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Deflagration Rate Measurements of Three Insensitive High Explosives: LLM-105, TATB, and DAAF

E. A. Glascoe, J. L. Maienschein, K. T. Lorenz, N. Tan, J. G. Koerner

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Deflagration Rate Measurements of Three Insensitive High Explosives: LLM-105, TATB, and DAAF

Elizabeth A. Glascoe, Jon L. Maienschein, K. Thomas Lorenz, Noel Tan, and Jake G. Koerner

Energetic Material Center
Lawrence Livermore National Laboratory
7000 East Ave, Livermore, CA 94550, USA

Abstract. The pressure dependent deflagration rates of LLM-105, DAAF and TATB based formulations were measured in the LLNL high pressure strand burner. The role of binder amount, explosive type, and thermal damage and their effects on the deflagration rate will be discussed. One DAAF formulation, two different formulations of LLM-105, and four formulations of TATB were studied; results indicate that binder amount and type play a minor role in the deflagration behavior. This is in sharp contrast to the HMX based formulations which strongly depend on binder amount and type. The effect of preheating these samples was considerably more dramatic. In the case of LLM-105, preheating the sample appears to have little effect on the deflagration rate. In contrast, preheating DAAF and TATB formulations causes the deflagration rate to accelerate. The thermal and mechanical properties of these formulations will be discussed in the context of their pressure and temperature dependent deflagration rates.

INTRODUCTION

The deflagration rates of energetic materials are important to the performance and safety of the material, especially in cook-off scenarios. Insensitive high explosives (IHE) are of particular interest to the explosives community because of they are less sensitive to thermal or impact stimuli relative to conventional HE's (e.g. HMX or RDX). TATB is the current material of choice for IHE formulations, however, testing of two new explosive, 2,6-Diamino-3,5-dinitropyrazine-1-oxide (referred to as LLM-105) and 4,4'-diamino-3,3'-azoxyfurazan (DAAF), indicate that these materials may eventually become superior candidates for IHE applications.

Both thermal and mechanical stimuli can initiate a reaction in an energetic material. In insulated and/or contained environments, the pressure and temperature can rise quickly as the material reacts resulting in an acceleration of the reaction until runaway conditions are reached. Accurate knowledge of the reaction rates at conditions typical of those in accelerating reactions is necessary to understand and predict the violence of the ensuing explosion. Hydrodynamic calculations indicate that reacting materials can achieve pressures in the hundreds of MPa range (several kbar) and higher. Therefore, measurements of the laminar deflagration rate at these pressures are particularly important in safety assessment and predictive modeling.

Preheating samples to various temperatures and durations allows for thermal damage to the material prior to burn ignition. Depending on the nature of the sample, preheating can result in phase transitions and introduce cracks, voids, and fissures. Sometimes, the damage induced by preheating can be subtle and not easily predicted based on conventional thermal analysis techniques (e.g. DSC or TMA), yet the changes in the burn behavior can be dramatic. Our results indicate that TATB and DAAF are both affected by preheating; the burn rate and predictability of the material burn change considerably. In contrast, LLM-105 based formulations tend to remain unaffected by preheating and the burn rates are nearly the same as the ambient temperature burn rates. Possible mechanisms for the accelerated burns in TATB and DAAF-based formulations are discussed.

EXPERIMENTAL METHOD

LLNL High Pressure Strand Burner

Deflagration rates are measured using the LLNL high pressure strand burner, shown in Figure F1. This experimental technique is described in detail in the literature.[1,2] Briefly, burns are performed under constant volume in an atmosphere of Argon. The pressure is measured in-situ throughout the burn and burn progress is monitored via silver break wires that are embedded within the sample. A typical sample consists of nine individual pellets (1/4 in diameter by 1/4 in tall) and 10 burn wires, the exterior surface is encapsulated by an organic-polymeric material to prevent flame spread down the sides. The sample is prepressurized to a desired pressure using Argon, the burn is initiated via an igniter train (igniter wire, $BKNO_3$ and a thin HNS pellet), and the sample burns resulting in a rise in pressure on the order of 3-5 times the initial pressure. Many towers may be burnt in order to investigate a pressure range of 10-600 MPa.

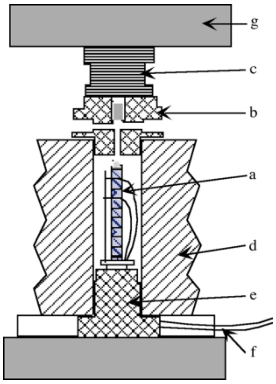

Figure F1. Strand burner schematic composed of a) nine segment burn sample with burn wires evenly spaced between segments (only two wires shown for clarity) and igniter on top, b) top plug with inlet and outlet ports and pressure transducer in center, c) load cell, d) pressure vessel, e) bottom plug with wire feed-throughs, f) signal wires to electronics, g) load frame (top and bottom).

Typical pressure and flame front time-of-arrival data are shown in Figure F2. These results represent a well behaved burn because the wires are burned in order and the pressure rise stops after the last burn wire. The burn wire data should cover the time span of the pressure signal, any significant deviation from this indicates anomalous behavior. For example, the report of all burn wires before the pressure reaches a maximum indicates that the deflagration front passed rapidly down the sample and left still-reacting material behind. This behavior is indicative of flame spread through the sample or of propagation of the flame down the side of the sample; although the epoxy coating should inhibit the latter.

To calculate deflagration rate as a function of pressure, the length and time-of-arrival for each pair of pellets is used, and the corresponding average pressure for this segment of the sample is calculated. The temporal pressure data can be used to calculate vivacity and surface area.[3-5]

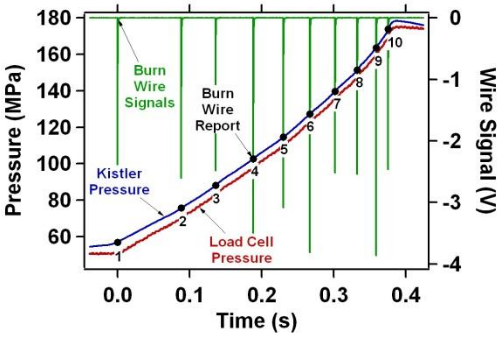

Figure F2. Typical strand burner data, showing temporal pressure behavior and flame-front time-of-arrival signals resulting from the burn wires.

Materials

Two different formulations of LLM-105 were studied in this work and are listed in Table T1. Both formulations were prepared from the same lot of LLM-105 (LLNL number PP-XV-89A). Typically a formulation contains about 28% ground (0.1 – 10 µm, bimodal distribution with maximum population at 0.27 µm and 2.9 µm) and 72% unground (10 – 110 µm, maximum population at 42 µm) particles. The theoretical maximum density (TMD) for each formulation was calculated assuming 4.8% 2,6-diamino-3,5-dinitropyrazine (ANPZ), a lower powered explosive that is a precursor in the synthesis of LLM-105. The calculated TMD for RX-55-AB and –AY are 1.9212 and 1.9096 g/cc, respectively. Both formulations were uniaxially pressed in a mechanical pressing die at 207 MPa (30 kPSI) and 105-110 °C (3x5 min dwell, 1 min break between dwells, 5 min heat soak prior to first dwell).

One formulation of DAAF was studied; the sample details are listed in Table T1. The material was supplied by Los Alamos National Laboratory as a powder and uniaxially pressed at LLNL in a mechanical pressing die at 207 MPa (30 kPSI) and 105-110 °C (3x5 min dwell, 1 min break between dwells, 5 min heat soak prior to first dwell).

Four different formulations of TATB were studied and variables include the binder type, binder amount and source of TATB; these formulations are listed in Table T1. In particular, the recrystallization solvent was found to improve the quality and size of the TATB crystals significantly over methods employed in the wet- and dry-aminated procedures.[6] LX-17 and RX-03-GP were uniaxially pressed in a mechanical pressing die at 207 MPa (30 kPSI) and 105 – 110 °C (3x5 min dwell, 1 min between dwells). RX-03-GO-IL4 was uniaxially pressed in a mechanical pressing die at 207 MPa (30 kPSI) and 135-139 °C (3x3 min dwell, 1 min between dwells, 5 min heat soak prior to first dwell).

Calculations

The pressure dependent deflagration rate is fit to the Vieille equation:

$$B = aP^n \tag{1}$$

where B is the burn rate (mm/s), a is the burn rate coefficient (mm/s•MPa), P is the pressure (MPa) and n is the pressure exponent (dimensionless).

Table T1. Formulation details and burn rate parameters[a]

Material Name	Formulation (wt %)	Density (g/cc)	TMD (%)	a (mm/s*MPa)	n
RX-55-AB	92 LLM-105 7.5 Kel-F 800	1.857	96.7	0.65 ± 0.09	0.77 ± 0.01
RX-55-AY	94 LLM-105 6 Viton A	1.835	96.1	0.8 ± 0.3	0.76 ± 0.02
RX-64-AA	95 DAAF 5 Viton A	1.684	96.4	0.8 ± 0.1	0.79 ± 0.01

LX-17	92.5 TATB[b] 7.5 Kel-F 800	1.898	97.6	0.184 ± 0.004	0.90 ± 0.01
PBX-9502	95 TATB[c] 5 Kel-F 800	1.887	97.1	0.23 ± 0.01	0.86 ± 0.01
RX-03-GO-IL4	92.5 TATB[d] 7.5 Cytop A	1.898	97.7	0.36 ± 0.07	0.75 ± 0.04
RX-03-GP	92.5 TATB[d] 7.5 Kel-F 800	1.905	98.0	0.32 ± 0.03	0.77 ± 0.03
LX-04	85 HMX 15 Viton A	1.861	98.5	1.1 ± 0.9	0.98 ± 0.01

[a] burn rate parameters correspond to the function $B = aP^n$; [b] wet-aminated; [c] dry-aminated; [d] ionic liquid re-crystallization (fine and course crystals)

RESULTS AND DISCUSSION

Ambient Temperature Measurements

The pressure dependent deflagration rates of the LLM-105 and DAAF formulations were measured between 0 and 300 MPa in a series of experiments. The results are plotted in Figure F3 along with the pressure dependent deflagration rates of LX-17 and LX-04; the burn rate parameters are listed in Table T1. The LLM-105 burn rates are within error of each other and more experiments would, likely, produce better overlap. The RX-55-AY data at 40-80 MPa is more erratic than any of the other burns, which is tentatively attributed to minor, random errors (e.g. minor delamination of the organic encapsulation), and is not expected to be significant or reproducible under repeated testing.

The DAAF formulation burns slightly faster than the LLM-105 formulations; however the burn equation parameters indicate that the materials are within error of each other. DAAF burn rates were measured previously by Son et al.[7] between 0.1 and 11 MPa; our burn rate exponents are similar, but not the same. As no standard deviation was reported previously, it is possible that our measurements fall within the error of their studies. Alternatively, the differences in burn rate exponents are most likely due to the difference in pressure and its affect on the mechanism of burning and flame structure.[8] Qualitatively, however, the relative burn rates of HMX-based, DAAF-based and TATB-based materials are similar to those reported previously[7] and in general, we consider our results to be consistent with Son et al.'s results.

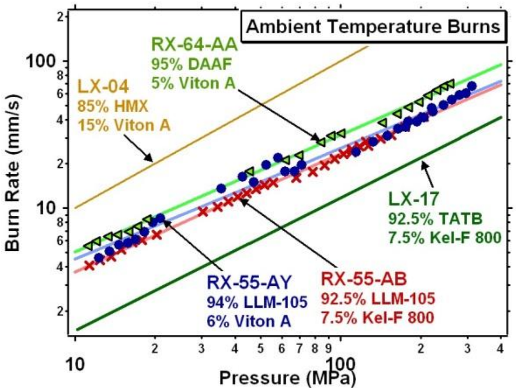

Figure F3. Pressure dependent deflagration rate measurements for LLM-105 and DAAF formulations. Refer to Table T1 for burn rate parameters.

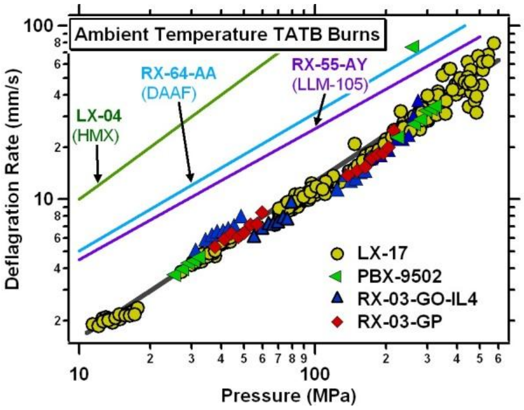

Figure F4. Pressure dependent deflagration rate measurements for TATB formulations. Refer to Table T1 for burn rate parameters.

Pressure dependent deflagration rates for all the TATB-formulations listed in Table T1 are show in Figure F4. LX-17 data was reported previously and is reproduced here.[9] Although there are a limited number of experiments of PBX-9502 and the two RX-03 formulations, all appear to burn in a well behaved manner and have similar burn rates to LX-17.

The criteria for a well-behaved burn are discussed in the experimental section. In general, there are a variety of possible random errors that can occur during a burn, however, the likelihood of significant random errors producing a well-behaved burn are small. Therefore, despite the limited number of experiments presented for each material in Figures F3 and F4, the orderly nature of the results indicate that these data are representative of an experiments that are free of significant random errors and reliable enough to draw preliminary conclusions.

Discussion of Ambient Temperature Results

It is interesting to compare the deflagration rates of HMX-, DAAF-, LLM-105- and TATB-formulations with their thermal decomposition properties. The temperature dependent heat-flow results from differential scanning calorimetry (DSC) on the neat explosives (i.e. no binder) are shown in Figure F5. Typically, a small amount of Viton-A, Kel-F 800, or Cytop-A will only shift these DSC peaks by a few degrees. Omitting the DAAF results, it appears that the relative thermal sensitivity of HMX, LLM-105 and TATB is similar to the relative burn rates. DAAF, however, breaks this trend and appears significantly more thermally sensitive than HMX, yet its deflagration rate is similar to LLM-105. Clearly, the trend in the decomposition thermodynamics (i.e. J/g for each explosive) is also inconsistent with the deflagration rate.

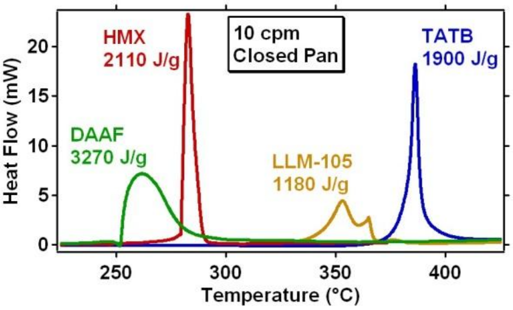

Figure F5. Differential scanning calorimetry results for four neat explosives (not formulations).

Constant volume explosion calculations using the program Cheetah 6.0 suggests a correlation between temperature, entropy and our experimentally measured relative burn rates. It is the transient species and products of deflagration that really dictate the temperature and entropy (and many other thermodynamic variables) of a deflagration. Hence these Cheetah results suggest that the specific molecular structure and molecular formula are the factors that drive the deflagration rate. Further work is necessary to establish whether the entropy and/or temperature predictions from Cheetah correlate with deflagration rates at elevated pressures.

Table T2. Constant vol. explosion calculation at material theoretical maximum density (TMD)[10]

Explosive	Oxygen balance (%)	Temp (°C)	ΔH_r (J/g)	ΔS_r (J/g)
HMX	-21.61	2853	9262	7.29
DAAF	-52.80	2709	7174	6.86
LLM-105	-37.02	2419	7869	6.48
TATB	-55.78	2147	7431	6.30

In all of the ambient temperature burns reported here, one of the key observations is the laminar nature of the burns. Burns of some HMX based formulations become extremely rapid and erratic at elevated pressures (i.e. P>150 MPa), in a process termed deconsolidative burning. The hypothesized mechanism behind these erratic burn rates is the physical deconsolidation of the material, which creates new cracks and voids and allows the flame to penetrate deep into the material. Materials that deconsolidatively burn at elevated pressures have been shown to be considerably more violent in confined heating experiments (i.e. cook-off scenarios).[11]

In HMX based materials, the binder type and volume fraction are important variables in determining if and when the material transitions to a deconsolidative burn. The mechanical properties of the material are heavily dictated by the binder type and amount, and studies have shown that increasing the binder amount increases the strain to failure and ultimate elongation[12] and decreases the likelihood of deconsolidation during burning.[1,2] LX-17 was shown previously to burn in a laminar fashion over a wide pressure range.[9] At this ratio of explosive to binder, a similar formulation made with HMX would deconsolidate above 150 MPa;[1] hence, the nature of the explosive, and, most likely, its burn temperature and burn rate, play an important role in the deconsolidation. In the case of the LLM-105 and DAAF formulations, the nature of the burn could not be predicted prior to experiments. The LLM-105 and DAAF formulations all have relatively low binder content and relatively stiff/brittle binders; an HMX formulation with the same binder type and amount would certainly deconsolidative burn at P > 150 MPa.

In the case of the novel TATB formulations (RX-03 formulations), the change in binder and crystal morphology were not expected to affect the burn rate dramatically. Cytop A is a perfluorinated polymer with a room-temperature ultimate strength and Young's Modulus that are between those of Viton A and Kel-F 800.[12] In addition, atomistic simulations predict that Cytop A will adhere to the TATB crystals better than Kel-F 800;[13] presumably this will reduce the likelihood of cracks forming between the binder and TATB. Hence, the stable, laminar burns observed for both RX-03 formulations are not surprising.

The nature of and ultimate cause of deconsolidative burning remains a puzzle. Clearly, the burn rate is one major factor in predicting whether a material deconsolidatively burns. Yet the mechanical properties of the material and probably the thermal transport and thermal expansion properties all play a role in the deconsolidation of the material. One could envision that at elevated pressures, the material will deconsolidate if the flame temperature is sufficiently high, and the pre-heated zone of unburnt explosive is short enough to create a short zone of material with a large thermal gradient. Such a situation could result in cracks that form in the material, ahead of the burn zone. If those cracks can sustain and propagate, the material may be able to deconsolidate and some convective burning may begin.

Elevated Temperature Measurements

Figure F6 shows the results of burning LLM-105 and DAAF-formulations at elevated temperatures after thermally soaking the sample. In these measurements, the experiment was assembled, the sample was pressurized, heated to a desired temperature (typically 1-2 °C/min), held for a desired length of time, and burned hot. For some materials, the order of heating and pressurizing can be important if there are material phase transitions that can occur under one set of conditions but not the other.[1] In the case of LLM-105 and DAAF, there are no known phase transitions in this temperature-pressure regime and the order of heating and pressurizing is not expected to affect the results.

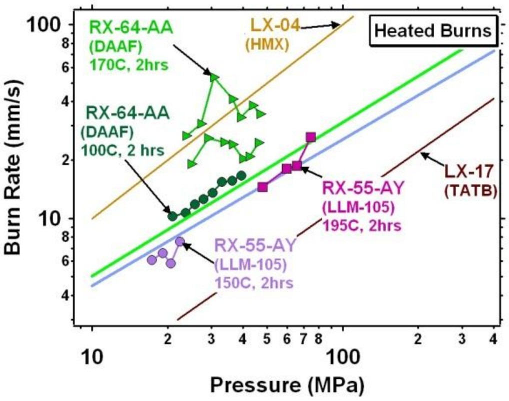

Figure F6. Deflagration rates of LLM-105 and DAAF formulations after heating (burns were initiated at the temperatures listed).

Figure F7 and F8 show the results of burning TATB-formulations at elevated temperatures after thermally soaking the sample. In most of the experiments, the sample was soaked at the indicated temperature for a designated period of time and then ignited hot. However, two LX-17 experiments (blue squares in Figure F7) were soaked at 195C for 2 hours, cooled back to room temperature and burned at ca. 22C. The LX-17 experiments at 225 °C, which are reproduced here from a previous study,[9] were all heated and then pressurized, all the other experiments were pressurized first, then heated. TATB has no known phase transitions in this temperature-pressure regime and the order of heating and pressurizing is not expected to affect the results. In addition, the LX-17 experiments at 225 °C were performed using band heaters around the pressure vessel and a small internal coil heater inside the pressure vessel (surrounding but not contacting or constricting the sample). The coil heater was later found to produce temperature gradients along the deflagration sample that spanned 16 °C[14] and was not used for any of the other experiments. In the coil-heater experiments, this temperature gradient can dramatically affect the experiment if the temperature spans a material phase transition or chemical decomposition.[14] For LX-17, 225 °C is well below any decomposition or phase transition, hence this 16 °C gradient is not expected to play a major role in the deflagration behavior. However, further work is underway to repeat some of these experiments without the coil heater.

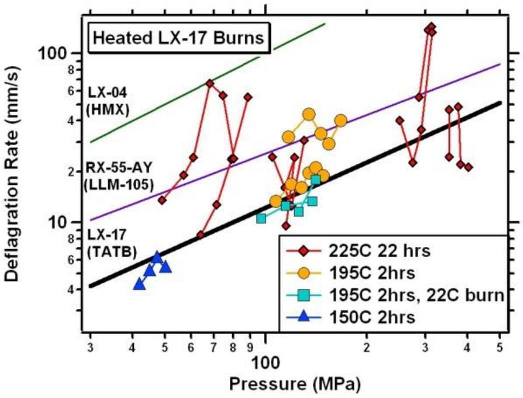

Figure F7. Deflagration rates of LX-17 (a TATB-formulation) after heating. All burns were initiated at the temperature listed except for the data in blue squares, in which samples were soaked at 195C for two hours and cooled to room temperature before burning. LX-17 burns at 225 °C are reproduced from previous work.[9]

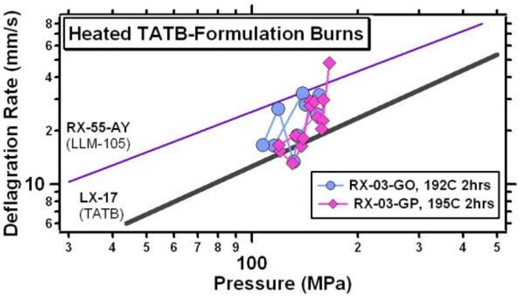

Figure F8. Deflagration rates of two TATB-formulations after heating. All burns were initiated at the temperature listed.

Discussion of Elevated Temperature Results

Heated deflagration rate measurements are particularly important to scenarios where an energetic material may have been thermally damaged and begins to cook-off. Previous studies of HMX based explosives demonstrate that heating the material above the β - δ phase transition of ca. 170 °C causes the material to burn at considerably higher rates. Burns of the same material below the β - δ phase transition, however, tend to behave similarly to ambient temperature burns.[1] These changes in burn rates are attributed to changes in the material structure rather than intrinsic changes in the decomposition and deflagration chemistry of the different phases.[15]

Neither DAAF, LLM-105, nor TATB has any known phase changes below the decomposition temperature, making the choice of temperatures somewhat arbitrary. DAAF, however, has a much lower onset temperature for thermal decomposition requiring more conservative thermal soaks than LLM-105 and TATB. In fact, when the DAAF formulation was heated to 195 °C the sample self-ignited after soaking for approximately 20 min. The DAAF experiments that were heated to 170C both appear to be rapid but not erratic, this is often indicative of material damage where the distribution of pores and voids is homogeneously distributed throughout the material (as opposed to deconsolidative cracking). When DAAF was heated to 100C the burn rate was relatively unaffected. Based on the thermal sensitivity of DAAF (see Figure F5), it is likely that at 170C the material experiences some small amount of decomposition which may either chemically change the material and/or introduce voids and small cracks in the material.

Our preliminary experiments of preheated LLM-105 indicate that the material burn rate does not change upon heating. These results are not surprising because there are no phase transitions below 195C and little material decomposition is expected based on the DSC results (see Figure F5).

In the TATB based burns, heating the sample appears to dramatically affect the burn behavior. The 22 hour, 225 °C burns of LX-17 were presented previously and it is clear that the material burns considerably faster and more erratically than the ambient temperature burns.[9] One could attribute some of this erratic burn behavior to the thermal gradients resulting from the coil heater. However, our preliminary data show that even under milder conditions (i.e. 2 hours at 195 °C) when only the band heaters were used (i.e. no coil heater, no thermal gradients), TATB formulations burn rapidly and erratically.

The source of this erratic burn behavior in heated TATB-formulations is puzzling. Previously, Koerner et al provided two possible explanations for why LX-17 burns erratically after 22hrs at 225 °C: either the anisotropic thermal expansion of TATB creates voids and cracks, or the elevated temperature assists in surmounting the energy barrier to decomposition causing an acceleration in the deflagration kinetics.[9] Based on our results of both LLM-105 and TATB formulations, the first hypothesis seems more plausible. Koerner et al. used the following basic Arrhenius analysis to estimate a chemical-decomposition rate at ambient and elevated temperature

$$\frac{k_2}{k_1} = exp\left[\frac{-E_a}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)\right] \qquad (2)$$

where k1 and k2 are the chemical-decomposition rates, Ea is the activation energy, R is the gas constant, and T1 and T2 are the flame temperatures at ambient and elevated temperatures, respectively.[9] The activation energy for LLM-105 and TATB are provided by Weese et al. (250 and 193 kJ/mol respectively)[16] and the flame temperatures are estimated using Cheetah 6.0 (see Table T2). The ratio of k2/k1 is 2.2 and 2.6 for LLM-105 and TATB respectively; based on this analysis one would expect both LLM-105 and TATB to accelerate by a similar amount at 200 °C relative to their ambient temperature results. Clearly the LLM-105 data is not accelerated at elevated temperatures, which eliminates the chemical kinetics hypothesis.

One notable trend in all the heated TATB burns was the fact that the wires often burned out of order. Figure F2 shows the basic criteria for a well behaved burn in which the wires burn in order and the pressure rise is well correlated with the wires, indicating that the material is burning in a sequential, laminar fashion. Figure F9 shows representative pressures and burn wire report times for a representative TATB-formulation experiment (this data came from an experiment where only the band heaters were used, no coil heaters, in order to avoid any potential problems with thermal gradients). In all the heated TATB based experiments, the wires burn out of order, however the pressure rise is usually relatively steady. This kind of scenario could occur if the flame is able to penetrate deeply into the sample without burning all the burn wires. A deep crack or fissure might create the path for the flame to penetrate, especially if the individual crystals anisotropically expand, there may be considerable changes in the packing arrangement of crystals and binders.

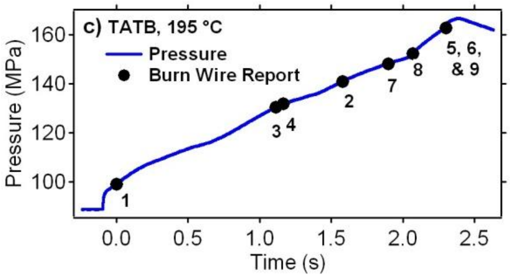

Figure F9. Pressure and burn wire report times for a heated TATB-based formulation.

Yet, the thermal expansion hypothesis seems less plausible when one considers the two experiments where TATB is soaked at 195 °C but cooled back to ambient temperature prior to burning. One would expect that the cooled material will retain many of the cracks and voids introduced from the thermal soak resulting in permanent, thermally induced damage in the sample. The fact that the heat-soaked and cooled samples burn at the same rate as the pristine samples indicates that whatever damage or material changes occur at 195 °C are reversible. This observation also eliminates the possibility of TATB sublimation at elevated temperatures because one would expect sublimation to be irreversible.

It is possible that the binder(s) characteristics change at elevated temperatures resulting in the erratic burn behavior of the TATB-formulations. Table T3 lists the glass and melt transition temperatures for three binders. At 195C, all three of binders are amorphous; hence simply the phase transition(s) is not the cause of the erratic burns in TATB-formulations. The mechanical strength the binder-explosive formulation may be the explanation. Further work is necessary to characterize the binder and/or formulation mechanical properties at 195C.

Table T3. Binder Properties

Binder	Glass Trans. Temp (°C)	Melt Trans. Temp (°C)	Source
Kel-F 800	30-31	82-107[a]	[17]
Viton A	-27	Not Obs.[b]	[18]
Cytop A	108	Not Obs.[b]	[18]

[a]depends on percent crystallinity of sample; [b]samples are mostly amorphous and have no melt transition

CONCLUSIONS

The deflagration rates of LLM-105, DAAF, and TATB based formulations are studied at various temperatures and pressures. This work is important in the assessment of safety and performance, in particular, in accidental heating scenarios (e.g. fires). The results of these studies indicate that none of the materials transition to deconsolidative burning when the sample is ignited at ambient temperature. This observation is important because deconsolidative burning has been correlated with significant violence in cook-off experiments.[11] Preheating these formulations changed the burn rates dramatically in the TATB and DAAF formulations, yet had little influence on the burn rates of the LLM-105 formulation.

Three TATB formulations were tested at elevated temperature and all three burned significantly faster and more erratically than the ambient temperature burns. The reason behind this burn behavior is unknown and multiple hypotheses were discussed yet none provided a satisfactory explanation. Further studies are necessary in order to understand why TATB-formulations burn so erratically at elevated temperatures. In particular, elevated temperature porosity measurements might demonstrate whether heating TATB introduces significant void structure and porosity in the samples. Mechanical properties of the binder and/or formulation at 195C might elucidate whether these properties are important to the heated TATB burns.

The DAAF-formulation also displayed burn rates at elevated temperatures. However, DAAF is thermally sensitive and decomposes at relatively low temperatures. It is plausible that preheating the DAAF formulation partially decomposes the sample which could either change the material chemically or structurally (via introduction of voids where material decomposed).

In contrast, heating the LLM-105 formulation prior to burning had little effect on the burn rate. These results are important because they indicate that under fire situations, LLM-105 based materials may be more stable and reliable.

ACKNOWLEDGEMENTS

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