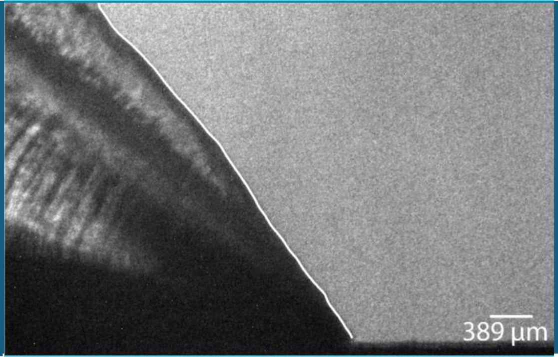
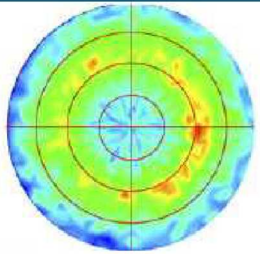
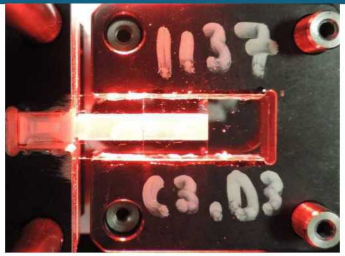
LDRD
Laboratory Directed Research and Development

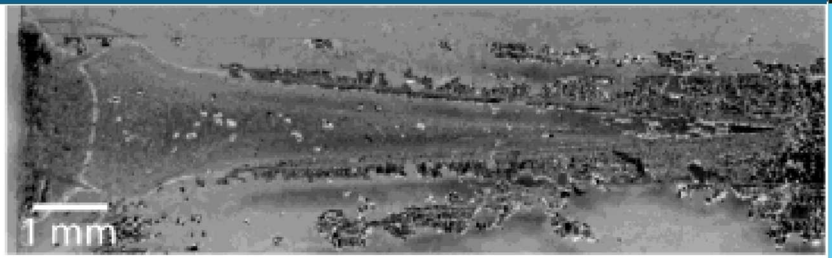
SAND2019-14516C

Functionally Grading Density in Thin Films of Energetic Materials for Detonation Wave Shaping









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PRESENTATION OUTLINE

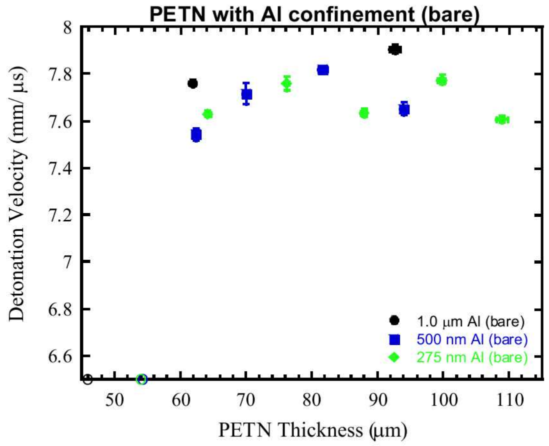
- Introduction and Background
- Experimental Approach
- Results
  - Energetic Film Characterization
    - Optical Microscopy
    - Density
    - SEM
    - XRD
  - Microdetonation Testing and Ultra-Fast Imaging
- Conclusion and Future Work

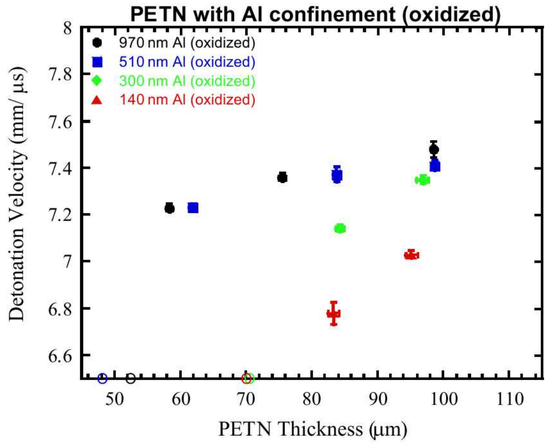
INTRODUCTION: Detonation Velocity Dependence on Density

- Microstructure and morphology of energetic materials play a key role in detonation characteristics such as initiation sensitivity and detonation wave velocity. Tradeoff between:
  - **Density**- dictates detonation velocity and output.
  - **Porosity and grain size**- influence sensitivity.
- Detonation wave velocity in explosive is related to the gradient of Chapman-Jouget (C-J) pressure with respect to specific volume and **unreacted material density**.
- Varying unreacted explosive material density in a single sample would enable localized control of detonation velocity.

$$D = \left[\frac{1}{\rho_0^2}\left(\frac{dP}{d\nu}\right)_{CJ}\right]^{1/2} \approx j + k\rho_0 \quad \text{where}$$

D = detonation velocity (km/s)
ρ_0 = unreacted explosive density (g/cm^3)
(Cooper, *Explosives Engineering*, 1996)

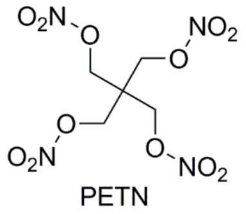




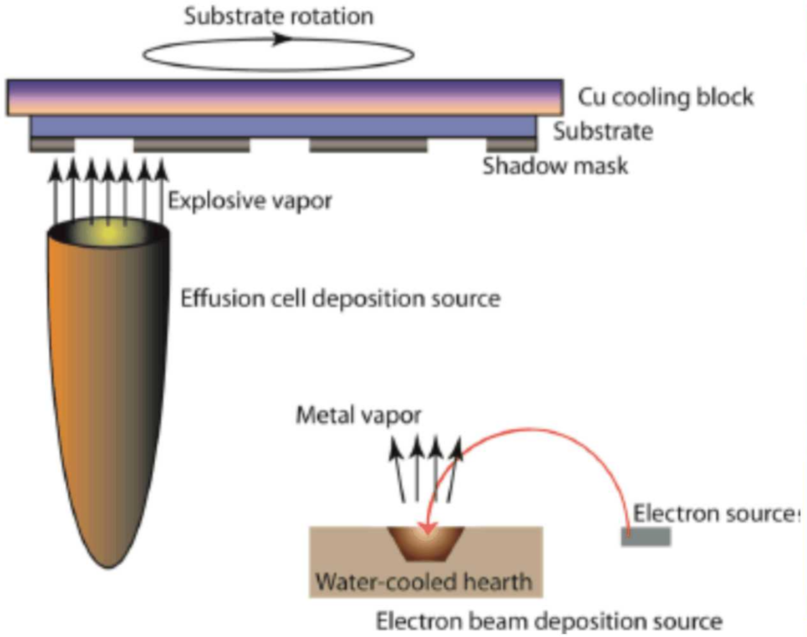
Effect of Density on Detonation Velocity in Pentaerythritol Tetranitrate (PETN). The top case (dense PETN) shows higher velocities than the bottom case (porous PETN). **(Knepper et al., *APS SCCM*, 2018)**

BACKGROUND: Thin-film Deposition of High Explosives

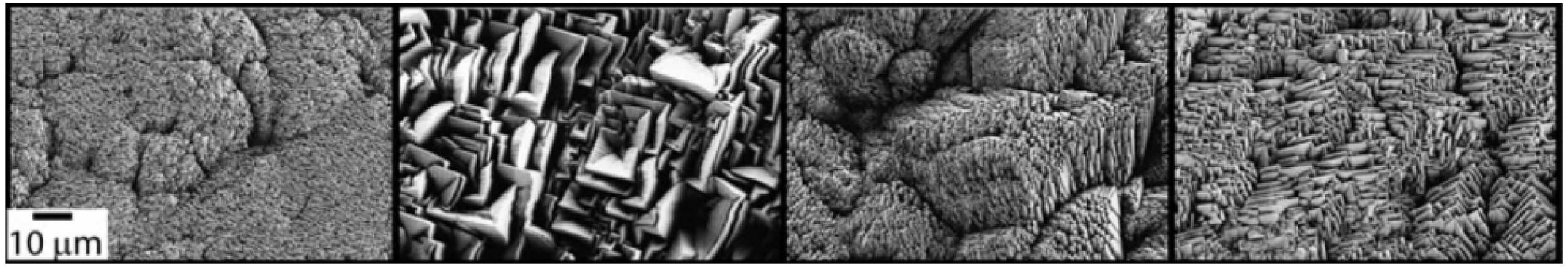
- Physical vapor deposition (PVD) of high explosives has enabled growth of samples for studying detonation phenomena.
- Pentaerythritol tetranitrate (PETN) is a secondary high explosive used in defense and mining.
  - Organic CHNO explosive can be deposited via PVD to create polycrystalline films of varying thickness.
  - Resultant microstructure and morphology largely dependent on deposition conditions and interfacial effects.



- Patterned aluminum deposition on substrates utilized to create localized high and low surface energy regions.
- PETN deposited onto:
  - Polycarbonate, polycarbonate/polyimide, polycarbonate/polyimide/aluminum.
  - PETN film thickness varied from ~10 μm to ~120 μm.



Schematic of the PETN deposition process.
(Knepper et al., *Int. Det. Symp.* 2014)



Variation in microstructure of PETN films due to varying substrate conditions (material and temperature).
(Knepper et al., *J. Mat. Res.*, 2011)

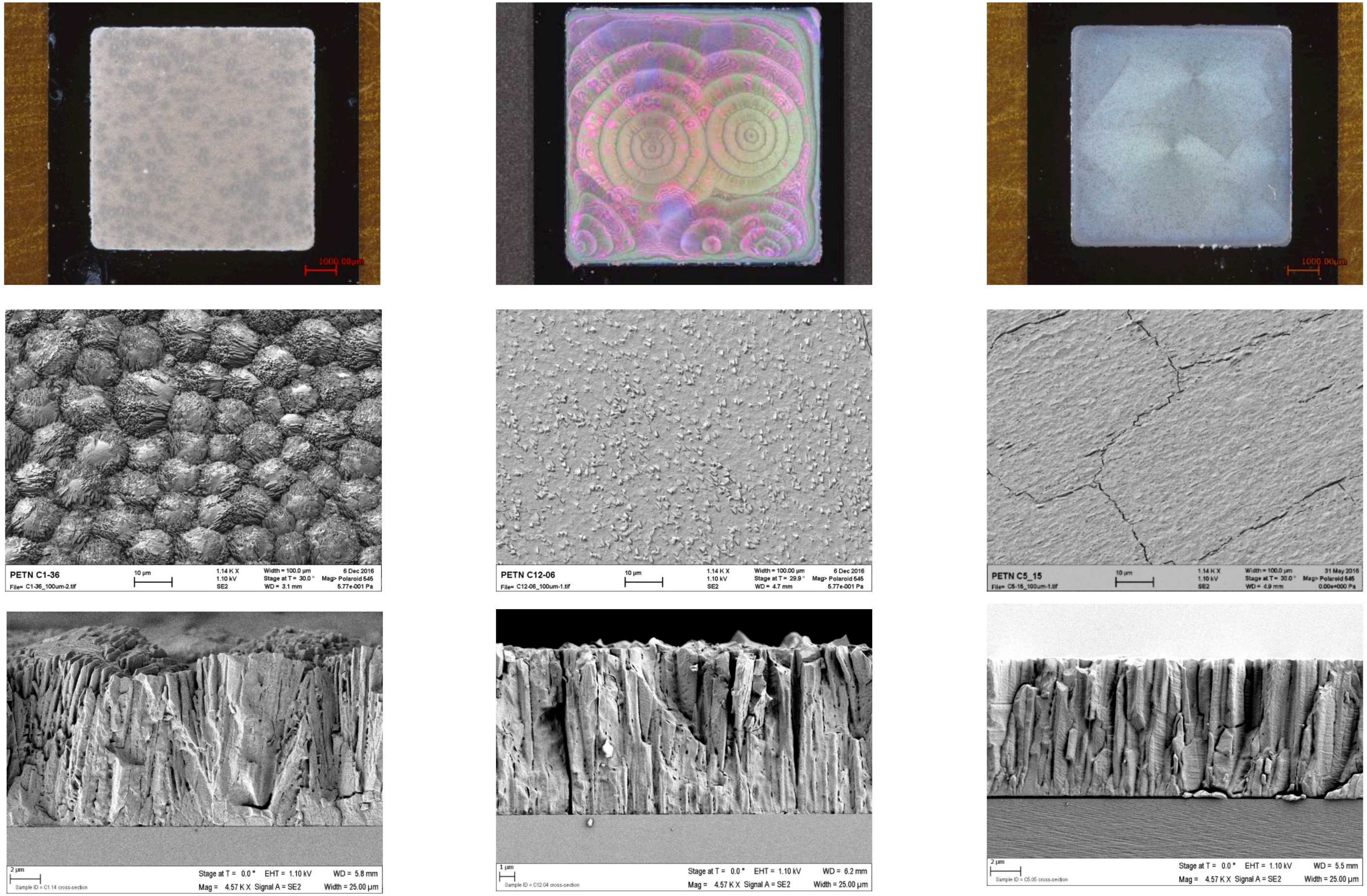
BACKGROUND: Surface Energy Effects on Explosive Films

Low E_s | Medium E_s | High E_s

Optical Microscopy (scale bar 1 mm)

SEM (1.14 kX, scale bar 10 µm)

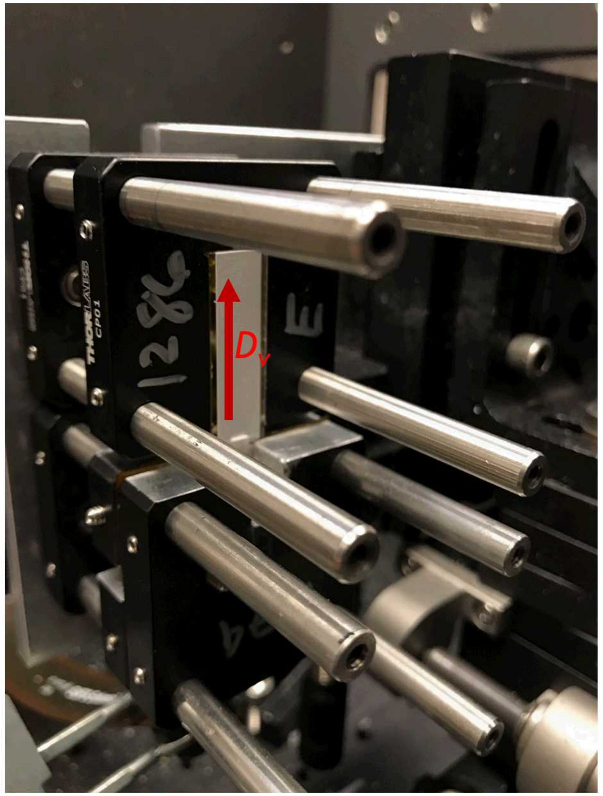
Fracture Cross-section SEM (4.57 kX, scale bar 2 µm, 1 µm, 2 µm)



Optical microscopy (top) and SEM images of surface (middle), and fracture cross-sections (bottom) of PETN films grown via PVD. Changes in morphology are due to interfacial energy alone. **(E. Forrest et al., *APS SCCM 2017*)**

EXPERIMENTAL: Microdetonation Testing

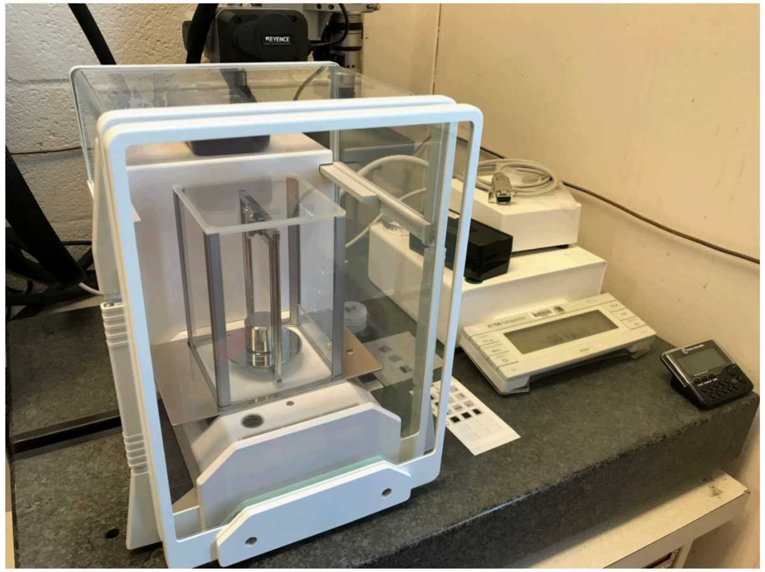
- Utilized existing laboratory-scale microdetonation test setup for conducting explosives testing of PETN samples.
- Ultra-high speed imaging to visualize detonation wave propagation in explosive sample.
  - SIMX-15 ultra-high speed framing camera (Specialised Imaging) used to capture detonation phenomena at frame rates up to 6.45 MHz (1/155 ns).
  - Imaged detonation light to estimate D_v.



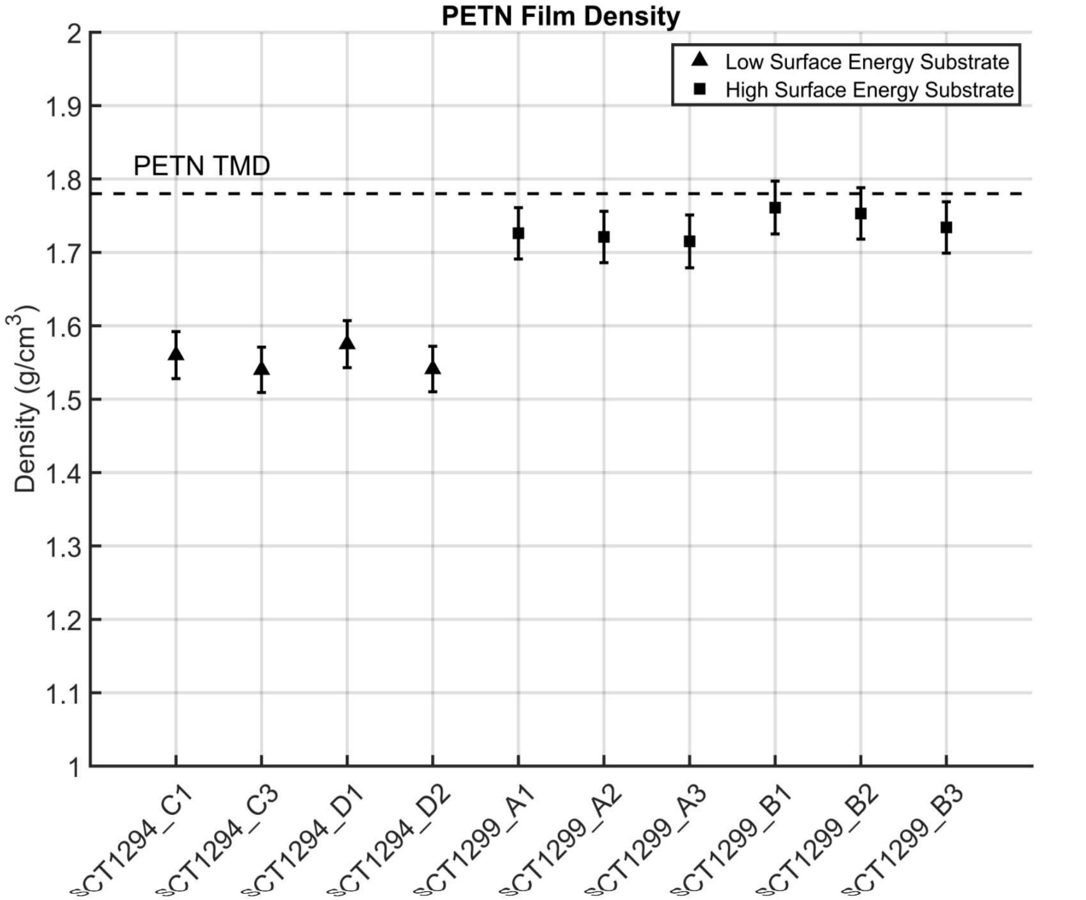
Photograph showing 1 cm × 3 cm sample mounted in fixture. The PETN film is initiated at the bottom and detonation propagates upward.

RESULTS: Film Density Measurement

- Film density measured with precision mass comparator.
  - Mettler Toledo AT106 with ±10 µg uncertainty.
  - *Accurate* measurement of film mass and volume enables resolving differences between low and high density PETN.



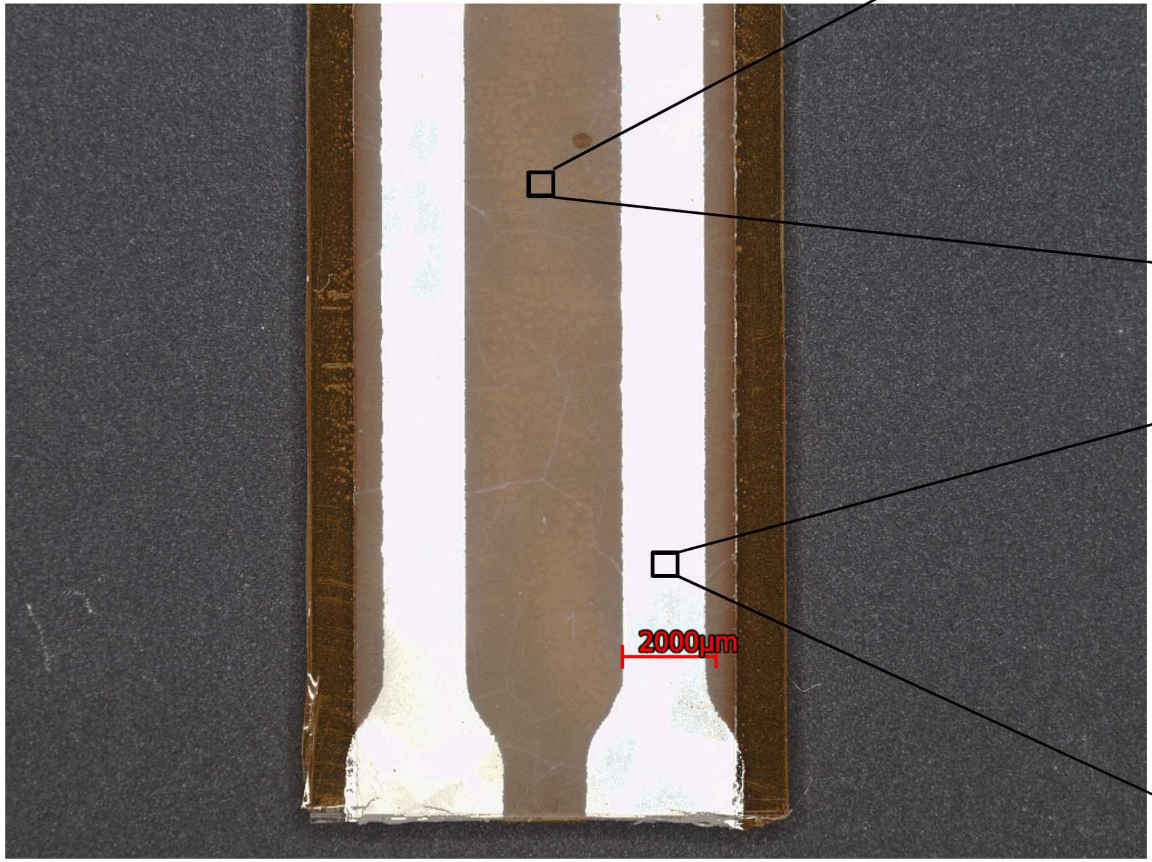
AT106 precision mass comparator (1 µg resolution). Estimated measurement uncertainty is ±10 µg.

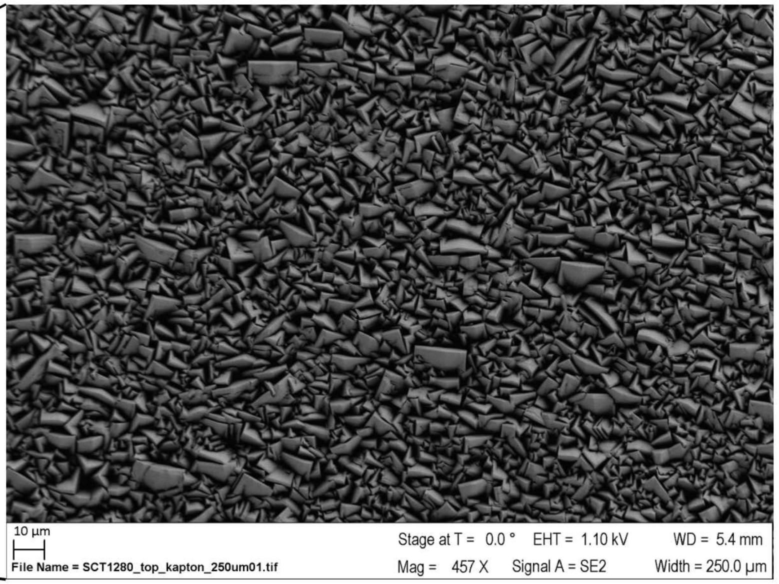


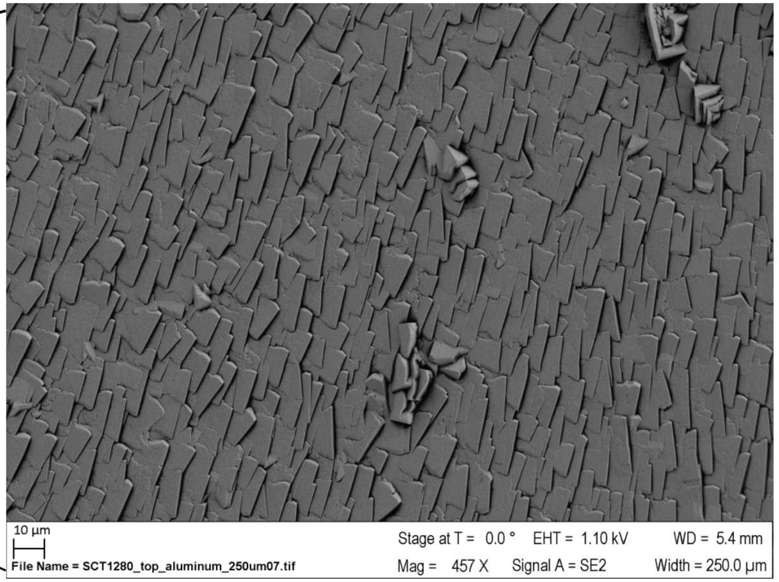
PETN density for ~60 µm-thick films grown on low and high surface energy substrates.

RESULTS: PETN Film Characterization

- Optical microscopy of patterned PETN film (on left) and SEM (on right).

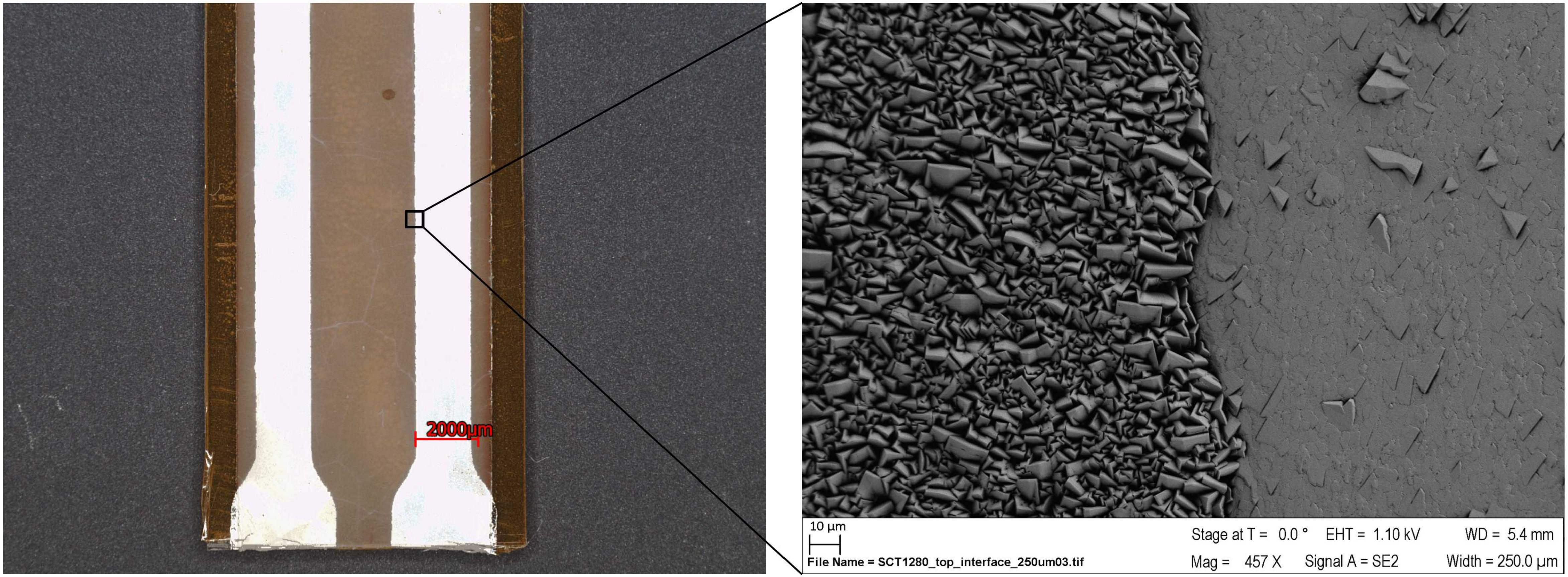






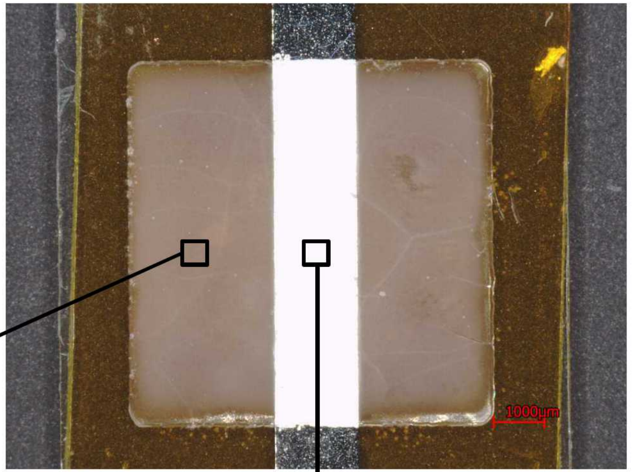
RESULTS: PETN Film Characterization

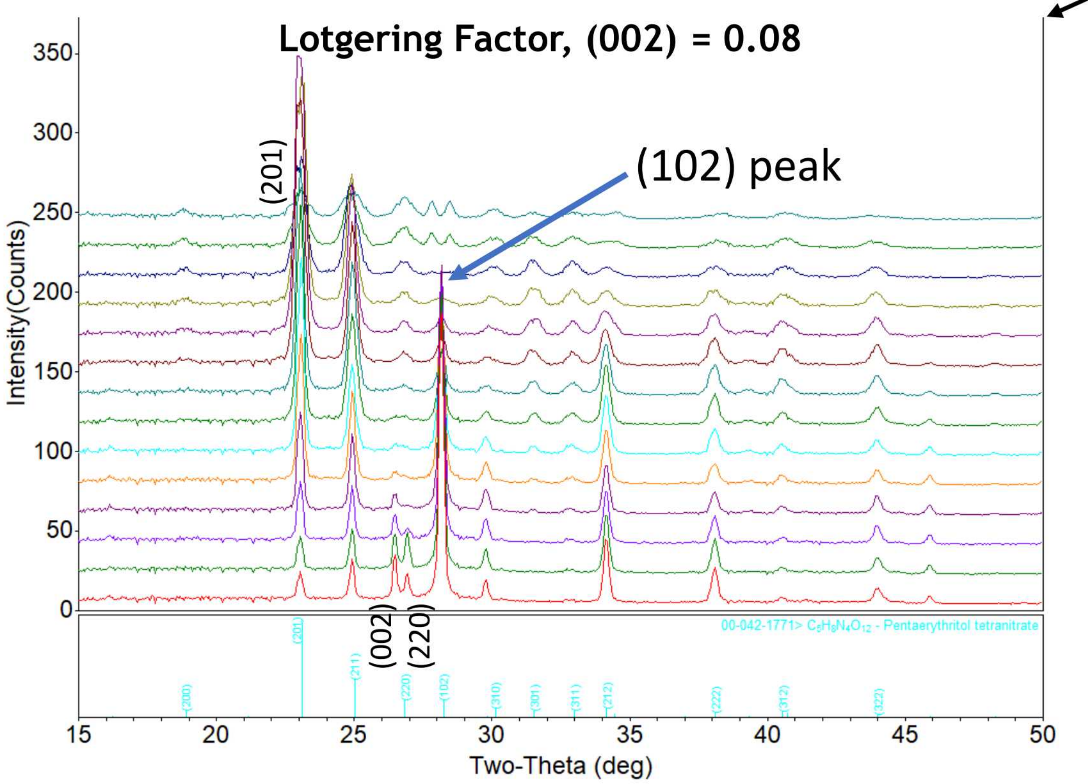
- Patterned high and low density PETN achieved in single deposition via different growth modes.



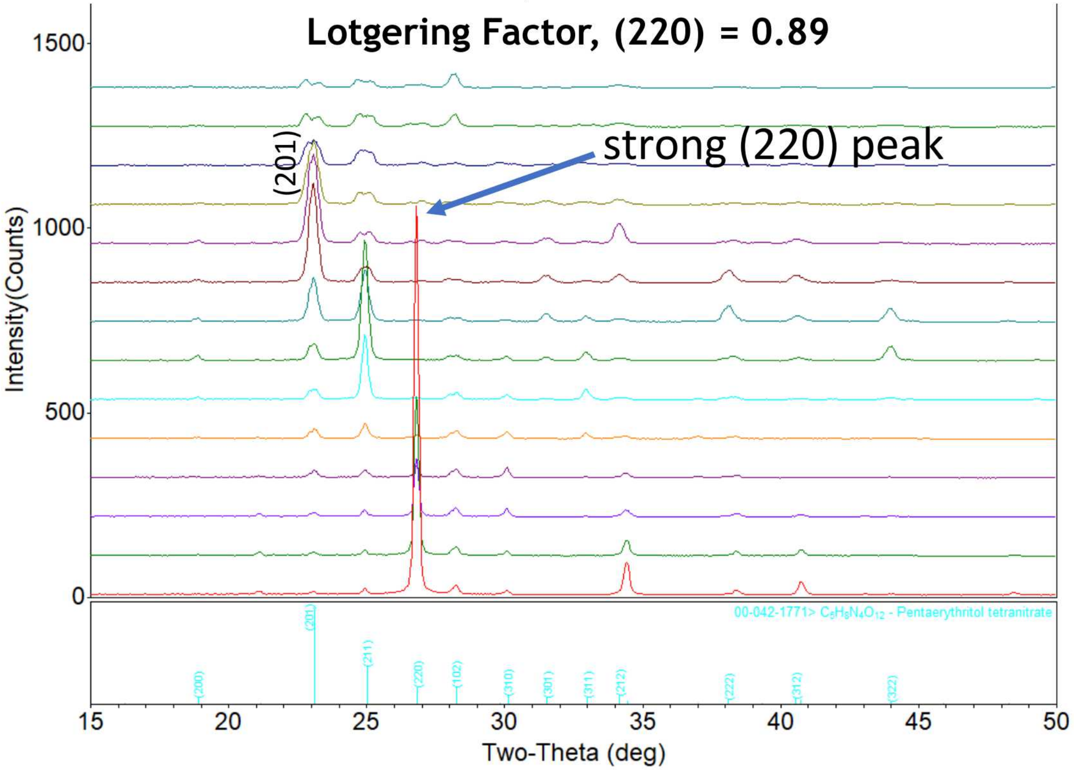
RESULTS: XRD on PETN

- XRD spectra indicate low density PETN with nearly random orientation, having some preference for (002) plane.
- XRD spectra confirm preferred (220) out-of-plane texture for denser PETN region.





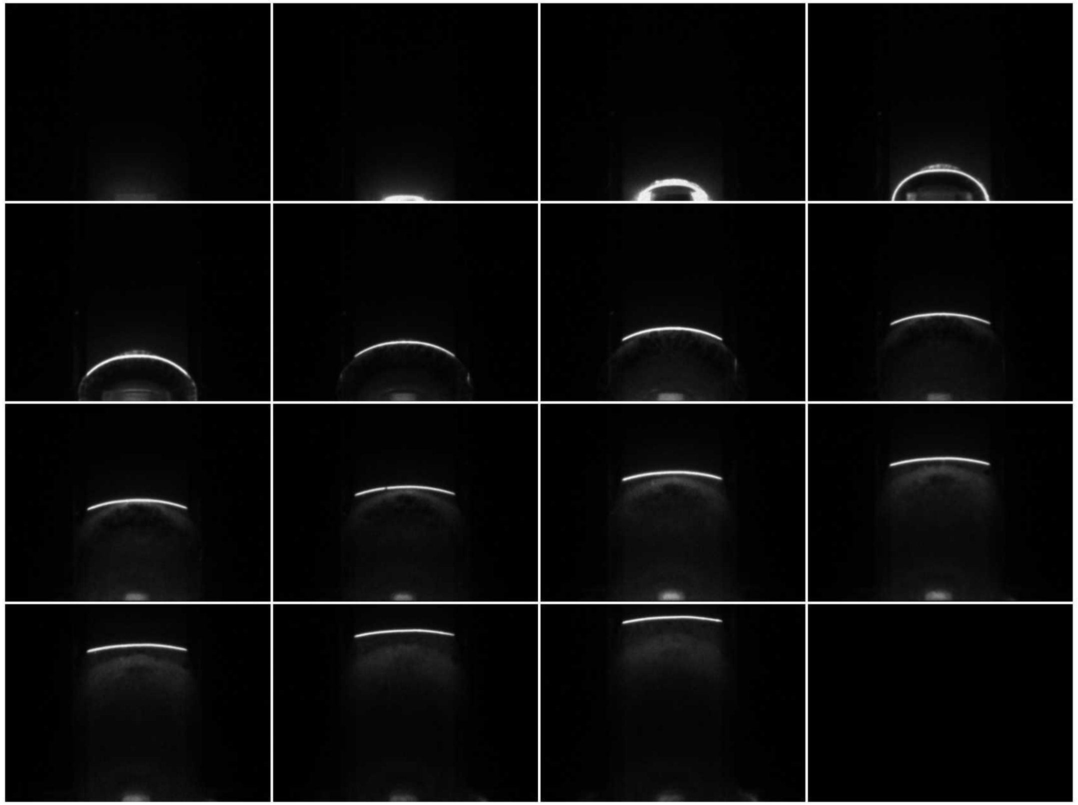
Phi-merged XRD scans of PETN on low surface energy region on substrate (low-density PETN).



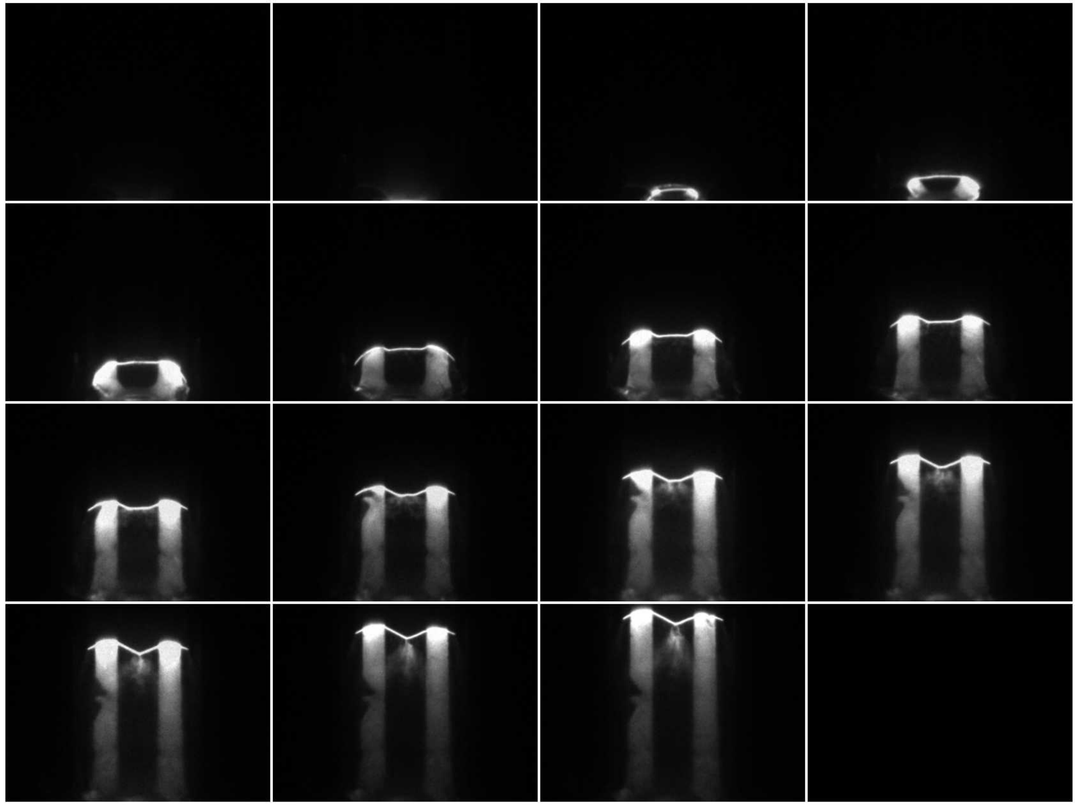
Phi-merged XRD scans of PETN on high surface energy region on substrate (high-density PETN).

RESULTS: Microdetonation Testing

- Investigated uniform-density PETN films (reference case) and variable-density films.

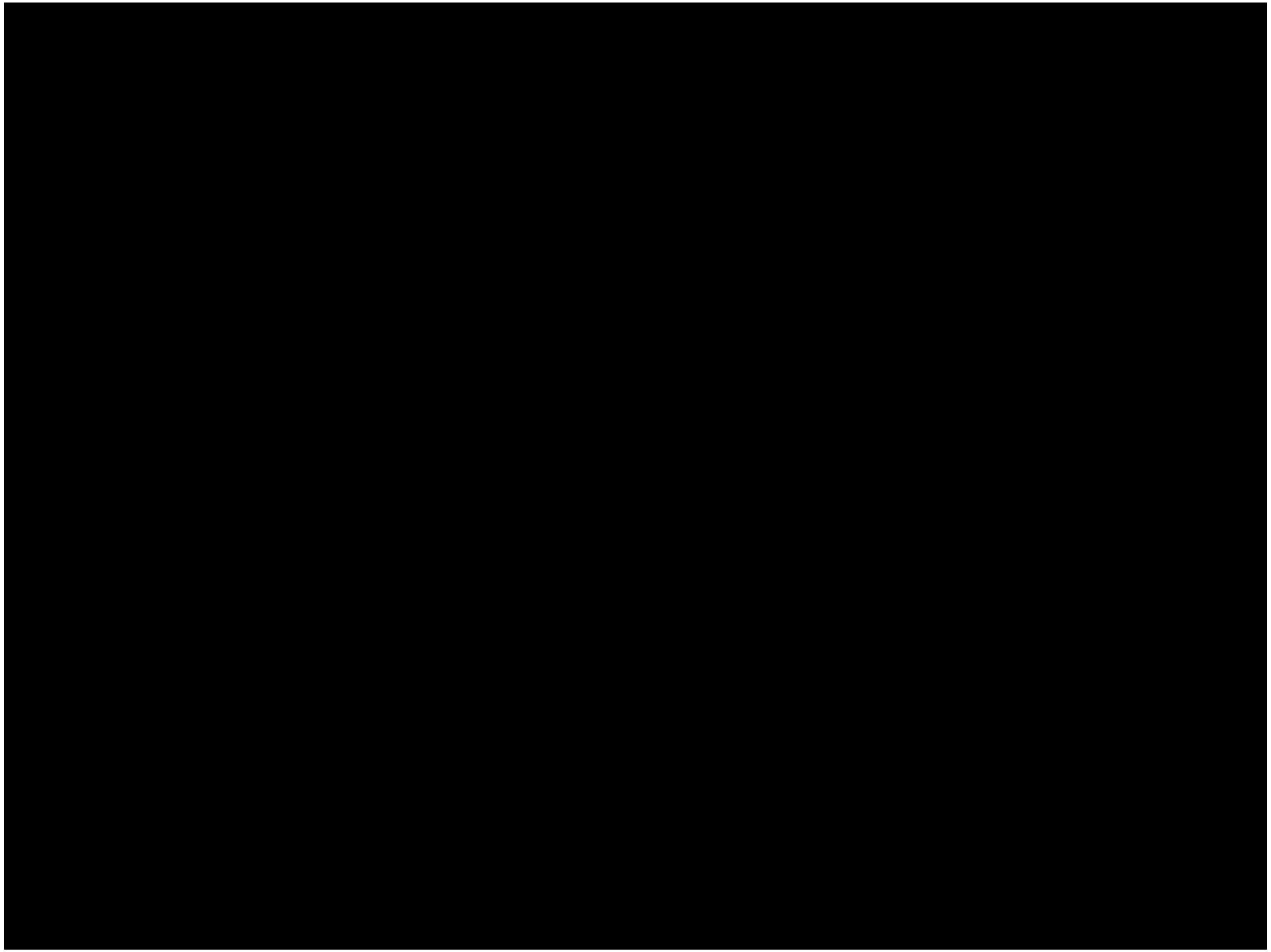


Detonation wave evolution for PETN film, all low density (reference case). FoV = 16.7 mm, 6.45 MHz (1/155 ns).

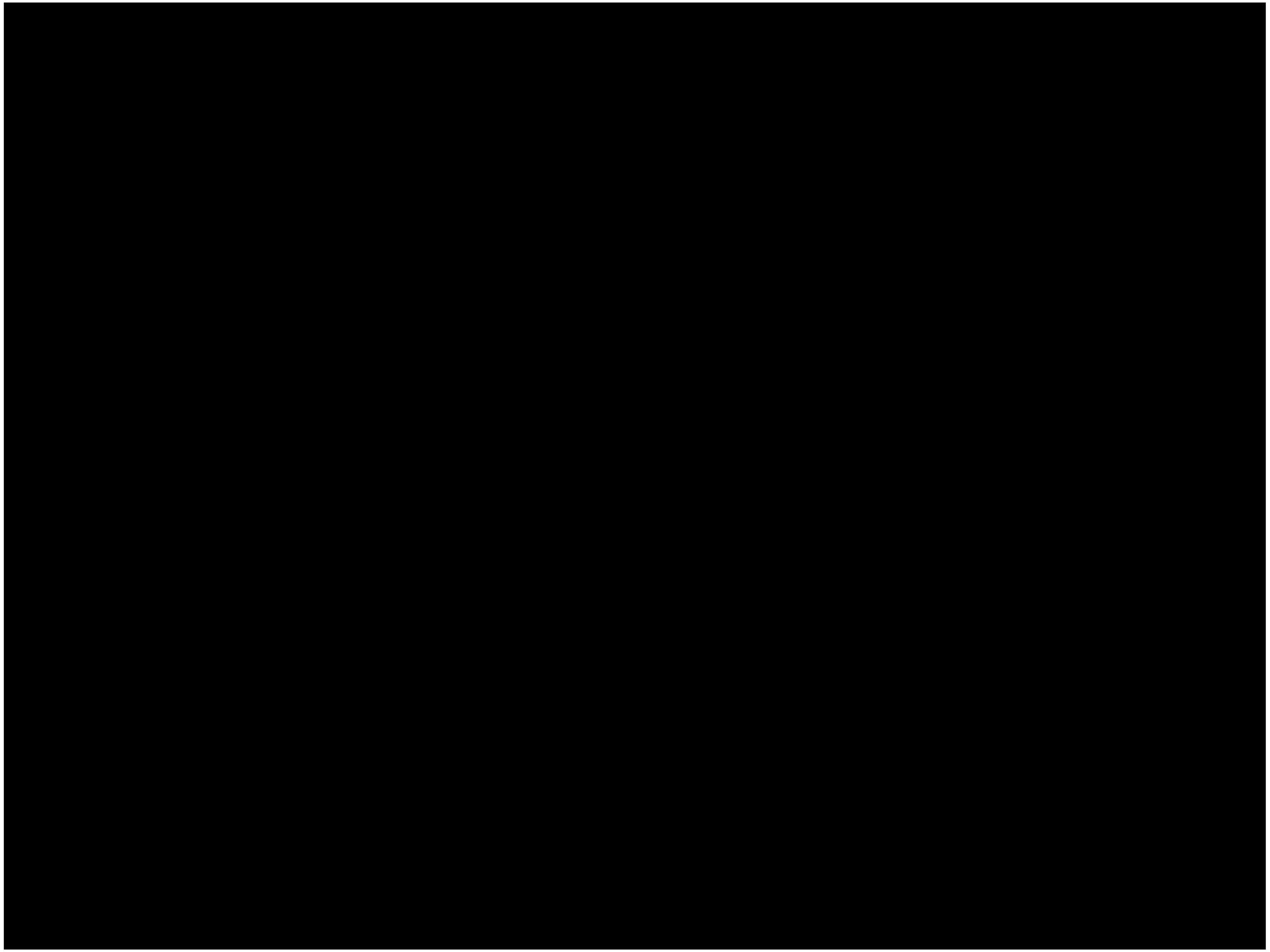


Detonation wave evolution for PETN film with 1.6 mm-wide high density outer lines and low density center region. FoV = 16.7 mm, 6.45 MHz (1/155 ns).

RESULTS: Reference Case



RESULTS: Variable Density PETN– 1.6 mm-wide Outer Stripes



CONCLUSION AND FUTURE WORK

- Localized control of substrate surface energy enables functional variation in energetic material density when grown via PVD.
- Controlled density variation in energetic material can be leveraged to locally alter detonation velocity.
  - Technique demonstrated for PETN, future work will explore technique for other energetic materials.
- Further work is needed to explore microstructure, grain size, and grain orientation effects on detonation velocity, especially at sub-millimeter scales.

ACKNOWLEDGEMENTS

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