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TEMPERATURE DEPENDENT EQUATION OF STATE FOR HMX-BASED COMPOSITES

M. R. Baer[1], S. Root[1], R. L. Gustavsen[2], T. Pierce[2], S. DeFisher[3], and B. Travers[3]

[1] *Sandia National Laboratories, Albuquerque, NM, 87185*
[2] *Los Alamos National Laboratories, Los Alamos NM 87545*
[3] *U.S. Army ARDEC, Picatinny Arsenal, NJ 07806-5000*

Abstract. In order to examine the temperature dependence of the equation of state (EOS) of HMX-based explosives, two energetic composites, PBX9501 and PBXN9, were subjected to shockless compression using the Sandia VELOCE magnetic compression system. Prior to compression, the energetic samples were heated to temperatures up to 155°C, presumed to be below the HMX β - δ phase transition at atmospheric pressure conditions. A Velocity Interferometer System for Any Reflector (VISAR) was used to measure particle velocity of the transmitted compression wave. Temperature corrections in the drive plates and windows were estimated and velocity profile data was analyzed using forward/backward integration methods along with an optimization method to determine unreacted Mie-Grüneisen EOS parameters.

Keywords: Isentropic compression, Z accelerator, polymer binders, energetic composites, CTH modeling.
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INTRODUCTION

In a prior study, HMX-based composites, PBX9501 and PBXN9, were subjected to identical ramp wave planar compression loads to assess material response at ambient (20°C) temperature conditions. Sandia's VELOCE magnetic compression facility [1] has a new capability to heat and cool target samples prior to the ramp loading. This capability was explored to assess the temperature dependence of the EOS of the energetic composites using data analysis of the measured particle velocities. Samples were heated up to 155°C, presumed to be below the HMX β - δ phase transition [2]. However, post data analysis revealed that the phase transition in the energetic composites likely occurred when heated to 155°C prior to the ramp loading.

EXPERIMENTAL CONFIGURATION

Isentropic compression experiments (ICE) were conducted at Sandia's VELOCE facility and details of the experimental setup can be found in Reference [1]. Figure 1 displays the modifications to the VELOCE target panel to accommodate preheating of the energetic composite sample.

A heater cartridge was attached to the drive panel and a temperature controller was used to

monitor the heating rate. Temperature variations in the panel were then measured using two thermocouples. A spring-mounted clamp kept a VISAR probe holder intact with the window/sample configuration during heating and ramp loading.

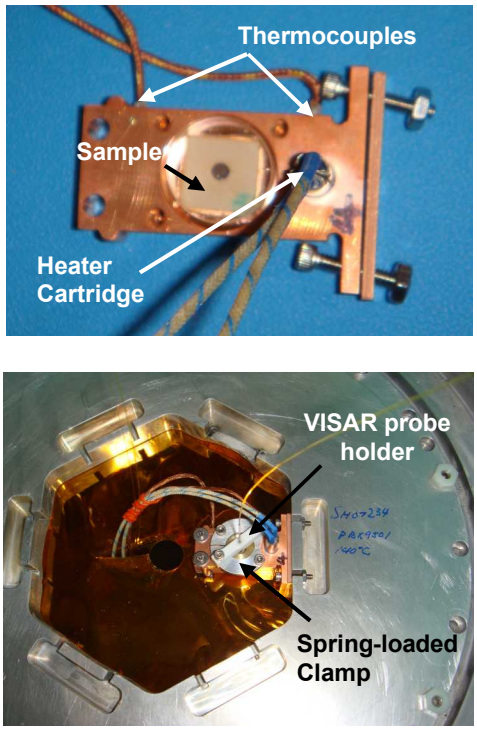


FIGURE 1. Heated panel configuration (top) and target assembled in VELOCE (bottom).

In this series of tests, ~400 μm thick samples of PBX9501, and PBXN9 were mounted on 1.5 mm Al-1100 drive panels and interfaced with 6mm LiF and NaCl. These assemblies were then heated at a rate of ~2°C /min to temperatures 55°C, 100°C and 155°C, respectively, and subjected to ramp loads up to ~50 Kbar over 250ns. VISAR particle velocity measurements were simultaneously taken at the composite/window interface location and at the opposing drive plate location. The drive measurements were corrected for window interactions and loading conditions were assessed using Hayes's backward analysis technique [3].

Data assessment of material response was based on forward and backward techniques using CTH/DAKOTA shock analysis and optimization methods as outlined in Reference [4]. In the sections to follow, temperature corrections for the drive plate and windows EOS is estimated and analysis of the heated PBX9501 and PBXN9 is presented.

TEMPERATURE CORRECTIONS

In these isentropic compression tests, temperature corrections to EOS of the Al-1100 and LiF / NaCl windows were determined to properly unravel the drive loading conditions and the material response of the energetic composites. Thermal expansion and specific heat property data at the various temperatures were obtained from historical reference data [5].

The Hugoniot sound speed, c_0, was estimated using a method given in Reference [6] using reference data of bulk modulus and thermal expansion. Variations of the Hugoniot slope, s, were assumed to be negligible. Similarly, the Al-1100 panel and window thicknesses were corrected to account for thermal expansion.

T (°C)	ρ (g/cc)	c_o (mm/μs)	s	Γ_o
20	2.709	5.335	1.35	1.97
55	2.704	5.313	1.35	1.97
100	2.695	5.277	1.35	1.98
155	2.684	5.231	1.35	1.99

TABLE 1 Al EOS parameters at various temperatures.

T (°C)	ρ (g/cc)	c_o (mm/μs)	s	Γ_o
20	2.165	3.528	1.34	1.6
55	2.163	3.586	1.34	1.6
100	2.158	3.667	1.34	1.6

155	2.153	3.752	1.34	1.61

TABLE 2 NaCl EOS parameters at various temperatures

T (°C)	ρ (g/cc)	c_o (mm/μs)	s	Γ_o
20	2.638	5.15	1.35	1.52
55	2.631	5.418	1.35	1.52
100	2.617	5.803	1.35	1.53
155	2.601	6.163	1.35	1.54

TABLE 3 LiF EOS parameters at various temperatures.

Table 1 displays the variation of the Al -1100 EOS parameters over the testing temperatures ranging from 20°C to 155°C. Similar variations are shown in Table 2 and 3 for the LiF and NaCl windows.

ICE tests at 20°C, 55°C and 100°C

The composite energetic material response was estimated assuming a Mie-Grüneisen form and material strength or rate-dependent effects were not considered. The EOS material response is represented in terms of a quadratic Hugoniot relationship:

$$U_s = c_0 + s_1 u_p + s_2 u_p^2 / c_0 . \qquad (1)$$

In prior Z tests [7], at 20°C, the EOS for PBX9501 was optimized using c_0=2.613[mm/μs], s_1=2.091 and s_2=-0.183. Density of this PBX9501 was taken as 1.837 [g/cc]. This optimization served as a baseline for the elevated temperature tests. Similarly, for PBXN9, the baseline EOS parameters c_0=2.495[mm/μs], s_1=2.127 and s_2=-0.331 were determined at a density of 1.75 [g/cc].

Additional isentropic compression tests were conducted higher temperature, 55°C and 100°C. These tests served to assess the repeatability of optimization technique and the consistency of sample preparation. Figure 2 and 3 display the overlay of forward analysis to the observed response at the elevated temperature for PBX9501 and PBXN5, respectively. In all of the simulations the 20°C EOS parameters were used without any modifications.

These comparisons indicate that the temperature corrections to the composite EOS are minor. Sensitivity analysis also indicated that the panel and window temperature corrections were negligible.

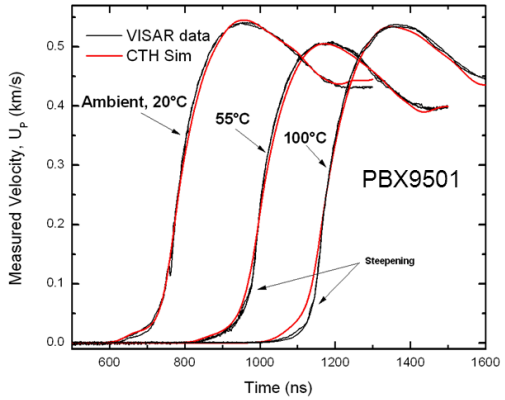


FIGURE 2. Particle velocities in PBX9501 at 20°C, 55°C and 100°C.

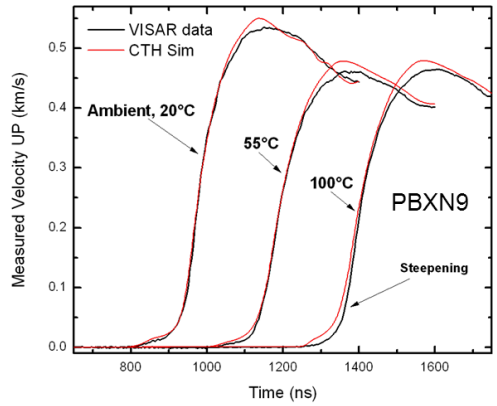


FIGURE 3. Particle velocities in PBN9 at 20°C, 55°C and 100°C.

ICE tests at 155°C

Isentropic compression tests were then conducted at 155°C with the intent of investigating phase transformation during ramp loading. Historical data suggests that the HMX β - δ phase

transition occurs above 160°C and it was suggested that the 5°C lower temperature differential was sufficient to prevent phase transformations during heating up to the testing temperature.

Both PBX9501 and PBXN9 samples were heated to 155°C and subjected to the ramp loading as described earlier. Figure 4 displays the input load and the measured particle velocity at the PBX9501/Lif window interface.

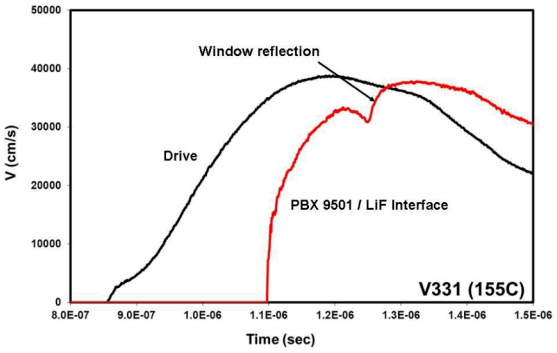
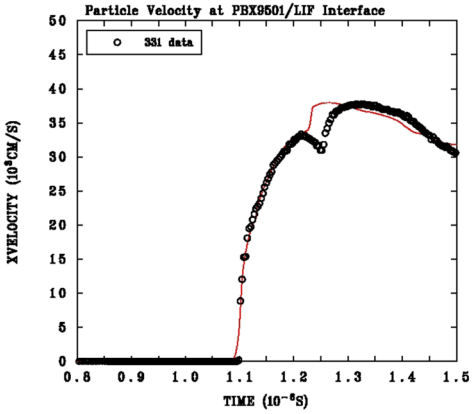


FIGURE 4. Particle velocities in the 400 μm PBX9501 sample subjected to the V331 ramp load.

FIGURE 5. Optimized data fit for the heated PBX9501 sample subjected to the V331 ramp load.

Figure 5 shows a comparison of the forward CTH/Dakota analysis to the observed measurements of particle velocity. The optimized parameters for EOS of PBX9501 were determined as c_0=1.646[mm/μs], s_1=2.61 and s_2=-0.1. The optimized sound speed was much lower than anticipated. Furthermore, the sample density was also included as an optimization parameter, (fixing the mass), and a lower density (1.648 [g/cc]) was determined. Similar implausible optimization parameters for the EOS were determined for the heated PBXN9 composite.

The greatly reduced density change was not consistent with existing thermal expansion data [8] and the HMX β - δ phase transition likely occurred during heating prior to the ramp loading. Hence, the temperature limit for phase transformation temperature appeared to be lower for the energetic composites as opposed to that of pure monolithic HMX crystals.



SUMMARY

In this study, isentropic ramp loading was applied to heated sample two HMX-based energetic composites. Equation of state parameters were determined from the material response data using forward analysis and optimization methods. At temperatures lower than 100°C, temperature effects appear to be minor effects. However, at 155°C, a compositional change, likely due to phase transformation, occurred prior to ramp loading. Further investigation requires additional diagnostics to assess the state of the material prior to isentropic loading.

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REFERENCES

1. Ao, T, C. et al, Rev. Scientific Instruments. **79**, 013903, 2008.
2. Levitas, V. I, et al, J. Phys. Chem, B. **110** (20), 2006, pp 10105-10119.
3. Hayes, D. B., Sandia National Laboratories Rpt SAND2001-1440, 2001.
4. Baer, M. R., et al, J. of Applied Physics, **101**, 034907, 2007.
5. Touloukian, Y.S. and M. Tadashi, **Thermophysical Properties of Matter**, Vol. 4 and 12, 1970.
6. Menikoff, R, **Shockwave Science and Technology Reference Library**, 2007, pp 143-188.
7. Baer, M. R., et al., Shock Compression of Condensed Matter, 2009 (M. Elert, M.D. Furnish, W. Anderson, W. Proud, W. Butler, eds.), part I, pp. 699-702.
8. Thompson, D, et al., LANL report, LA-UR-09-05002, 2009.