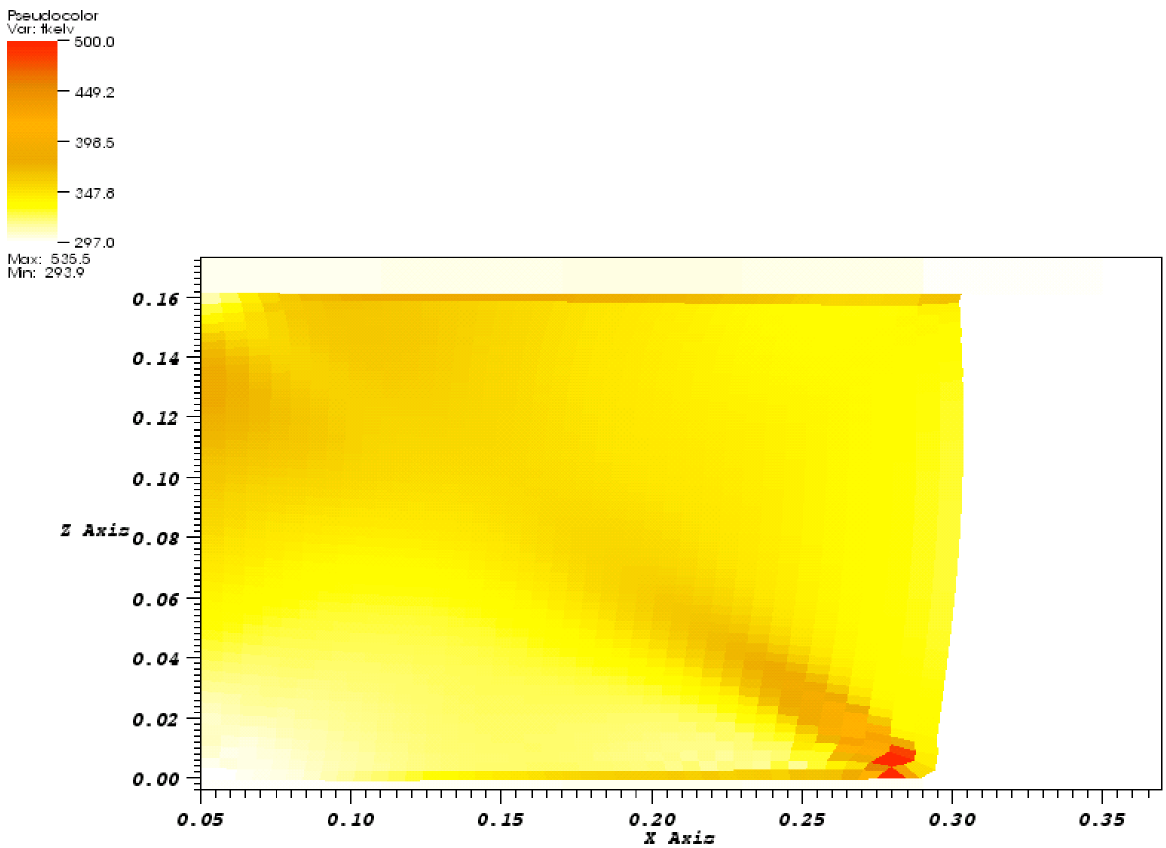

Figure 5. Pressure profile of JA2 obtained from a five-center inside burn model.

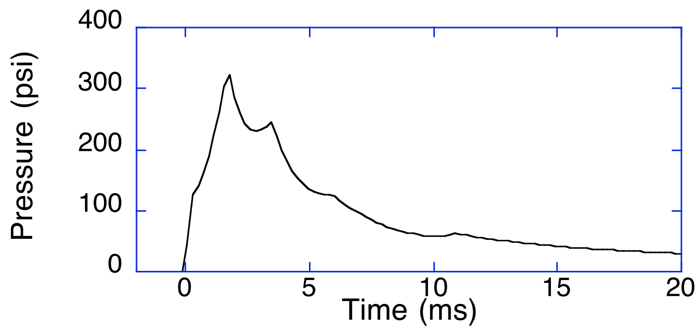

Figure 6. Modeled pressure profiles of BIC tests as a function of sample mass.