SAND2016-12830C

Growth to detonation in hexanitrostilbene (HNS)

Joseph Olles, Ryan R. Wixom, Robert Knepper, Alexander S. Tappan, and Cole D. Yarrington,
Sandia National Laboratories, Albuquerque, NM, U.S.A.

Abstract—Explosive properties, such as run-distance or detonation velocity, are typically found using wedge tests or embedded gauges. The growth to detonation and equation of state of an explosive are crucial for predicting performance and parameterizing hydrodynamic simulations. The short distance for growth to detonation in some explosives renders most conventional tests inadequate. By instead using thin vapor-deposited films and initiating with an electrically driven flyer, hexanitrostilbene (HNS) has been observed to grow from an inert shock to full detonation within 100 μm. The plastic flyers (Parylene-C) used to initiate the thin HNS films are driven to a few km/s by exploding a thin metal foil via a high voltage capacitive discharge unit. By varying the size of the flyer and the discharged voltage supplied to burst the foil, the impact conditions are modified. To quantify the flight of the flyer, frequency shifted photonic Doppler velocimetry (PDV) is used and analyzed with short-time Fourier transform methods along with other digital filtering schemes. The measured impact and shock durations correlate well to shock physics simulations.

Keywords—hexanitrostilbene, HNS, energetics, vapor deposition, flyer, growth to detonation.

I. Introduction

TO simulate the run up to detonation in explosives, reactive burn models are used in hydrocodes. The burn model is typically calibrated to experimental data in order to properly capture the transition from a shocked state to a detonation. In the past the growth to detonation of explosives has been measured using wedge tests, or embedded gauges [1] . These techniques are often impractical for certain explosives, such as HNS, where the run distance is of the same order as a typical embedded gauge thickness. Recently, it has been shown that certain explosives possess characteristics lending them to be vapor-deposited [2]–[4] . Physical vapor deposition is a process capable of producing sub-millimeter explosive samples with precise control of thickness. The HNS films used in this work were deposited on substrates using a custom high-vacuum deposition system.

Using thin vapor-deposited HNS films measuring the growth to detonation becomes realizable. To initiate the HNS films, plastic flyers are driven electrically from a large capacitive discharge unit by bursting an underlying metal foil bridge. Due to the time scales on which the shock-detonation occurs, photonic Doppler velocimetry (PDV) [5] is utilized to measure particle velocity from the explosive shock into a PMMA substrate. By using the measured particle velocity from PDV, and pressure from Rankine-Hugoniot jump conditions of PMMA, parameters of reactive burn models can be tuned empirically.

II. Experimental Setup

To accurately control the thickness of HNS, a custom high-vacuum deposition system is employed. By prescribing the deposition rate, masks, and temperature of the substrate, HNS film density, geometry, and thicknesses are regulated. The HNS is deposited from 30–150 μm, in increments of 30 μm, onto aluminized polymethyl methacrylate (PMMA, Spartech Polycast Poly II MIL-P-5425). An aluminum layer was vapor-deposited nominally at 2 μm thick onto one surface of a cylindrical PMMA substrate. The aluminum coating provides a reflective surface for PDV with minimal attenuation of particle velocity.

To initiate the HNS films the free surface of the films were impacted with electrically driven flyers. Flyers herein were made by vapor-depositing metal foil bridges on an alumina substrate and then coating with Parylene-C. To burst the metal foil a high voltage capacitive discharge unit is used. The flyer velocities at varying discharge voltages are characterized through PDV prior to impacting the HNS.

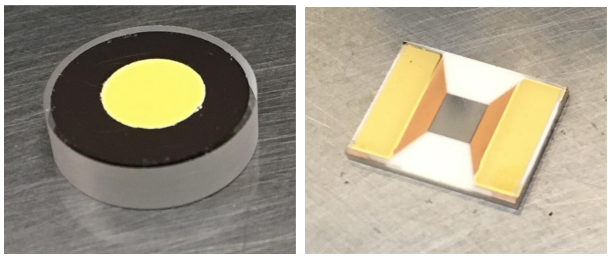

Fig. 1. A representative sample of an HNS vapor deposited film on aluminized PMMA window (left) and a Parylene-C coated chip slapper (right).

For all of these experiments, frequency-shifted PDV (up-shifted to $\sim$6 GHz) is utilized. This is done by using two fiber lasers slightly off frequency from one another near 1550 nm, one send and one reference laser. One single mode collimated gradient-index (GRIN) lens probe, having a 0.5 mm spot size at 15 mm, is used for send and receive light by passing through a circulator. The return and reference light are then combined to create a beat frequency in a 20 GHz fiber optic receiver, then digitized and recorded with an oscilloscope having at least 12 GHz of bandwidth.

PDV is used to record the particle velocity history at the explosive/substrate interface. By varying the flyer impact velocity and deposition thickness, data was captured at states along the build-up to detonation. Figure 2 shows a schematic of the experimental setup used. Analysis of PDV traces was done in MATLAB using a frequency bandpass and short time Fourier transforms (STFT). STFT analysis windows were typically taken to be 1 ns with a 90% overlap on the advancing window.

Manuscript received December 20, 2016.

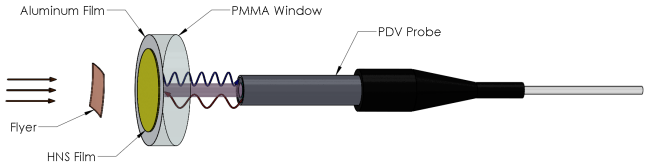

Fig. 2. Schematic of experimental setup. A plastic flyer shown (red) is incoming from the left to impact the HNS film (yellow). The HNS film is shown on a cylindrical PMMA substrate with an aluminum coating on one surface. On the right is a single mode GRIN lens PDV probe, which is sending light and receiving reflected light.

III. Results and Discussion

To ensure that the proper density and grain morphology were used in continuum and mesoscale simulations, HNS film cross-sections were analyzed. An SEM image of an ion polished cross-section of a vapor-deposited HNS film on a PMMA substrate is shown in Figure 3. Through image analysis of grain and pore size, the bulk density of the sample is calculated to be 87% TMD. This cross-section represents a typical sample used in these experiments.

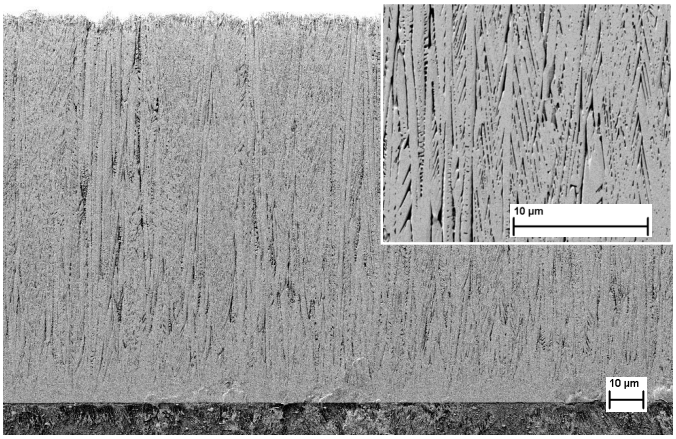

Fig. 3. SEM images of an ion polished cross-section of a vapor-deposited HNS film on a PMMA substrate (shown near the bottom, dark in color). Top of the image shows the HNS free surface. Inset shows a magnified region of the cross-section. Through image analysis of grain and pore size, the bulk density of the sample is calculated to be 87% TMD.

For slow flyer velocities, which do not cause significant reaction to occur in the HNS film, a shock transits and is measured with PDV. An unreacted state is found from 1D CTH [6] simulations using a density functional theory (DFT) based equation of state table for HNS set to 87% TMD with a p-alpha model. This unreacted state is shown as a dashed line in Figure 4. As the flyer impact velocity is increased, the explosive will transition to a partial and then a full detonation. Using the Chapman-Jouguet (C-J) pressure for densified, fully detonating HNS [6], the peak particle velocity in PMMA is expected to be ∼2400 m/s. Figure 4 shows a trend of the peak particle velocity in PMMA as a function of the flyer impact velocity. There is a monotonic rise with each velocity, which follows the predicted line of an unreacted state, then a departure as the flyer impact velocity approaches 3000 m/s. Figure 4 clearly shows that HNS at 120 μm is fully detonating with a flyer impact velocity above 3000 m/s, and at least partial detonation is occuring in films as thin as 60 μm.

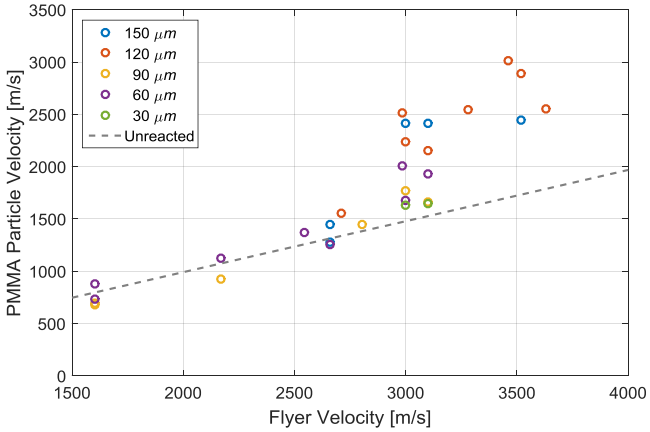

Fig. 4. Measured peak particle velocity versus flyer impact velocity. The dashed line shows the predicted unreacted response obtained from continuum hydrocode simulations. Uncertainty in the flyer impact and the measured peak velocity was calculated to be no more than 50 m/s and 35 m/s [7], respectively.

Interesting behavior is seen with a couple of the measured peak particle velocities, where they indicate pressures that are above the C-J prediction. The fidelity of the PDV diagnostic is below 0.1 ns/point. If the reaction zone takes longer than 0.1 ns to cross the explosive/window interface, it would be possible to measure particle velocities associated with pressures greater than C-J. Our hydrodynamic simulations predict that particle velocities resulting from the von Neumann spike would be ≥3000 m/s. While the von Neumann spike is not likely resolved in these experiments, the data does indicate measured velocities approaching that value.

A peak particle velocity-based calibration for a burn model is able to capture gross effects of the explosive, suitable for continuum simulations; however, for higher fidelity the entire velocity trace is needed. As the explosive builds up to a detonation, a measured velocity trace in time is believed to show an unreacted pulse for a discrete duration followed by an increase in velocity. This pulse will grow until the explosive is fully detonating, and the trace is at or above the velocity associated with the C-J pressure. Figure 5 shows simulated velocity traces of inert HNS films. The inert traces are shown based on a 3000 m/s flyer impact into films of 30–150 μm thick. Figure 6 shows particle velocity traces of 30–150 μm thick HNS films, in 30 μm increments, measured in PMMA. Each film was impacted with a flyer at 3000 m/s (shown with solid lines) and 3100 m/s (shown with dashed lines). These traces are associated with the data points in Figure 4. Simulated velocity traces can be compared with these data to validate equations of state and burn model parameters, or model parameters can be calibrated to match the experimental data [8]–[10].

IV. Conclusion

With the availability of vapor-deposited HNS films, experimental data show build-up to detonation on the micron scale.

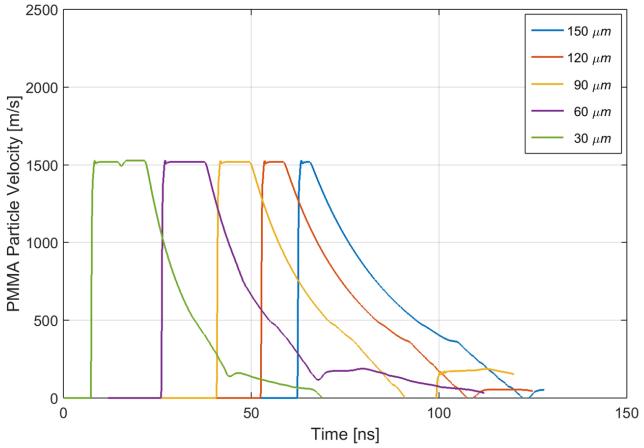

Fig. 5. Simulated particle velocity traces of 30–150 μm thick inert HNS films, in 30 μm increments, in PMMA. Each film was impacted with a flyer at 3000 m/s. These traces are associated with the unreacted line in Figure 4. The traces are time shifted for clarity based on peak particle velocity and film thickness.

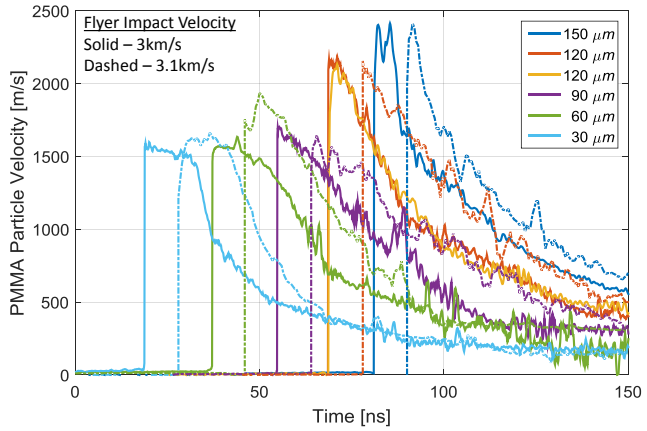

Fig. 6. Particle velocity traces of 30–150 μm thick HNS films, in 30 μm increments, measured in PMMA. Each film was impacted with a flyer at 3000 m/s (shown with solid lines) and 3100 m/s (shown with dashed lines). These traces are associated with the data points in Figure 4. The traces are time shifted for clarity based on peak particle velocity and film thickness.

By using PDV to measure the particle velocity of a reflective PMMA/explosive interface, velocity traces are obtained from a flyer impact initiation. These data should allow for a more accurate calibration of the models used in predictive, reactive flow simulations of HNS-based explosives. Further work will be done in characterizing the flyer geometry at impact and additional data will collected for varying film thicknesses.

Acknowledgment

The authors wish to thank Michael P. Marquez, James Patrick Ball, M. Barry Ritchey, and Matt Zelenok for experimental support. This work was funded in part by the Joint Department of Defense/Department of Energy Munitions Technology Development Program as well as Sandia's Laboratory Directed Research and Development program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

References

[1] Gibbs, T. R., *LASL Explosive Property Data*, Vol. 4., Univ. of California Press, 1980.

[2] Knepper, R., Wixom, R. R., Marquez, M. P., and Tappan, A. S., *Near-Failure Detonation Behavior of Vapor-Deposited Hexanitrostilbene (HNS) Films*, Shock Compression of Condensed Matter, AIP Conf. Proc., 2015.

[3] Knepper, R., Browning, K., Wixom, R. R., Tappan, A. S., Rodriguez, M. A., and Alam, M. K., *Microstructure Evolution during Crystallization of Vapor-Deposited Hexanitroazobenzene Films*, Vol. 37 No. 4, Propellants, Explosives, Pyrotechnics, WILEY-VCH Verlag, 2012.

[4] Knepper, R., Tappan, A. S., Wixom, R. R., and Rodriguez, M. A., *Controlling the microstructure of vapor-deposited pentaerythritol tetranitrate films*, Vol. 26 Iss. 13, Journal of Materials Research, July 2011.

[5] Jensen, B. J., Holtkamp, D. B., Rigg, P. A., and Dolan, D. H., *Accuracy limits and window corrections for photon Doppler velocimetry*, Vol. 101 No. 1, Journal of Applied Physics, 2007.

[6] *CTH Shock Physics*, http://www.sandia.gov/CTH/ 09/14/2015,

[7] Dolan, D. H., *Accuracy and precision in photonic Doppler velocimetry*, Vol. 81 No. 5, Review of Scientific Instruments, AIP Publishing, 2010.

[8] Yarrington, C., Wixom, R. R., and Damm, D. L., *Mesoscale Simulations Using Realistic Microstructure and First Principles Equation of State.*, JANNAF Subcommittee Meeting, Monterey, CA., Dec. 2012.

[9] Damm, D. L., Welle, E. J., and Dudley, E. C., *Characterization of Physical Processes During Thin-Pulse Initiation of Energetic Materials.*, 14th International Detonation Symposium, Coeur d'Alene, ID, Apr. 2010.

[10] Damm, D. L., Yarrington, C., and Wixom, R. R., *Development of a Grain-Scale Model for Initiation of HNS.*, 15th International Detonation Symposium, San Franscisco, CA, July 2014.