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Mechanical Damage and Combustion of TNT and Composition-B

by Robert J. Lieb, John J. Starkenberg, William Lawrence, and Patrick J. Baker

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Abstract

Fracture damage was introduced into trinitrotoluene (TNT) and Composition-B (Comp-B) through uniaxial compression applied at controlled strain rates from 0.1 to 100 s^{-1}. The mechanical response was measured with parameters that have been used to characterize the fracture response of gun propellant during its development over the last decade. The damaged high explosive was burned in a small closed bomb in an effort to characterize the fracture surface area that resulted from the uniaxial compression. However, the brittle nature of both the TNT and Comp-B, and the burning character of these materials prevented a completely successful characterization and correlation with the mechanical response. The brittle mechanical response produced wide scatter in the measured parameters, and the apparently erratic burning behavior of the TNT and Comp-B prevented accurate surface area determination from the damaged high explosive. There were some trends that were noted for the mechanical response as a function of strain rate, and an idea of the nature of the fracture damage was attained. However, the roles that fracture play in the violence of the response of high explosive materials to impact and combustion threats remains unclear.

Acknowledgments

Michael G. Leadore (ARL, APG, MD) performed all of the mechanical properties tests and conducted all of the closed-bomb firings. His skill and patience with the equipment during this difficult test series is greatly appreciated.

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1. Introduction

The susceptibility to fracture damage of high explosives may play a role in their vulnerability response and in the evolution to violent scenarios. The mechanical response of gun propellant has been correlated with the fracture damage that was suffered under controlled compression of that propellant. This correlation was made with a parameter called the failure modulus that measured the material susceptibility to fracture and a method that successfully determined the fracture generated surface area [1, 2]. This same damage evaluation technique was attempted for the explosive materials trinitrotoluene (TNT) and Composition-B (Comp-B). In this technique, the failure parameter (failure modulus) for the material is measured under specific conditions. Usually the strain rate, temperature, and amount of strain are the parameters that determine the degree of fracture under uniaxial loading conditions. In these experiments, the temperature and amount of strain were held fixed, and the strain rate was varied over four orders of magnitude. The failure modulus was measured, along with other parameters that characterize the response of the material, and then the damaged material was collected and burned within a closed bomb in an effort to determine the correlation between the measured response and the fracture surface area produced.

The technique used to measure the surface area involves establishing the burning rate of the material as a function of pressure using undamaged specimens. Then, damaged material is burned, and using the established burning rates, the exposed surface area can be calculated from the pressure-time curve. Certain assumptions about burning must hold in order to successfully use this procedure. These assumptions will be addressed.

In addition to the experimental analysis previously outlined, a damage model was constructed. The model is a comprehensive theoretical foundation for modeling coupled damage and reaction in energetic materials. Although reaction is not expected, these models may be applicable to the description of material damage produced in the servohydraulic tester used to compress the specimens. The degree of damage (which varies from zero to some value near unity) represents additional surface area that is available to support reaction.

2. Experimental

2.1 Mechanical Response Measurements

The mechanical response was measured using a specially designed servohydraulic tester [3] shown schematically in Figure 1. The machine allows compression measurements to be performed at controlled rates as great as 1000 s^{-1} for a specimen with a nominal length of 1 cm. Compression is arrested when contact occurs between the impact bell and cone. Therefore, setting the anvil height can accurately predetermine the amount of specimen compression. This contact between bell and cone not only stops the specimen compression, but it also shunts the force around the specimen. The nitrogen spring absorbs the decelerating force of the massive ram and extends its duration. The force applied to the specimen is measured using the quartz piezoelectric gauge inside the impact bell. During compressive response measurements, displacement is measured with a linear variable differential transformer (LVDT) in the actuator column and is corrected for machine stiffness.

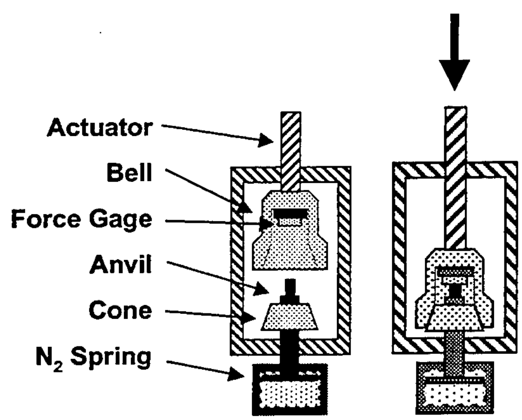


Figure 1. High-rate servohydraulic tester.

The specimens were prepared from cast, solid, right-circular cylinders of TNT and Comp-B. The specimen preparation procedure began by cutting the sample with a diamond saw to a length of 1.00 cm. The ends were cut flat, parallel, and perpendicular to the grain axis according to the specifications in a proposed NATO draft Standard Agreement entitled "Uniaxial Compressive Test," which is an updated version of the test published in CPIA Publication 21 [4]. The specimen was then placed on the anvil and tested at 21 °C.

The distance between the anvil and the force gauge when the bell and cone surfaces were mated determines the final strain to which the specimens were taken. That distance was determined by placing a lead specimen on the anvil and performing compression. This allowed any dynamic effects to be taken into account that may have been overlooked in a static measurement. The percentage strain used in these tests was initially selected to be 80%. However, during initial testing, it was observed that initial failure occurred before 10% strain, which showed that all support within the specimen was lost (Figure 2). This indicated that the damage from the initial contact was completed before 10% strain and that any further compression would increase the damage by means of secondary compression of the specimen fragments. This would add to the initial damage and could weaken the correlation between the initial mechanical conditions and the resulting fracture. As a result of this observation, all specimen compression was halted at 10% strain for specimens burned.

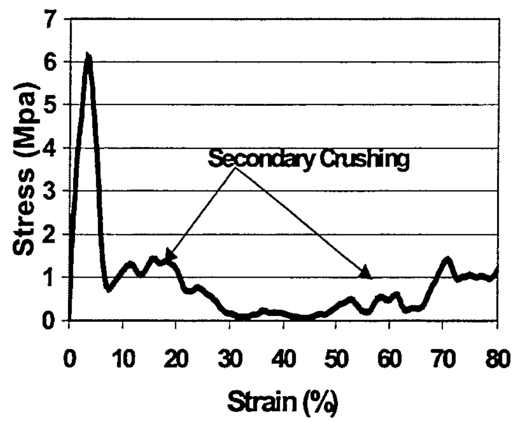


Figure 2. Individual compression curve.

The parameters measured in a response characterization test are (1) the modulus, (2) maximum stress, (3) strain at maximum stress, (4) stress at failure, (5) strain at failure, and (6) failure modulus. These parameters and an indication of their origin are illustrated in Figure 3. The first three parameters have the traditional engineering definitions. The failure stress, failure strain, and failure modulus have special values. The failure modulus is the slope of the stress-strain curve in the near linear region between strain at maximum stress, and twice that value. The failure modulus values were established from averaging the values determined from five response curves. The point of failure, from which the stress at failure and strain at failure values were determined, is defined by the intersection of the two lines that determine the modulus and failure modulus. The strain at the intersection of those lines defines the strain at failure; the corresponding stress on the response curve defines the stress at failure. The specimen strain rate for these tests was chosen to be 0.1 s^{-1}, 1 s^{-1}, 10 s^{-1}, or 100 s^{-1}.

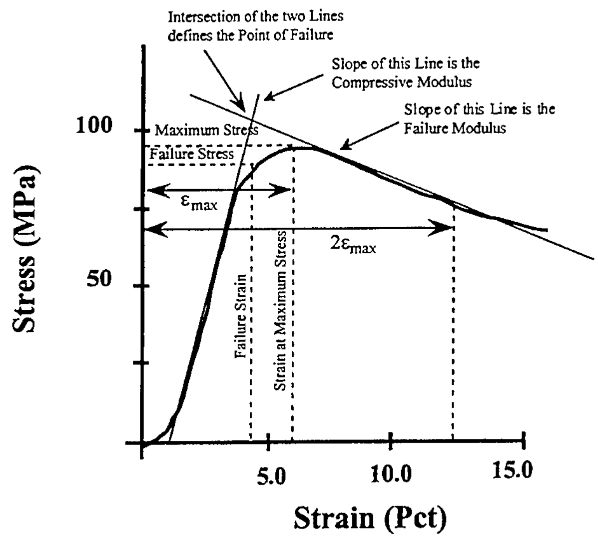


Figure 3. Characterization parameters.

It was hoped that a difference in fracture susceptibility could be established over this range of strain rates.

2.2 Fracture-Generated Surface Area Measurement

The shards of the grains that were damaged by uniaxial compression, as previously outlined, were carefully collected and burned in a small-volume (about 25 cc) closed bomb called the dynamic closed bomb (DCB). The bomb was used in an attempt to determine the effect that the mechanical damage had on the rate of pressure generation of the material. In normal propellant burning, the rate of pressurization during combustion is controlled by the intrinsic burning rate of the energetic material and the surface area exposed to the flame. The burning rate or the surface area can be determined from the pressure-time curve if the other is assumed or known. Once the burning rate has been established from undamaged specimens, it is possible to determine the surface area from the combustion pressure-time data.

Undamaged specimens were burned in the DCB at the same loading density that was used in the damaged grain firings. These pressure-time traces were analyzed using the closed-bomb reduction code, BRLCB [5], to establish the burning rates for the TNT and Comp-B used in these tests. Once established, the surface area from all the pressure-time histories can be determined using the same code by selecting the surface area analysis option. The output from the code provides pressure in MPa and the corresponding surface area in square centimeters. This output was converted to intrinsic parameters of fraction burned and surface area ratio (S/S_0), respectively, by dividing the pressure by the maximum pressure and the surface area by the initial surface area of the undamaged grain. This permitted closed bomb runs with different charges, pressures, etc., to be compared. Enough material was damaged to provide two closed bomb firings for each strain rate.

3. Results

3.1 Mechanical Response Measurements

As previously mentioned, a typical compressive stress-strain curve for Comp-B is shown in Figure 2. Secondary compression of the shards of the high explosive specimen is indicated in this figure, and because of this secondary compression, the experiment was stopped at 10% strain. The specimens were then burned in the DCB to determine the surface area caused by the fracture. The initial portion of the uniaxial compressive response of Comp-B at the strain rate of 100 s^{-1} is shown in Figure 4.

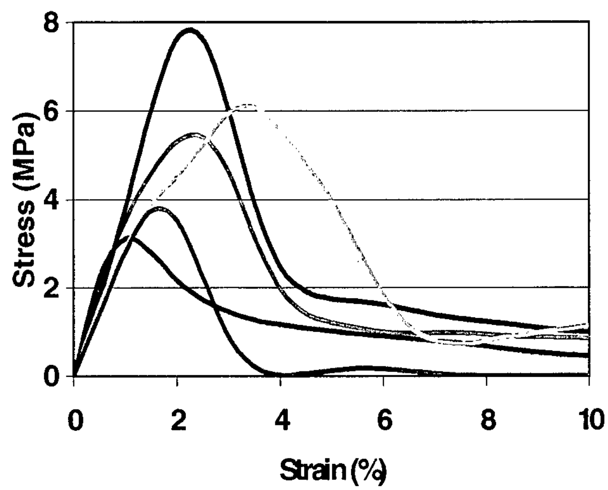


Figure 4. Response of Comp-B at 100 s^{-1}.

These curves were very representative of all the compressive tests that were performed on either material (TNT or Comp-B) at any rate. The response shown in Figure 4 is very brittle, as shown by the dramatic loss of strength after maximum stress. It is also very weak, indicated by the very low values of maximum stress, as compared to curves of conventional energetic materials (gun propellants) that are routinely tested at the U.S. Army Research Laboratory (ARL) [3]. Because the response is severely brittle, there is significant scatter in the maximum stress values, and the curve shapes show significant deviation from each other with some curves (none shown here) displaying double stress peaks, indicating significant local failure before general brittle failure. Curves such as these indicate very brittle response and great likelihood of material failure in very low-level stress environments. However, attempts were made to characterize the response from these curves by averaging the values for the modulus and failure modulus at each strain rate, which indicate the material resistance to deformation and its fracture susceptibility. These two quantities were calculated for each curve and averaged. These averages and scatter are indicated in Figure 5. The maximum stress, the stress at failure, and the associated strains were not averaged because of the wide scatter in the measured results. From these plots, the indication is that brittle fracture occurs at all strain rates. Figure 6 shows the specimens after uniaxial compression.

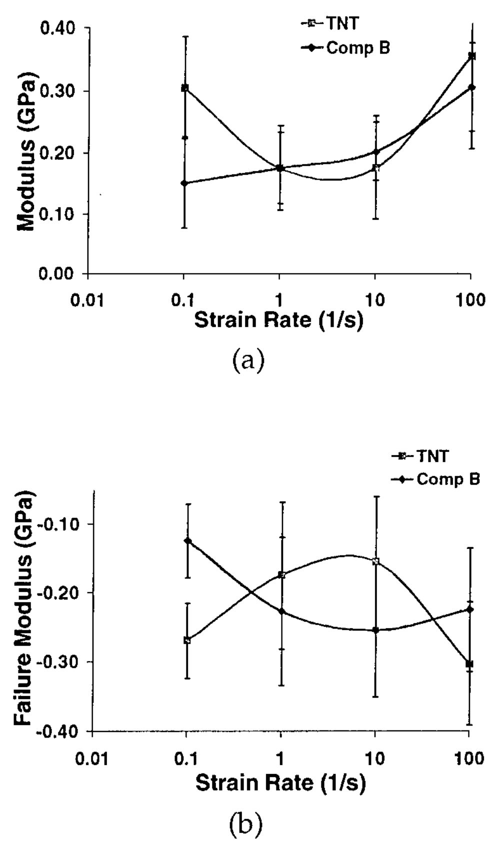


Figure 5. Average values for TNT and Comp-B.

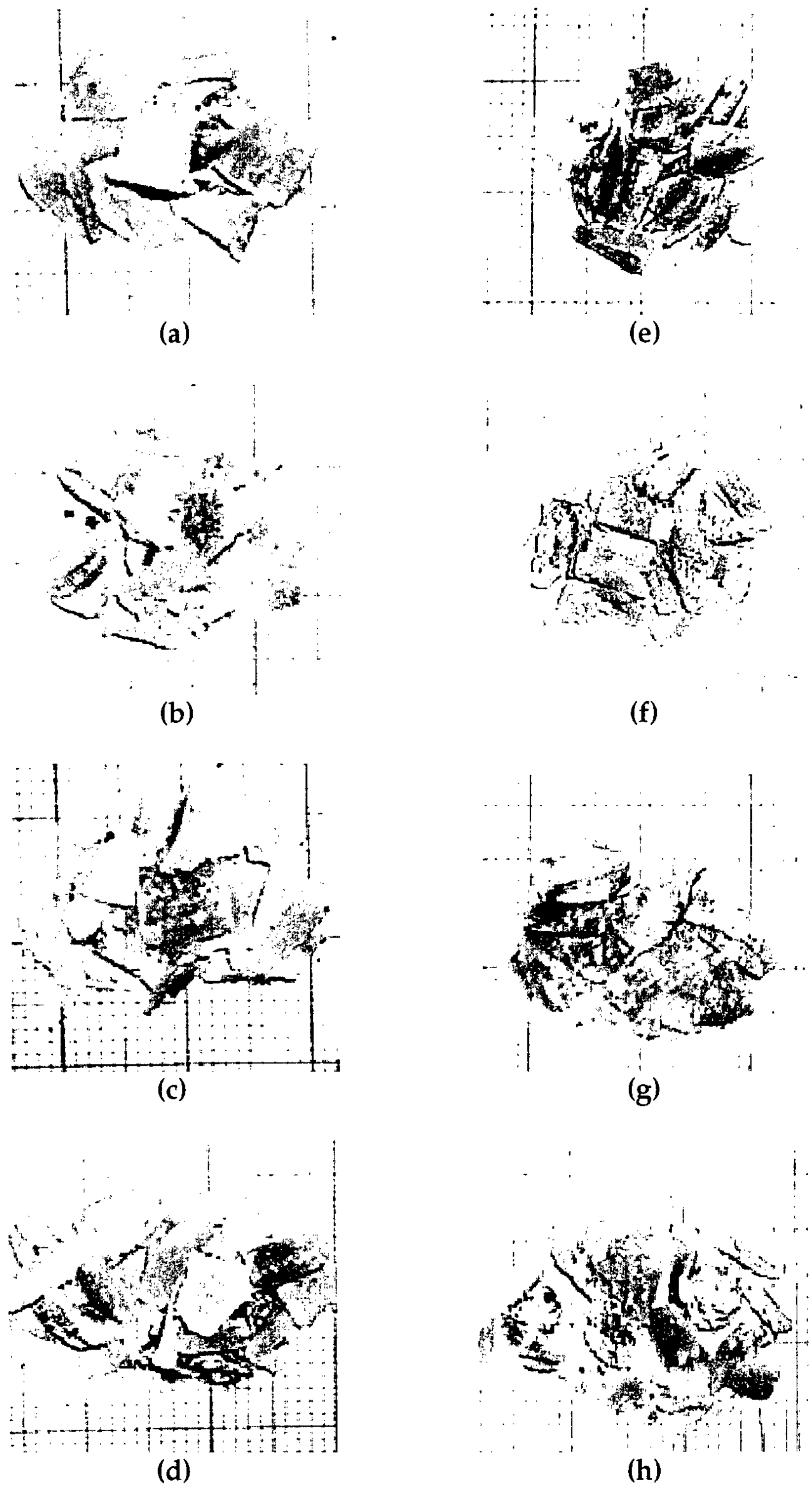
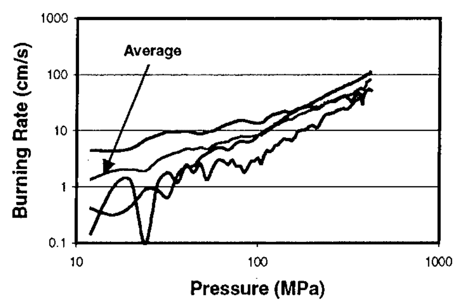


Figure 6. Tested specimens of TNT and Comp-B.

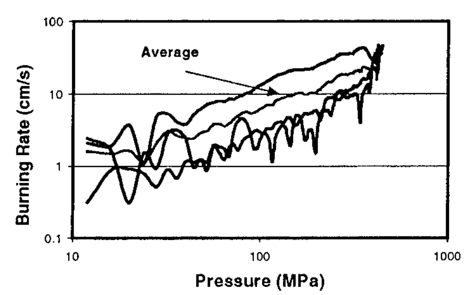
3.2 Closed-Bomb Firings

The closed-bomb portion of the experimental procedure posed quite a problem. Previous attempts to characterize the burning of TNT and Comp-B [6, 7] were met with very limited success. Conclusions from these references state that TNT and Comp-B both demonstrate "in-depth" burning. TNT seems to break up during the burning process and spew particles of various sizes into the combustion zone. Comp-B reportedly burns on the surface, as normal gun propellants are assumed to do, but transitions to an in-depth process at some pressure. These burning characteristics do not provide encouragement to analysts using these methods, which have been shown to provide invaluable insight into gun propellant-fracture analysis. However, the attempt to determine the burning rates was made using the procedure outlined in section 1. The results for the individual tests are shown in Figure 7. Note the large differences in slope and magnitude observed for some of the curves, and the fluctuations found in the low-pressure portion of the curves. The average values of these curves (shown on the plots) were used in the surface area analysis of the damaged grains.



TNT

(a)

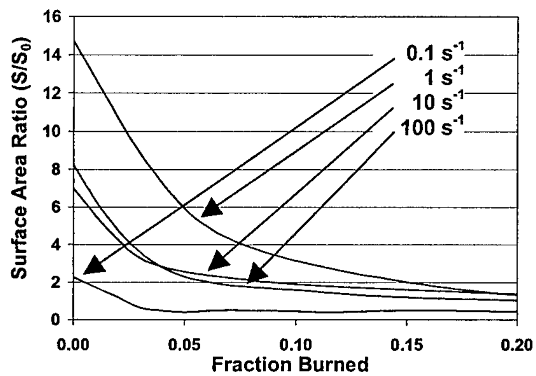


Comp-B

(b)

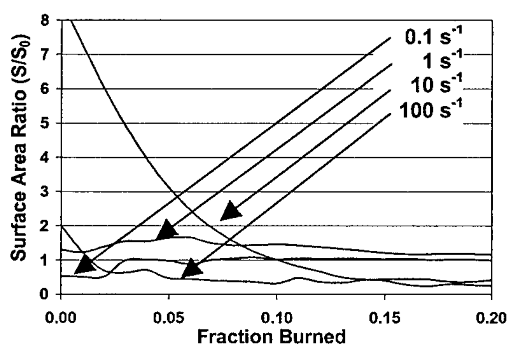
Figure 7. Individual and average burning rate curves.

The surface area reductions are shown in Figure 8. The values of S/S_0 at fraction-burned values of zero are extrapolated from the trend as the fraction burned approaches zero. The first value of surface area is calculated for fraction-burned values beginning from 2-3%, based on the assumptions used in BRLCB. This feature of the output program requires an estimate of the initial surface area since the initial area is assumed to be the undamaged area of the specimen with its original dimensions.



TNT

(a)



Comp-B

(b)

Figure 8. Surface area profiles (surface area ratio vs. fraction burned).

4. Analysis

4.1 Mechanical Response

The overall mechanical response of the materials is very brittle, as mentioned previously. The brittleness was compounded by the very low strength of the material. Rarely did the failure strength exceed 10 MPa. The failure strain was also very low, not exceeding 5%. However, some minor trends were observed in the response of the specimens.

Comp-B tended to show increased modulus values with increased strain rate, while the failure modulus decreased at increasing strain rate. The exception to this was at the highest strain rate, where the failure modulus becomes less negative (see Figure 5). A greater negative value for the failure modulus indicates a more brittle response. Therefore, this trend of parameters indicates that for Comp-B, as strain rate increases the material becomes more brittle until the strain rate approaches 100 s^{-1}. At that point, a slight strengthening occurs that may be reflected in reduced surface area production upon failure. However, the nature of the materials is still very brittle, as is the case whenever the failure modulus has the same magnitude as the modulus. Therefore, any effect of reduced brittleness may be lost in the overall brittle nature of the material. This is especially true considering the scatter observed in the magnitude of the calculated parameters.

TNT showed the same overall brittleness, but demonstrated a different trend. The magnitude of the failure modulus and the modulus seemed to match at each strain rate, i.e., higher modulus values were matched with higher brittleness. This would predict that maximum fracture occurred at maximum stiffness, a trend that indicates a simple relationship. Again, the scatter in the individual measurements is large, so this trend may not be obviously reflected.

These trends were minor and did not affect fracture significantly. In fact, the deduced surface area measurements do not strongly reflect any of these mechanical response observations, as will be discussed.

4.2 Closed-Bomb Firings

It should be noted that in order for the burning rates to have good physical meaning, the assumptions made in the analysis program BRLCB must be met. The key assumptions of the data reduction code are the following:

- The igniter material is completely consumed before the energetic materials begin to burn.

- The material begins to burn with all exposed surfaces ignited.
- The mass generation (of gas) is a result of combustion from surface phenomena (no in-depth burning or particle spewing into the flame).

No gun propellant or any other material follows these rules strictly. Deviations from these assumptions include residual igniter material that burns while the energetic material begins to burn, flame spreading, burning irregularities, and mechanical damage. However, the closer the material being burned comes to abiding by these assumptions, the closer the results reflect valid analysis. Some indications that these assumptions were not closely abided in this series include:

- Significant variation in burning rate at low pressure. This indicates that nonuniform, incomplete, or unstable combustion was occurring on the exposed surfaces. (These effects may also be responsible for initial S/S_0 values of less than one.)
- Significant variation in burning rate levels at the same pressure. This indicates that different burning processes may have been occurring at various pressures during combustion (i.e., in-depth combustion or deconsolidation of the surface).
- Different slopes for curves at the same pressure. This may indicate an unstable transition in combustion processes (e.g., going from a process that is primarily surface combustion to another, such as an in-depth process).
- Multiple peaks in the pressure-time plot. Several closed-bomb runs had to be discarded because a low-pressure peak was followed by renewed burning and a second peak, which indicated that the specimens had burned unevenly (e.g., some grains were significantly consumed before others were fully ignited).

While all combustion processes are different and occur in various combinations, the degree of deviation from the assumptions is usually manageably small. With these results, the degree of adherence is difficult to determine without more extensive testing.

The surface area profiles (Figure 8) show additional surface area present in almost all cases. Figure 9 shows the regressive profile of the undamaged specimens. The profile starts at one and gradually decreases as the specimen is consumed. Near the end, it rapidly goes to zero. Although the damaged specimen profiles show additional surface area produced during the burning, the predictions based on mechanical properties are not reflected in the TNT profiles. The lowest and highest strain rates should produce the most surface area (Figure 5b), but the profile suggests that the order jumps from low at low rate to high at the next level, and then produces the same profile at 10 s^{-1} and 100 s^{-1}. Comp-B profiles (Figure 8) show a similar difference. Mechanical properties indicate a steady increase in surface area with strain rate, with a leveling at the higher rates. The measured profiles show a steady increase up to 10 s^{-1}, but then

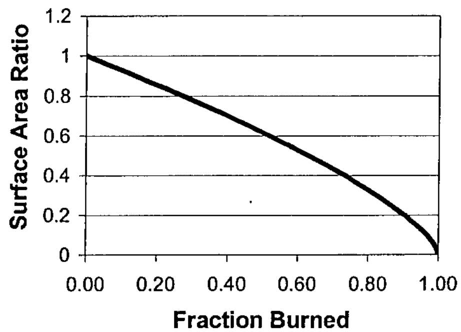


Figure 9. Surface area profile of solid right circular cylindrical specimens.

the surface area generation is dramatically lowered at 100 s^{-1}. This mismatch between mechanical properties prediction and observed results allows reflection on the influence of the irregular burning observations noted earlier.

4.3 The Modeling Effort

A comprehensive theoretical foundation for modeling damage, reaction, and the coupling between these two quantities in energetic materials has been developed. Under this formulation, Matheson's tensile distension and damage (TDD) model [8] is used to drive both the viscous-elastic-plastic (VEP) model [9] and an extended version of the multiphase burn (MPB) model of Baer and Nunziato [10]. Although reaction is not expected, these models may be applicable to the description of material damage produced in the servohydraulic tester. It is notable, however, that damage due to shear is not included in TDD. The degree of damage (which varies from zero to some value near unity) represents additional surface area that is available to support reaction.

The models have been implemented in a developmental version of Sandia National Laboratory's CTH software [11], but have not yet been calibrated for application to a wide variety of energetic materials. We have exercised CTH in a simulation of the nonreactive response of a sample in the servohydraulic tester. In order to obtain a significant amount of strain in a short period of time, we chose a strain rate of 200 s^{-1}. We ran the simulation for 250 µs to achieve a maximum nominal strain of 5%. The model calibrations that we used were supplied by Sandia with the developmental code, and the response of the associated material may not be representative of that of TNT or Comp-B. In spite of this, the results are informative. Shown in Figure 10 are plots of damage (on the right) and displacement of the material (on the left) at 50-µs intervals, corresponding to 1% intervals in overall strain. The ram is at the top of the plots and the anvil at the bottom. These show that damage initially appears at the top and, to a lesser extent, bottom of the sample. Through the first 150 µs, damage propagates through the upper quarter of the sample at a moderate pace. During

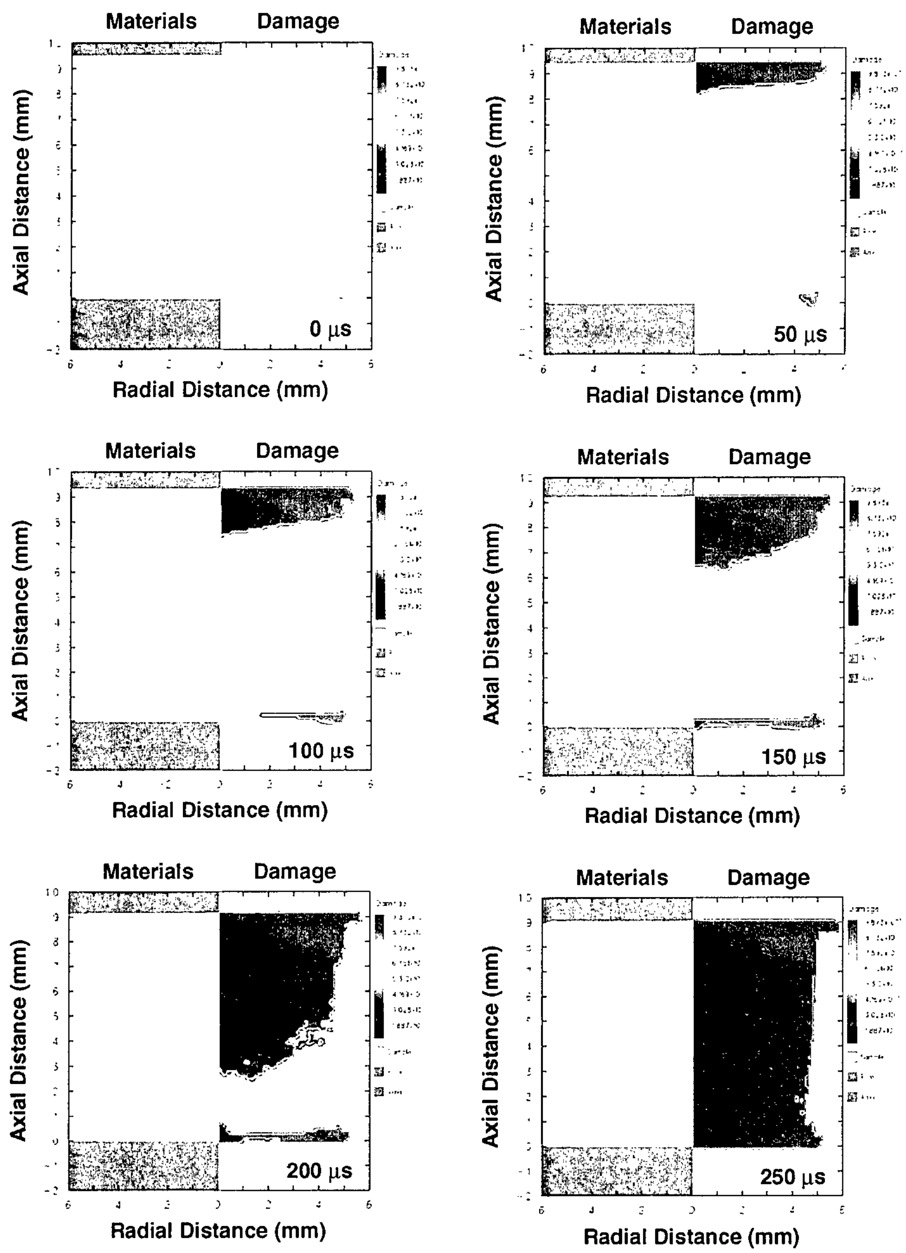


Figure 10. Plots of damage (right) and material deformation (left) at 50-μs (1%) intervals.

the last 100 μs, damage propagates at an accelerated pace through the rest of the sample. The highest damage level is found in the region adjacent to the ram and, to a lesser extent, the anvil. Levels of damage in other regions are nearly as high. Regions of low or moderate damage are extremely limited. These predictions reflect the actual damage observed, as shown in Figure 6.

5. Conclusions

The mechanical response of TNT and Comp-B was measured over four decades of strain rate. The response of both high explosive formulations was very brittle and weak, compared to gun propellants measured under similar conditions within ARL. The failure modulus, a measure of the fracture susceptibility, was about the same magnitude as the modulus of the material. In previous measurements, if an energetic material had a failure modulus one-tenth the magnitude of the modulus, the material was considered very brittle and unsuited for use in gun firings. However, the conditions under which gun propellant is used are much different from that of high explosive materials, and the criteria for acceptable use must be independently established. The strength of the high explosive material was also about one tenth of the conventional gun propellants. This implied that the high explosive would fail in a brittle fashion under a relatively low stress environment.

In an attempt to measure the degree by which the fracture damage produced the fracture-generated surface area, a technique was employed that established a correlation between a mechanical failure parameter (the failure modulus) and the amount of surface area generated under uniaxial compression. In this technique, the material damaged under the well-defined uniaxial load was burned in a small closed vessel. The rate of pressurization was analyzed using the closed-bomb code BRLCB and established burning rates for undamaged material, and surface area was extracted. In a successful procedure, a correlation is established between the failure response and the surface area generated.

In this series of tests, the extreme brittleness of the TNT and Comp-B produced mechanical characterization parameters that varied widely under similar test conditions. In addition, burning the high explosive material in the closed vessel proved erratic. The material was difficult to ignite (there were some successful ignitions of the primer without subsequent combustion of the high explosive), and it seemed to burn differently from one experiment to the next under similar ignition conditions. This may be due to deconsolidation during combustion or in-depth burning reported by others, but the effect of the exposed fracture generated surface area on the pressurization was diminished by these burning characteristics.

It was determined, however, that TNT and Comp-B are very brittle and are reduced to rubble after about 5% compression, regardless of the rate of deformation. The actual increase in exposed surface area is unknown, although measured values for increase in initial surface area are over ten times the initial undamaged value. However, it seems as though ignition difficulty would serve to reduce the calculated surface area value, while any deconsolidation during combustion would tend to amplify that value. The difficulty is gauging by how much each process affects the mass generation of the combustion material.

One strongly positive result is the model that was established. It predicted the mechanical behavior of the materials very well and characterized the failure. By examining the shards in Figure 6 and the predicted damage in Figure 10, it is clear that the model shows the extent and type of damage observed in these experiments. The mechanical response has been shown to be very brittle over a wide range of strain rates, and the mechanical properties do not seem to vary widely in this strain rate domain. Further development of this model to incorporate the combustion phase promises to offer additional insights into the behavior of the material under operational and threat conditions.

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Fracture damage was introduced into trinitrotoluene (TNT) and Composition-B (Comp-B) through uniaxial compression applied at controlled strain rates from 0.1 to 100 s^{-1}. The mechanical response was measured with parameters that have been used to characterize the fracture response of gun propellant during its development over the last decade. The damaged high explosive was burned in a small closed bomb in an effort to characterize the fracture surface area that resulted from the uniaxial compression. However, the brittle nature of both the TNT and Comp-B, and the burning character of these materials prevented a completely successful characterization and correlation with the mechanical response. The brittle mechanical response produced wide scatter in the measured parameters, and the apparently erratic burning behavior of the TNT and Comp-B prevented accurate surface area determination from the damaged high explosive. There were some trends that were noted for the mechanical response as a function of strain rate, and an idea of the nature of the fracture damage was attained. However, the roles that fracture play in the violence of the response of high explosive materials to impact and combustion threats remains unclear.

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