

Benchtop energetics: Detection of hyperthermal species

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BENCHTOP ENERGETICS: DETECTION OF HYPERTHERMAL SPECIES

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Abstract. We present a novel scheme for monitoring the transition between deflagration and “detonation-like” behavior of small-scale explosive samples subjected to shock stimuli. The intended geometry for this setup incorporates a laser-driven-flyer impact technique to generate a pure mechanical input. However, we report results here using a simplified geometry for purposes of evaluating the time-of-flight mass spectrometric (TOFMS) diagnostics using direct laser ablation of solid aluminum and of an aluminum mirror coated with a small amount (~1 μg) of PETN. This manuscript presents the TOFMS detection of fast aluminum atoms (>10 km/s) resulting from laser ablation, confirming our ability to detect hyperthermal species. Preliminary results from pentaerythritol tetranitrate (PETN) experiments reveal a transition from species consistent with deflagration (primarily NO_2) at low laser fluence, to those consistent with detonation-like events (N_2 , CO , CO_2) at higher laser fluence. At this time, due to several unknown parameters in the current setup, we will not posit the exact physical details which cause this transition (e.g. shock pressures, temperatures, etc.). However, these results indicate that such a transition can be detected using the Benchtop Energetics TOFMS diagnostics setup, where future, more controlled and/or characterized energetic events may lead to better understanding of initiation/ignition thresholds of candidate materials.

Keywords: Detonation, deflagration, TOFMS, laser ablation, laser initiation

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INTRODUCTION

Over the past half-century, a number of research groups have pioneered investigations involving ever-decreasing sample sizes, motivated by the inherent limitations of large-scale testing, and interest in exploring fundamental detonation phenomena and practical applications at smaller scales [1]. Traditional large-scale explosive testing relies primarily on mechanical, electronic, photographic, interferometric, and radiographic techniques [2] which yield little or no direct “chemical” information, e.g.: temperatures, molecular species identities and abundances or reaction pathways. Furthermore, large-scale testing logistically limits the number of energetic

events possible in a reasonable amount of time. Small-scale (< g) explosives testing enables working in a controlled laboratory environment, with lower hazard exposures for delicate equipment and personnel, and as sample sizes are decreased, tens to hundreds of events within a single day or even minutes become feasible.

The approach presented herein utilizes ~ μg scale samples initiated in vacuum, allowing us to measure directly the product chemical identities and abundances *via* time-of-flight mass spectrometry (TOFMS), and thus to determine the extent of reaction achieved for a given sample configuration and ignition stimulus. Deflagration of simple organic explosives in vacuum should produce slow reaction *intermediates*, as expansion

into vacuum would quench the reaction. In contrast detonation-like events (not necessarily achieving steady-state) are expected to produce *final products* (e.g. PETN final products being H_2O , N_2 , CO , CO_2) [3] as the high temperature and pressure conditions allow reactions to proceed to completion prior to expansion, and for products to be accelerated to hyperthermal speeds -- as has been observed when a detonation wave reaches an explosive-vacuum interface [4]. Thus, we propose to exploit these differences in product chemical identities and velocities to provide a chemically-based diagnostic for distinguishing between deflagration and detonation-like events.

Using a first generation apparatus [5,6] we were able to observe products of in-vacuum deflagration of PETN samples [7] shock initiated by laser-driven flyers [8]. However, we did not observe the hyperthermal final products expected from detonation-like events. The results of these PETN experiments prompted the work presented herein to confirm our ability to detect hyperthermal species, if present.

EXPERIMENTAL PROCEDURE

Experiments are conducted under vacuum (base pressure $\sim 10^{-6}$ torr) and we form a molecular beam of gaseous products originating from an event at the center of the main chamber through a pair of skimmers at the entrance/exit of a differential pumping section, into a third chamber (base pressure $\sim 10^{-8}$ torr) for TOFMS analysis, similar to the LANL Detonation Chemistry Apparatus [9]. Pulsed TOF scans every 20 μs glean time-resolved mass spectra of the arriving products in the molecular beam. The distance from the center of the main chamber to the center of the ionization region is $X = 0.68$ m, which allows us to infer velocity of incoming species by the time resolved spectra.

Laser ablation/ignition was performed using a 1064 nm, 9 ns pulse duration Nd:YAG laser for two different experimental configurations. The first setup is simply a piece of 1-mm-thick 99.9% pure Al, where the laser incident at a 45° angle forms a 1.5 mm x 1.0 mm ellipse and the ablation spot is on a line-of-sight with the skimmers and the TOFMS ionization region. The second setup consists of PETN that has been dissolved in

acetone and drop-wise deposited onto an Al/glass mirror (6-mm-thick soda lime glass with 250-nm-thick Al coating protected by 50-nm-thick SiO) leaving ~ 1 μg of PETN at each sample spot after evaporation of the solvent. A 1.4-mm-diameter laser spot is incident through the glass to the Al-glass interface at 90° , and the opposite side of the Al/SiO/PETN-layered sample is exposed to vacuum. Rastering each coupon through the fixed laser beam using the “nanoshock target array” approach [10] for producing rapid repetitive events, with 4 mm spacing we obtain 187 individual “events” per coupon. A $|B| \approx 1$ mT transverse magnetic field, produced by a stack of rare-earth magnets at the exit of the main chamber, serves to deflect the majority of charged species from the molecular beam.

Ions are created in the TOFMS chamber through 70 eV electron-impact ionization and are extracted vertically from the ion source region at the upper voltage limit of the instrument (3800 V) to minimize flight times and thus horizontal drift in the flight tube. A bias voltage, V_{XY} can be applied to the “upstream” deflection plate serving to steer the ions onto the 40-mm-diameter MCP detector. Ions produced from background neutrals (e.g. $\langle v \rangle = 0$) require a small repulsive “kick” ($V_{XY} > 0$) to impact the MCP due to the “downstream” offset of the detector from the ionization region. Conversely, ions produced from fast neutrals in the molecular beam require an attractive negative bias ($V_{XY} < 0$) to reduce their transverse momentum.

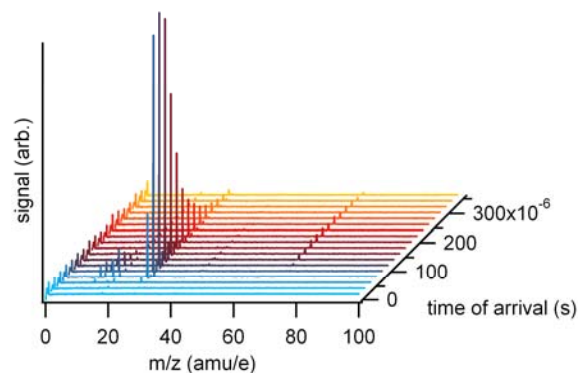


Figure 1. Aluminum ablation TOFMS data plotted vs. ion m/z , for $V_{XY} = -100$ V. The data have been transformed from TOF to mass and are shown binned into a histogram of signal vs. ion m/z at a resolution of 0.1 amu/e.

RESULTS AND DISCUSSION

Fig. 1 shows representative data from aluminum ablation experiments using a laser energy of 20 mJ. The deflection voltage in this representative case is $V_{XY} = -100$ V which decelerates the ions and provides optimum detection efficiency near the peak of the Al atom time-of-arrival distribution.

A “slice” through Fig. 1 at the 27 amu/e peak along the t_{TOA} direction represents the time-ordered arrival of Al atoms at the ionization region; such cuts are shown in Fig. 2 (top) for three different values of V_{XY} . The inset shows the first statistically significant Al^+ signal above baseline (95 % confidence), appearing at $t_{TOA} = 42.7$ μs , corresponding to $v_{neutral} = 15.9$ km/s. Below is a contour plot of the integrated Al^+ peak intensities plotted vs. both V_{XY} and t_{TOA} , illustrating the dependence of the measured Al^+ signal on the ion deflection voltage, V_{XY} . The signals for the slowest species are maximized for small repulsive values of V_{XY} , whereas efficient detection of the fastest species requires large attractive values of V_{XY} . The sensitivity of the TOFMS is preferential to slow-moving species due to velocity-dependent ionization (having an inverse relationship) and the horizontal drift within the flight tube, which cannot be entirely overcome by adjustments to V_{XY} . Corrections to the data are suggested in ref. [11].

In the case of the second experimental configuration (PETN experiments) we observe a threshold for detection of gaseous products at laser energies of about 20 mJ/pulse ($\sim 10^{12}$ W/m²). Some representative results of PETN experiments are shown in Fig. 3 where three prominent mass signals (amu/e = 28, 44, and 46) vs. t_{TOA} are shown for a single V_{XY} (-200V) and two laser energy conditions. A transition is apparent between products consistent with deflagration (primarily NO_2 which we assign to the $m/z=46$ peak) at low laser fluence, to those consistent with detonation-like events (N_2/CO and CO_2 for $m/z = 28$ and 44) at higher laser fluence. At this time, due to several unknown parameters in the current setup such as PETN morphology/density, as well as the extent of laser interaction with the sample, we will not posit the exact physical details which cause this transition (e.g. shock pressures, temperatures, etc.). However, these results indicate that such a

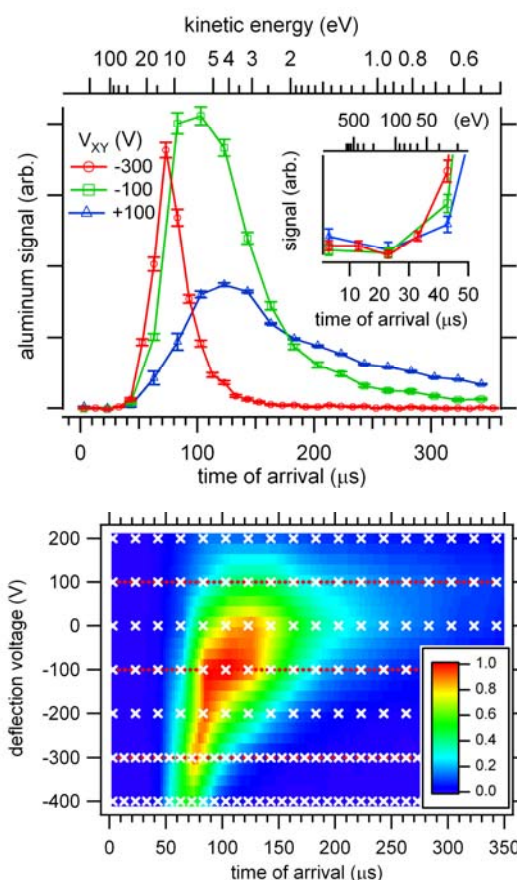


Figure 2. Al atom time-of-arrival signals, i.e. Al^+ peak integrated intensities vs. t_{TOA} , as measured for $V_{XY} = -300$, -100 and $+100$ V (top) and as represented on a contour plot for $-400 < V_{XY} < +200$ V (bottom). White x's denote the actual data and red dotted lines represent the slices displayed in the top figure (integral over a 0.75-amu/e-wide bin centered on $m/z = 27$ amu/e, averaged over 50 ablation events). The error bars represent the standard error of the means ($SE = \sigma / \sqrt{50}$).

transition can be detected using this setup, where more controlled and/or characterized energetic events may lead to a better understanding of initiation/ignition thresholds of candidate materials.

We note that experiments conducted with direct laser irradiation of the vacuum-exposed PETN rather than through the glass yielded no discernable peaks above baseline at comparable laser energies. It is hypothesized that excessive ionization of the PETN products precluded the detection of the products, as ionic species are

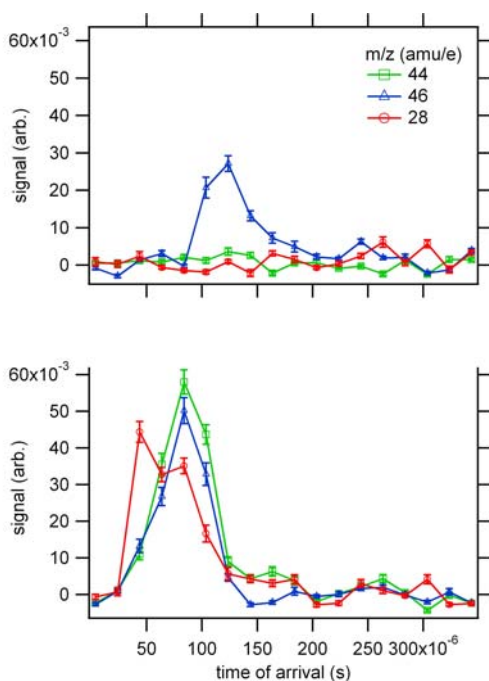


Figure 3. Integrated intensities for peaks at $m/z=28$, 44, and 46 amu/e vs. t_{TOA} ($V_{\text{XY}} = -200$ V) for a laser energy of 20 mJ (top) and 150 mJ (bottom). (Integral is over a 0.75-amu/e-wide bin centered on m/z , averaged over 10 events. Error bars: standard error of mean.)

deflected from the molecular beam prior to arrival at the TOFMS detection region.

CONCLUSIONS

We report results using an improved configuration of the Benchtop Energetics apparatus capable of detecting hyperthermal products. The laser-driven-flyer technique was temporarily abandoned in lieu of a simple method of creating fast species via direct laser ablation. Laser ablated aluminum atoms and the resulting mass spectra were presented to show the ability to detect hyperthermal velocity species and present the dependence on various instrument parameters. Finally, we presented observation of hyperthermal PETN products consistent with both deflagration and detonation-like events using direct laser irradiation of aluminum in physical contact with the energetic sample. While the mechanism of this type of initiation is complex we conclude that this

apparatus is capable of detecting such a transition by direct observation of product species.

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