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INITIATION OF HEATED PBX-9501 EXPLOSIVE WHEN EXPOSED TO DYNAMIC LOADING

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Abstract. Shock initiation experiments on the heated PBX9501 explosive (95% HMX, 2.5% estane, and 2.5% nitro-plasticizer by weight) were performed at temperatures 150°C and 180°C to obtain in-situ pressure gauge data. A 101 mm diameter propellant driven gas gun was utilized to initiate the PBX9501 explosive and manganin piezo-resistive pressure gauge packages were placed between sample slices to measure time resolved local pressure histories. The run-distance-to-detonation points on the Pop-plot for these experiments showed the sensitivity of the heated material to shock loading. This work shows that heated PBX-9501 is more shock sensitive than it is at ambient conditions. Proper Ignition and Growth modeling parameters were obtained to fit the experimental data. This parameter set will allow accurate code predictions to be calculated for safety scenarios involving PBX9501 explosives at temperatures close to those at which experiments were performed. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.
INTRODUCTION

A considerable interest exist in studying safety aspects of exposing heated energetic materials to dynamic loading conditions. Of particular interest are the HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) based explosives such as the commonly used PBX 9501 (95% HMX, 2.5% estane, and 2.5% nitroplasticizer by weight) and LX-04 (85% octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazine (HMX) with 15% Viton binder) when they are exposed to elevated temperatures prior to their dynamic loading such as a shock wave. The work on LX-04 has been described earlier in several publications [1-3] with the latest overview still in press [4]. Prior studies on PBX-9501 include wedge tests [5], embedded particle velocity gauges [6-8], and VISAR at low input shock pressures [9,10], and embedded manganin gauges [11,12] at both ambient and elevated temperature. In this paper an attempt was made to extend the heating temperature to that beyond the polymorphic phase transformation of HMX from $\beta$ to $\delta$ phase and show how shock sensitivity of PBX-9501 is affected by this increase in temperature.

EXPERIMENT

Shock initiation experiments were performed on the explosive PBX 9501 using the 101 mm diameter propellant driven gas gun at Lawrence Livermore National Laboratory (LLNL), which allows close control of the projectile velocity and of the loading pressure imposed on the energetic materials (EM) target.

The target assembly, shown in Fig. 1, consisted of several discs of different thickness. Gauge packages containing manganin pressure gauges were embedded between individual discs. The gauges were armored with thin (125 $\mu$m) Teflon insulation on both sides to prevent shorting of the gauges in a conductive medium when the material becomes reactive. Other details of the manganin pressure gauges were described in our previous publications [13-17]. For better control of the impact pressure a thin buffer plate of the same material as the impact plate is placed in front of the target assembly for symmetrical impact. Also included in the target assembly are six tilt pins placed around the periphery of the target flush with the impact surface to measure tilt of the impact plate as it strikes the target, and two velocity pins sticking out some known distance from the target to measure velocity of the impact plate just before it strikes the target.

During the heated experiments nichrome foil spiral heaters were placed on both sides of the target separated by a thin aluminum disc for better heat distribution into the material under study. In this case gauge packages also contained thermocouples (TC) for better monitoring of the target temperature distribution during the heating cycle. The heating rate of the target was usually held constant initially at 3$^\circ$C/min until about 10$^\circ$C below the desired temperature. Then it was changed to 1$^\circ$C/min until the final desired temperature is reached where it was held as long as necessary before the gun was fired.

Figure 2 illustrates the temperature record during the heating cycle of the experiment to the temperature of 150$^\circ$C with traces representing the records of thermocouples at various locations within the target assembly.
EXPERIMENTAL RECORDS

Following are the types of pressure records obtained from the gun experiments on shock initiation of PBX-9501 explosive heated to different initial temperatures. Figure 3 shows the pressure records of shock loaded PBX-9501 initially at ambient temperature impacted by an aluminum flyer at a velocity of 0.697 mm/\(\mu\)s yielding an impact pressure of 3.3 GPa. Figures 4 and 5 illustrate the pressure records for the same explosive initially at 52 and 50 degrees Centigrade impacted by an aluminum flyer at 0.8 and 0.64 mm/\(\mu\)s respectively generating corresponding pressures of 3.9 and 2.95 GPa. Figures 6 and 7 show pressure records when PBX-9501 was initially heated to 150˚C and impacted by an aluminum flyer at velocities 0.73 and 0.55 mm/\(\mu\)s yielding impact pressures of 3.0 and 2.1 GPa respectively.

Experiments at higher initial temperature turned out very noisy due to the polymorphous transformation of HMX from a \(\beta\) to \(\delta\) phase. This phase change has lead to a density increase of the samples, creating new voids and a loss of integrity of the target assembly, causing noisy performance of the gauges. The evidence of HMX phase transformation is illustrated in the temperature records taken during heating of explosive to the temperature of 180˚C shown in Fig. 8. Here, the phase transition can easily be observed to start at above 170˚C and last for more than 30 minutes. Thus, due to the severity of the environment, the pressure records of heated PBX-9501, just as they were in LX-04, are quite noisy and will not be shown here. However, the pertinent information for such experiment was retrieved from these records by looking at each trace separately.

The relative shock sensitivity of PBX-9501 at various initial temperatures is illustrated on the “Pop Plot” [18] shown in Fig. 9. The “Pop Plot” represents a plot of run distance to detonation as a function of impact pressure in a log-log space. The closer the points are to the origin of the plot the more sensitive the explosive is to pressure impact. Included in the Pop Plot are the results of previous studies by the Los Alamos group as well as our present work with the results previously published by the LLNL group. The data of both groups agree very well for all published results. The data point for PBX-9501 heated to 180˚C with large error bars is also in a good agreement with the data of another HMX based explosive, LX-04, heated to 190˚C.

REACTIVE FLOW MODELING

Since not all shock initiation scenarios can be experimentally tested, the Ignition and Growth reactive flow hydrodynamic computer code model of shock initiation and detonation has been developed based on the embedded gauge experiments discussed above to predict the results for such scenarios [19].

The Ignition and Growth reactive flow model uses two Jones-Wilkins-Lee (JWL) equations of state, one for the un-reacted explosive and another one for the reaction products, in the form:
where \( p \) is pressure in Megabars, \( V \) is relative volume, \( T \) is temperature, \( w \) is the Gruneisen coefficient, \( C_V \) is the average heat capacity, and \( A, B, R_1 \) and \( R_2 \) are constants. The equations of state are fitted to the available shock Hugoniot data. Table 1 contains the modeling parameters for these experiments.

**Table I.** Ignition and Growth modeling parameters for PBX 9501 at 150°C.

<table>
<thead>
<tr>
<th></th>
<th>UNREACTED JWL</th>
<th>PRODUCT JWL</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A )</td>
<td>7320 Mbar</td>
<td>16.689 Mbar</td>
</tr>
<tr>
<td>( B )</td>
<td>-0.065278 Mbar</td>
<td>0.5969 Mbar</td>
</tr>
<tr>
<td>( R_1 )</td>
<td>14.1</td>
<td>5.9</td>
</tr>
<tr>
<td>( R_2 )</td>
<td>1.41</td>
<td>2.1</td>
</tr>
<tr>
<td>( \omega )</td>
<td>0.8867</td>
<td>0.45</td>
</tr>
<tr>
<td>( C_V )</td>
<td>2.786x10^{-5} Mbar/K</td>
<td>1.0x10^{-5} Mbar/K</td>
</tr>
<tr>
<td>( T_0 )</td>
<td>423 K</td>
<td></td>
</tr>
<tr>
<td>Shear Modulus</td>
<td>0.0352 Mbar</td>
<td>-</td>
</tr>
<tr>
<td>Yield Strength</td>
<td>0.002 Mbar</td>
<td>-</td>
</tr>
</tbody>
</table>

The reaction rate equation is:

\[
\frac{dF}{dt} = I(1-F)^b \left( \frac{\rho}{\rho_0} - 1 - a \right)^x + G_1(1-F)^c F^{-d} p^y + G_2(1-F)^e F^{-f} p^z \tag{2}
\]

where \( F \) is the fraction reacted, \( t \) is time in ms, \( \rho \) is the current density in g/cm\(^3\), \( \rho_0 \) is the initial density, \( p \) is pressure in Mbars, and \( I, G_1, G_2, a, b, c, d, e, g, x, y, \) and \( z \) are constants. This reaction rate law models the three stages of reaction generally observed during shock initiation of solid explosives.

Reaction rate constants used in this modeling are listed in Table 2.

**Table II.** Reaction rate constants.

<table>
<thead>
<tr>
<th></th>
<th>REACTION RATES</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>0</td>
</tr>
<tr>
<td>( b )</td>
<td>0.667</td>
</tr>
<tr>
<td>( c )</td>
<td>0.277</td>
</tr>
<tr>
<td>( d )</td>
<td>0.667</td>
</tr>
<tr>
<td>( e )</td>
<td>0.333</td>
</tr>
<tr>
<td>( g )</td>
<td>1.0</td>
</tr>
<tr>
<td>( I )</td>
<td>1.4x10^{11} \mu s^{-1}</td>
</tr>
<tr>
<td>( G_1 )</td>
<td>190 Mbar^{-2} \mu s^{-1}</td>
</tr>
<tr>
<td>( G_2 )</td>
<td>400 Mbar^{-2} \mu s^{-1}</td>
</tr>
</tbody>
</table>

\( \mu s^{-1} \) is microsecond^{-1}.
The Grueneisen parameters used for the inert materials are listed in Table 3.

Table III. Grueneisen parameters for inert materials.

<table>
<thead>
<tr>
<th>INERT</th>
<th>( \rho_0 ) (g/cc)</th>
<th>( C ) (km/s)</th>
<th>( S_1 )</th>
<th>( S_2 )</th>
<th>( S_3 )</th>
<th>( \gamma_0 )</th>
<th>( a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>6061-T6 Al</td>
<td>2.703</td>
<td>5.24</td>
<td>1.4</td>
<td>0.0</td>
<td>0.0</td>
<td>1.97</td>
<td>0.48</td>
</tr>
<tr>
<td>Teflon</td>
<td>2.15</td>
<td>1.68</td>
<td>1.123</td>
<td>3.98</td>
<td>-5.8</td>
<td>0.59</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The Ignition and Growth simulation of the shock initiation of PBX 9501 at 25, 50 and 150°C are illustrated in Figs. 10 - 12 respectively. From these figures it is quite evident that the Ignition and Growth model simulates experimental records quite well and can be reliably used to calculate safety scenarios involving PBX-9501 explosive at temperatures from ambient to 180°C. While most of the modeling constants remain unchanged, only few of them require a change depending on the temperature. These constants are shown in Table 4.

Table IV. Ignition and Growth parameter changes for 25°C, 50°C and 150°C PBX 9501

<table>
<thead>
<tr>
<th>( T_0 ) (°C)</th>
<th>Density (g/cm(^3))</th>
<th>Unreacted B (Mbar)</th>
<th>( G_1 ) (Mbar(^{-2})µs(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.83</td>
<td>-0.052654</td>
<td>130.0</td>
</tr>
<tr>
<td>50</td>
<td>1.82</td>
<td>-0.055179</td>
<td>130.0</td>
</tr>
<tr>
<td>150</td>
<td>1.762</td>
<td>-0.065278</td>
<td>190.0</td>
</tr>
</tbody>
</table>

**SUMMARY**

Previously published shock initiation experiments on the explosive PBX-9501 were reviewed and extended to initial temperature of 180°C. The use of the Ignition and Growth model for the explosive works well and can be used to calculate safety scenarios involving this explosive for the range of temperatures between ambient and 180°C.

**ACKNOWLEDGEMENTS**

The High Explosives Response program provided funding for this research. Special thanks go to the 101 mm gun crew in the High Explosives Application Facility (HEAF) including Rich Villafâna, Steve Kenitzer, and Gary Steinhour. This work was performed under the auspices of the U. S. Department of Energy by the University of
REFERENCES


FIGURE CAPTIONS

**Figure 1** Experimental set-up used to study initiation process in heterogeneous solid explosives. It depicts a moment as the projectile with an impactor leaves the gun barrel just before striking the target assembly. The target assembly is fitted with manganin pressure gauges and thermocouples at various depth of the target and with pins ahead of the target to measure the impact velocity and the tilt of the impact.

**Figure 2** Pressure histories in hot 150°C LX-04 impacted by an aluminum flyer at 0.701 km/s.

**Figure 3** Pressure histories in ambient PBX-9501 impacted by an aluminum flyer with a velocity of 0.607 mm/µs.

**Figure 4** Pressure histories in PBX-9501 heated to 52°C and impacted by an aluminum flyer with a velocity of 0.8005 mm/µs.

**Figure 5** Pressure histories in PBX-9501 heated to 50°C and impacted by an aluminum flyer with a velocity of 0.649 mm/µs.

**Figure 6** Pressure histories in PBX-9501 heated to 150°C and impacted by an aluminum flyer with a velocity of 0.73 mm/µs.

**Figure 7** Pressure histories in PBX-9501 heated to 150°C and impacted by an aluminum flyer with a velocity of 0.55 mm/µs.

**Figure 8** Thermal traces at various depth of the target during the heating process to the desired temperature of 190°C. The figure shows a distinct evidence of the b to d phase transition process in HMX occurring above 175°C.

**Figure 9** “Pop Plot” for PBX-9501 at various initial temperatures demonstrating its sensitivity to impact pressure.

**Figure 10** Experimental (solid) and calculated (dashed) pressure profiles in ambient PBX-9501 impacted by an aluminum flyer with a velocity of 0.607 mm/µs.

**Figure 11** Experimental (solid) and calculated (dashed) pressure profiles in heated to 50°C PBX-9501 impacted by an aluminum flyer with a velocity of 0.649 mm/µs.

**Figure 12** Experimental (solid) and calculated (dashed) pressure profiles in heated to 150°C PBX-9501 impacted by an aluminum flyer with a velocity of 0.55 mm/µs.
Figure 1

Flyer Plate

Pressure Gauges and Thermocouples

Heaters

Target

Figure 2

Experiment 4664 Temperature Profile, 150°C PBX9501

Temperature (°C)

Time (minutes)
Figure 3

SHOT 4521, PBX 9501, Amb.
Al 6061 => PBX 9501
ufp = 0.607 mm/µs

Gauge 1 at 0 mm
Gauge 2 at 5.31 mm
Gauge 3 at 7.63 mm
Gauge 4 at 9.96 mm
Gauge 5 at 13.28 mm
Gauge 6 at 16.59 mm

Figure 4

SHOT 4522, PBX 9501,
To = 52˚C
Al 6061 => PBX 9501
ufp = 0.8005 mm/µs

Gauge 1 at 0 mm
Gauge 2 at 3.33 mm
Gauge 4 at 7.97 mm
Gauge 5 at 11.28 mm
Figure 5

SHOT 4523, PBX 9501, To = 50°C
Al 6061 -> PBX 501
ufp = 0.649 mm/µs

Pressure (kbar)

<table>
<thead>
<tr>
<th>300</th>
<th>250</th>
<th>200</th>
<th>150</th>
<th>100</th>
<th>50</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>26</td>
<td>24</td>
<td>22</td>
<td>20</td>
<td>18</td>
<td>16</td>
<td>14</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gauge 1 at 0 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauge 2 at 5.33 mm</td>
</tr>
<tr>
<td>Gauge 3 at 10.65 mm</td>
</tr>
<tr>
<td>Gauge 4 at 12.97 mm</td>
</tr>
<tr>
<td>Gauge 5 at 15.30 mm</td>
</tr>
<tr>
<td>Gauge 6 at 18.62 mm</td>
</tr>
</tbody>
</table>

Figure 6

Shot 4663 Hot 9501, T=150°C
Al 6061 flyer, ufp=0.73mm/µs

Pressure (kbar)

<table>
<thead>
<tr>
<th>250</th>
<th>200</th>
<th>150</th>
<th>100</th>
<th>50</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>20</td>
<td>18</td>
<td>16</td>
<td>14</td>
<td>12</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>g 1 at 0 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>g 2 at 5.38 mm</td>
</tr>
<tr>
<td>g 5 at 7.72 mm</td>
</tr>
<tr>
<td>g 7 at 11.09 mm</td>
</tr>
<tr>
<td>g 9 at 16.48 mm</td>
</tr>
<tr>
<td>g 10 at 21.86 mm</td>
</tr>
</tbody>
</table>

Time (µs)
Shot 4664, Hot PBX9501 (T=150°C)
Al Flyer, ufp=0.55 mm/µs

gauge 1 at 0 mm
gauge 2 at 5.37 mm
gauge 4 at 10.75 mm
gauge 6 at 13.09 mm
gauge 8 at 15.44 mm
gauge 10 at 18.8 mm
gauge 12 at 22.69 mm

Figure 7

Temperature (°C)

Evidence of Phase Transformation

TC's with the heaters

TC's inside of HE samples

Figure 8
Figure 9

Figure 10
Figure 11

50°C PBX 9501 3 GPa initial pressure
Experiment - solid lines
Calculation - dashed lines

- 0 mm
- 5 mm
- 10 mm
- 12 mm
- 14 mm
- 17 mm

Figure 12