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Quasi-Isentropic Compression of Vapor-Deposited HNAB – Experiments and Analysis

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20th Biennial Conference of the APS Topical Group on
Shock Compression of Condensed Matter,
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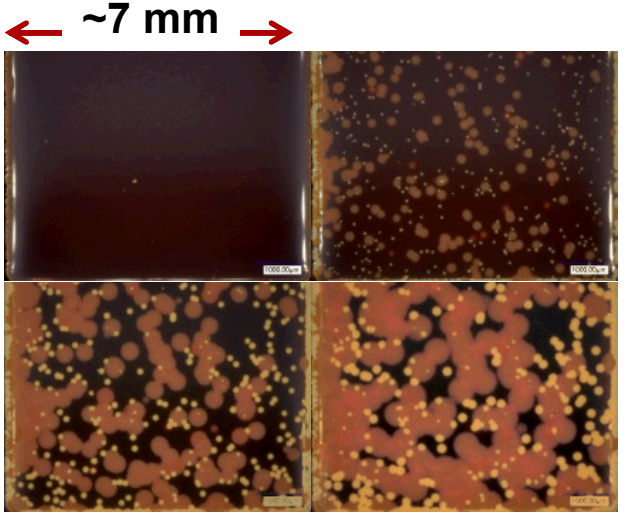
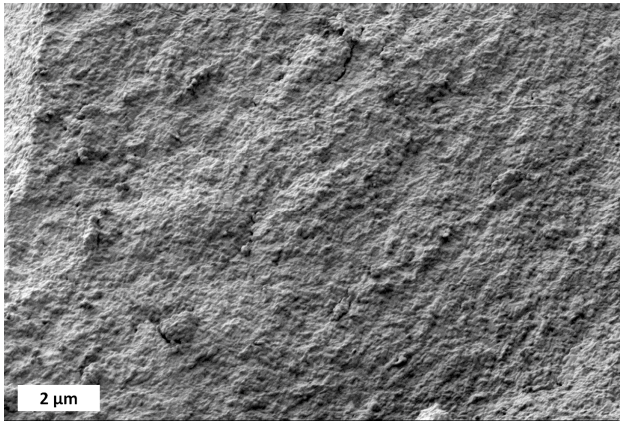
HNAB explosive films

- Vapor-deposited hexanitroazobenzene (HNAB)
- Amorphous (as deposited) then crystallizes (days to weeks)
- Final films are principally HNAB-II, isotropic, nanocrystalline, and >99.5% dense



HNAB crystallization, time-lapse 65 °C, 24 min./image.



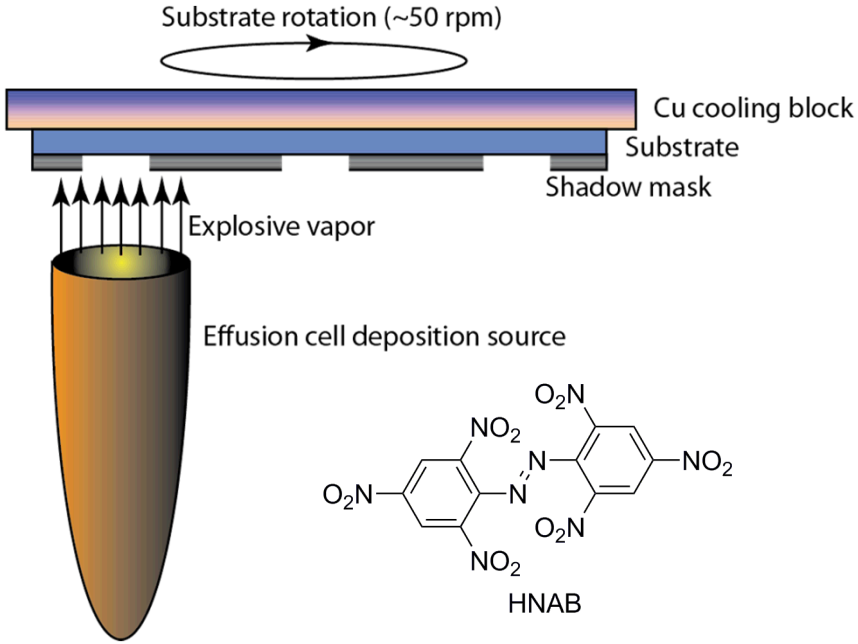
Fracture cross-section micrograph of 35 °C crystallized HNAB.

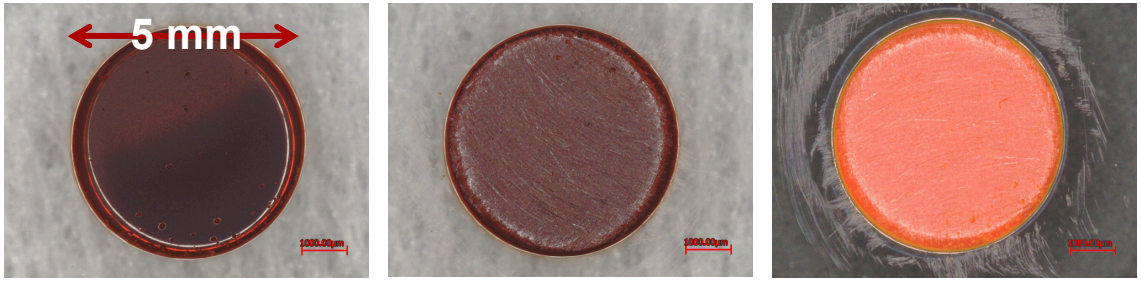
Knepper, R., Browning, K., Wixom, R.R., Tappan, A.S., Rodriguez, M.A., and Alam, M.K., "Microstructure Evolution during Crystallization of Vapor-Deposited Hexanitroazobenzene Films," *Propellants, Explosives, Pyrotechnics,* vol. 37, pp. 459 – 467, 2012.

Tappan, A.S., Wixom, R.R., and Knepper, R., "Geometry effects on detonation in vapor-deposited hexanitroazobenzene (HNAB)," *AIP Conference Proceedings,* vol. 1793, no. 1, p. 030036, 2017/01/13, 2015.

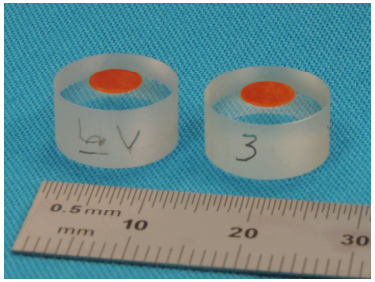
HNAB physical vapor deposition

- Vacuum thermal evaporation
- Cooled substrate holder
- 0.2 to 0.3 µm Al reflector
- 189 and 169 µm HNAB
- Crystallization of amorphous HNAB nucleated by gentle roughening





Optical micrographs of HNAB after deposition (left), after roughening (middle) and after crystallization.



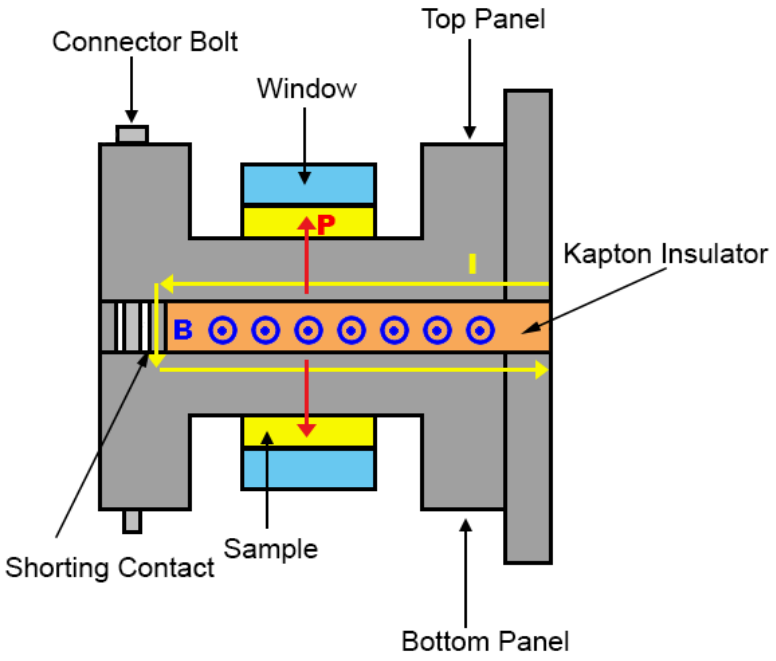
HNAB films on PMMA and LiF.

Quasi-Isentropic Compression

- A continuous measurement of the HNAB quasi-isentrope was obtained through magnetic ramp compression
  - Quasi-isentropic because not completely reversible
- Current flow generates a magnetic field between the top and bottom panels
  - The resulting Lorenz force, **P** = **I** x **B**, compresses the sample [1]

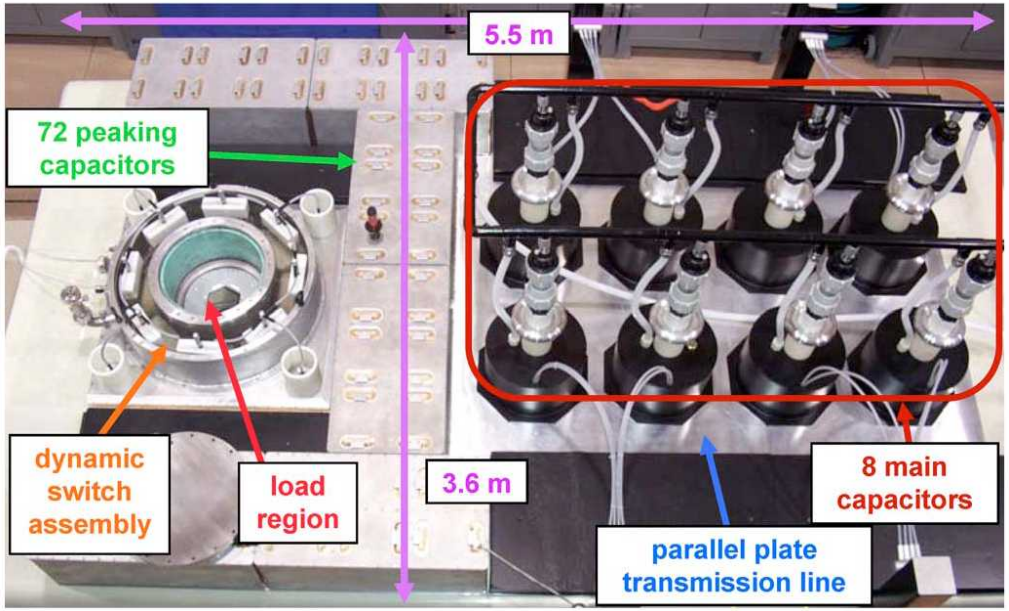
$$P = k_e \frac{B^2}{2\mu} = k_e \frac{\mu}{2}\left(\frac{I}{w}\right)^2$$

- Experiments performed on the VELOCE Pulsed Power Machine [1] at Sandia National Laboratories



VELOCE Pulsed Power Machine

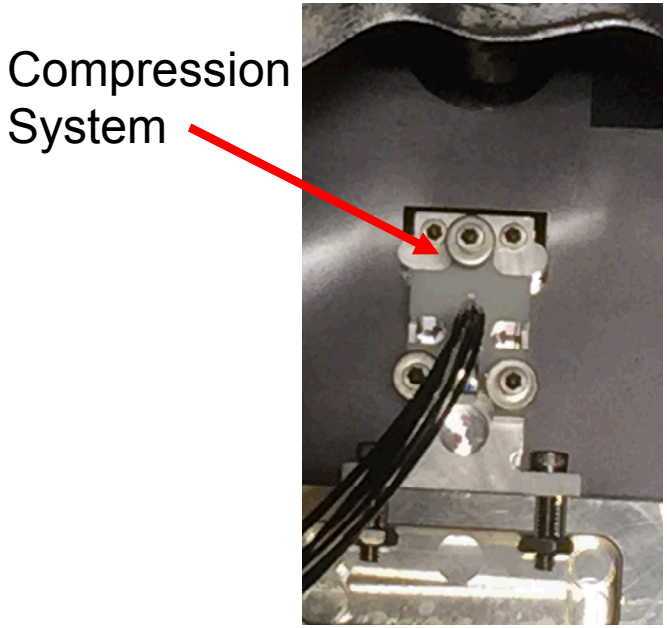
- VELOCE [1] is a compact pulsed power machine located at the Dynamic Integrated Compression Experimental (DICE) facility at Sandia National Laboratories
  - 3 MA of current
  - Rise times from 440 to 550 ns
  - Pressures from 5 -20 GPa

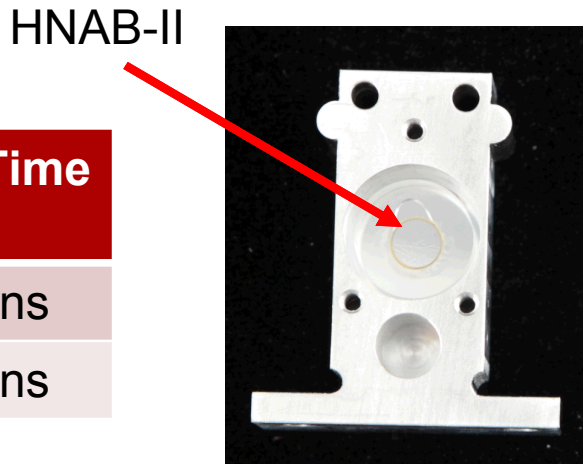


From T. Ao et al., Rev. Sci. Instrum. **79**, 013903 (2008).

Experimental Parameters

- Al 6061 panels with a 1.5 mm floor thickness
- Samples were bonded to the panel with Sylgard® 527 silicone and secured with a compression system
- Velocity records were recorded with both VISAR and PDV

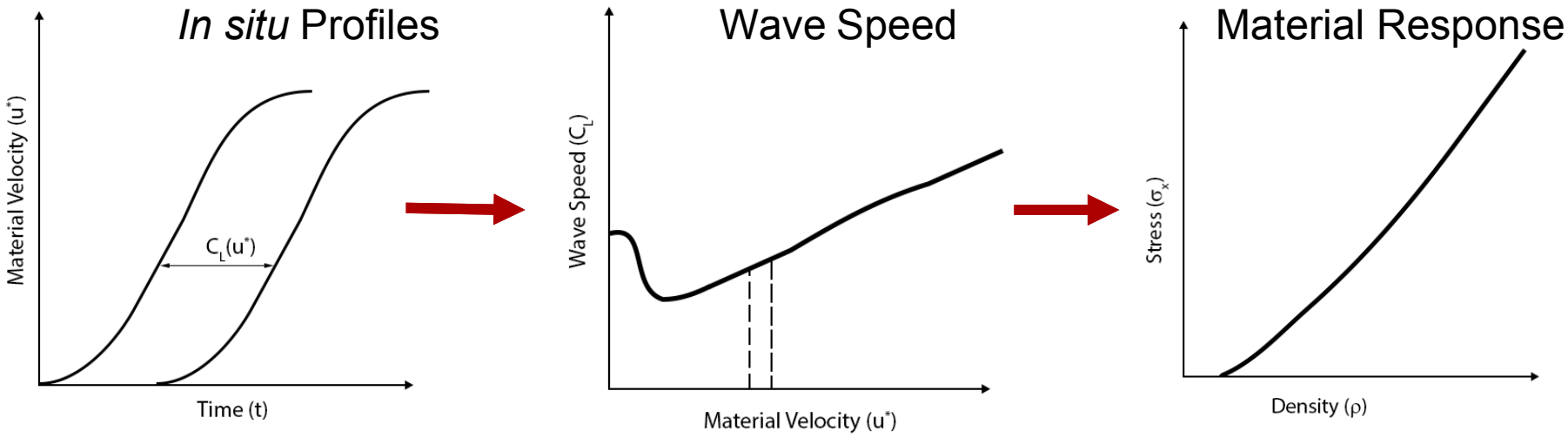




Experiment	HNAB Thickness	Window	Current	Rise Time
1	169 µm	LiF	1.9 MA	493 ns
2	189 µm	PMMA	2.1 MA	504 ns

Quasi-Isentrope Determination

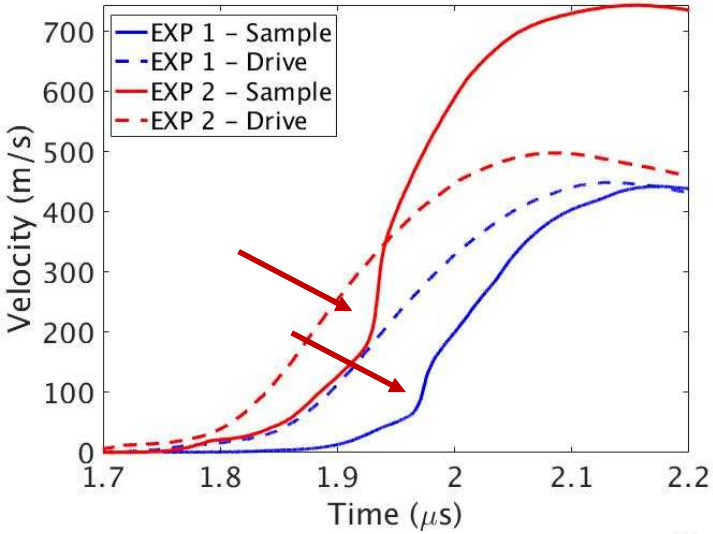
- Quasi-isentrope is determined with Lagrangian, or *in situ*, material velocities at two locations in the sample [2]
  - Direct Lagrangian analysis
    - $dv = -\frac{-du^*}{\rho_0 C_L(u^*)} \qquad d\sigma_x = \rho_0 C_L(u^*) du^*$
- Usually velocimetry measurements are at window interfaces and must be mapped to *in situ* velocities
  - Inverse Lagrangian analysis (ILA) [2]

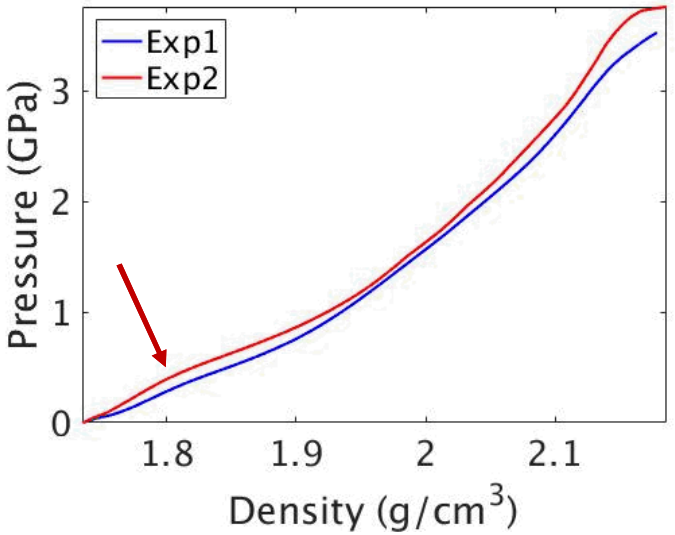


[2] J.P. Davis et al. J. Appl. Phys. **116**, 204903 (2014).

Experimental Results

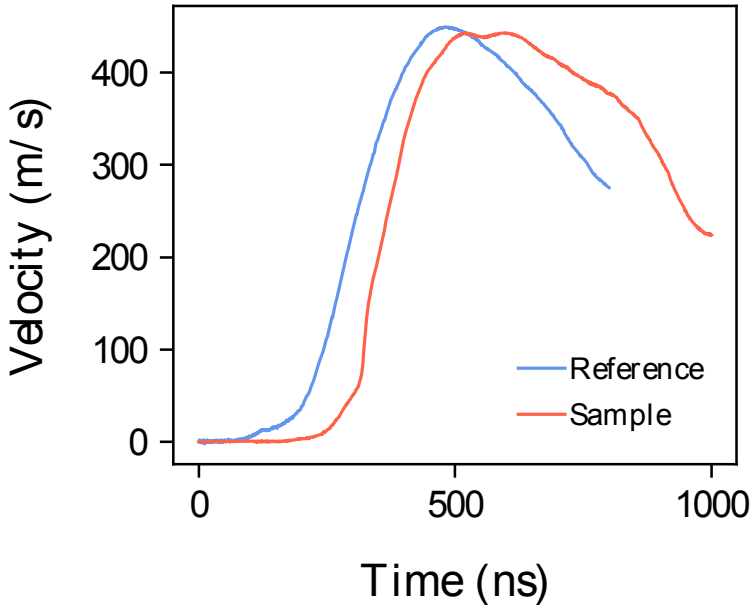
- Interface velocity records from each experiment indicated a low pressure (~ 0.6 GPa) phase change in HNAB-II
- Phase transition cast doubt on the obtained quasi-isentrope
  - Invalidates the isentropic flow assumptions underlying the analysis method
  - Current efforts are underway to perform ILA through phase transitions

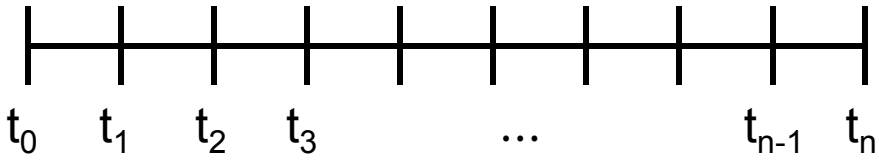




EOS – Alternate Determination Methods

- Backward integration technique (Hayes, 2001)
  - Time partitioned
  - Equations of motion marched backwards in space
  - Visar record is initial condition
  - Must know material response of reference material
- Each veloce shot has sample side (HNAB-II) and reference side (1100-Al) that are subjected to the same drive conditions

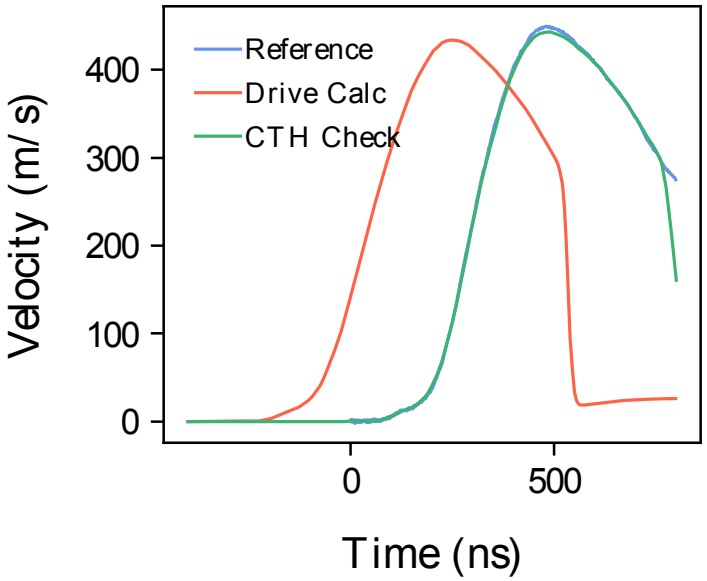


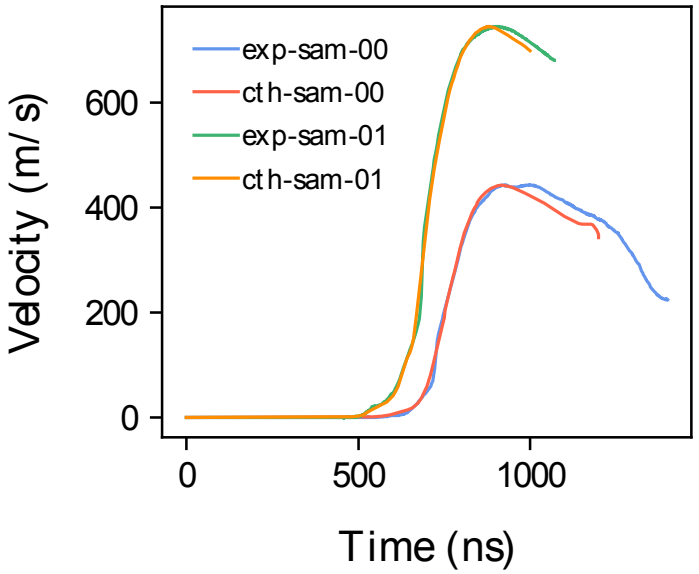


Each iteration takes the solution back dx, until the drive surface is reached

Drive Verification and EOS determination

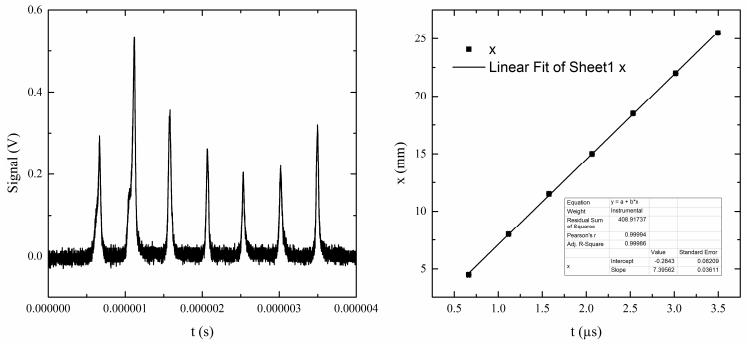
- The drive conditions are verified by running a standard forward calculation using the drive stress history
- Sample geometry run in a forward calculation with unknown EOS and constitutive model
- DAKOTA is used to optimize Mie-Gruneisen and EPPVM constitutive model parameters



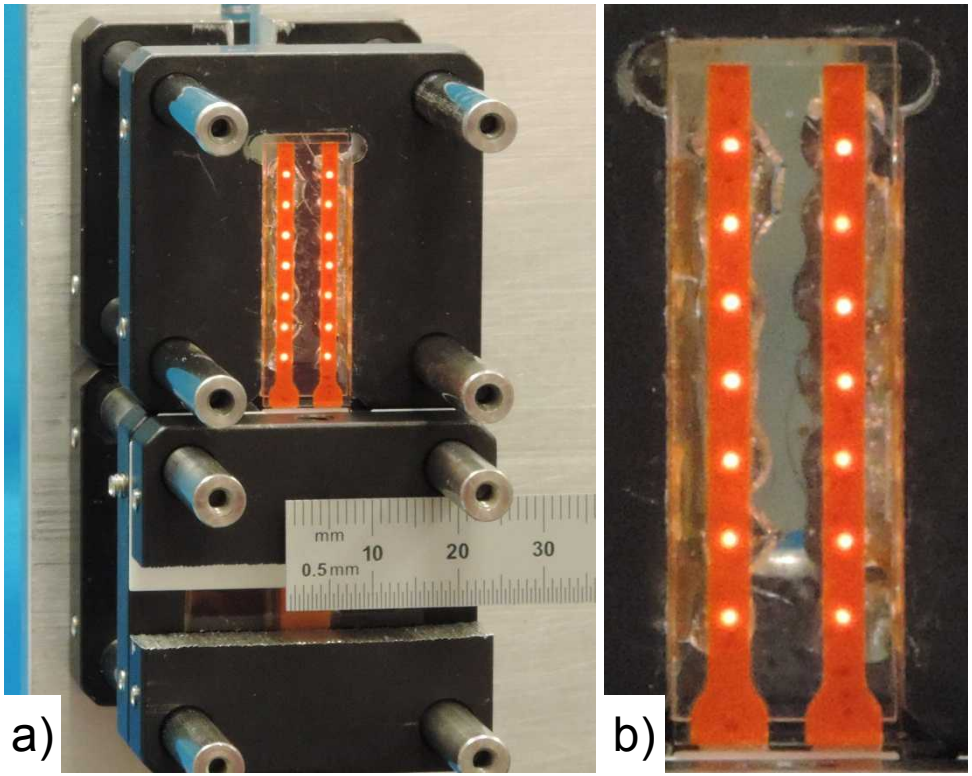


Critical detonation thickness experiment

- Two experiments (HNAB lines) each shot
- Optical fibers deliver detonation light to photodetector



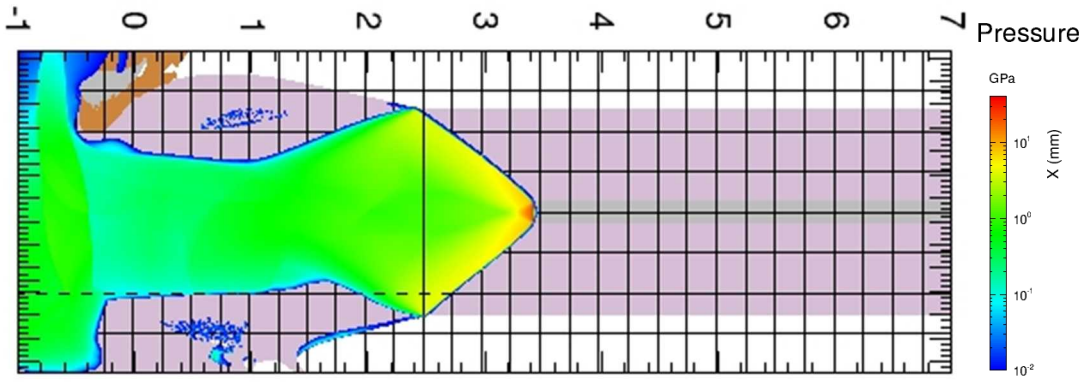
Optical fiber data is used to produce a linear fit to position versus time, where the slope is the velocity.

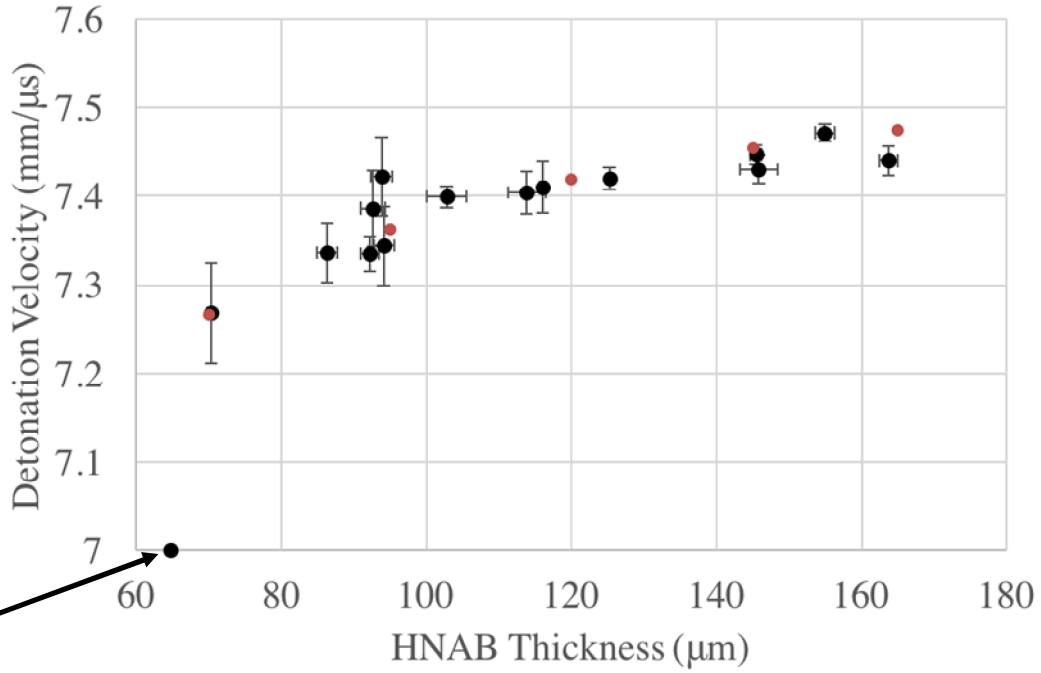


Photographs of critical detonation thickness experiment. Optical fibers illuminated to highlight position.

Model Fitting and Results

- Density: 1.735 g/cm^3
- Steady roll off in velocity at decreased thicknesses
- Failure to propagate at thickness < 65 µm
- Two material PETN model for detonator to match average density
- Cross sectional 2D model (assumed infinite width)
- Detonation velocity deficit captured well using Arrhenius Reactive Burn
- Detonation failure not captured
  - Similar to Hexanitrostilbene (HNS)
  - 3D effects
  - Density resolution in booster





Conclusions

- Amorphous deposited HNAB crystallized at room temperature through gentle abrasive nucleation
- VELOCE crystalline HNAB-II samples prepared through deposition on LiF windows
- Backward integration used to define drive conditions
- HNAB-II EOS and strength parameterization obtained through optimization of continuum model with the VISAR data
- ARB model optimized against experimental velocity vs. thickness data
- Good match to performance data obtained, however further refinement needed to capture failure

Acknowledgements

- Michael P. Marquez, Nicole Cofer, and M. Barry Ritchey
- DICE team
  - Randy Hickman, Keith Hodge, Nicole Cofer, and Joshua Usher
- The Joint Department of Defense/Department of Energy Munitions Technology Development Program
- Laboratory Directed Research and Development

Backup slides

Sandia National Laboratories

Sample Identifier	HNAB Thickness	HNAB Thickness standard deviation	Window material	Notes
	μm	μm		
SCT928_6	189	1	PMMA	PMMA window #6
SCT951_3	169	4	LiF	LiF window #3

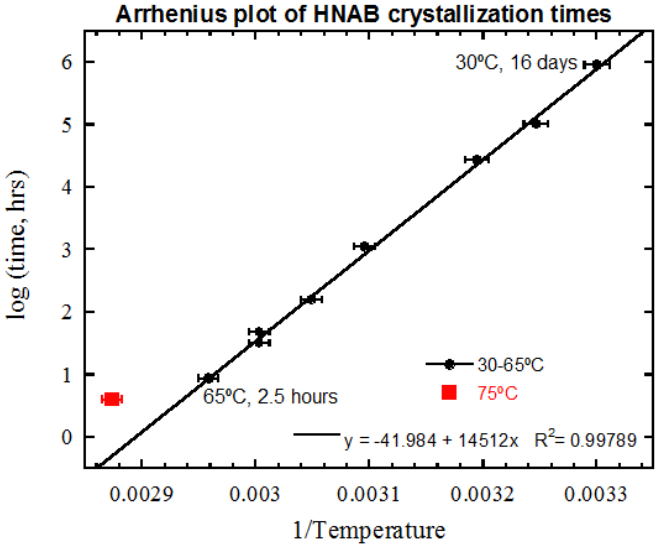
Previous work on vapor deposited HNAB shows that the HNAB crystallizes principally to the HNAB-II polymorph, which has an unstrained crystal density of 1.744 g/cm3.[1] The density of vapor deposited HNAB-II films is estimated to be 99.5% (1.735 g/cm^3) from ion-polished cross-section data.[2, 3]

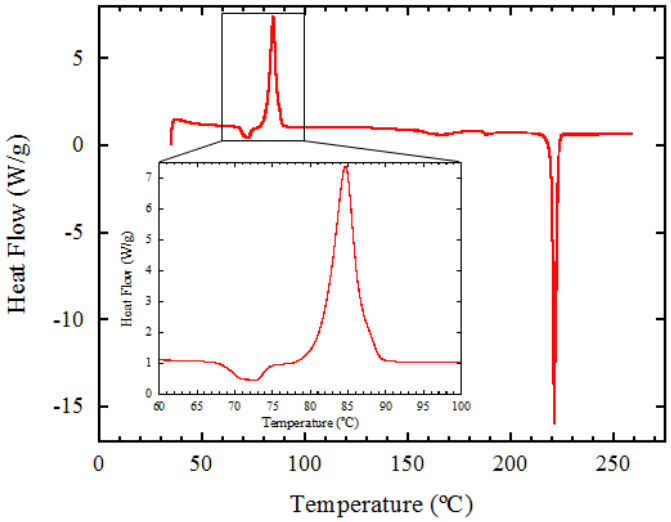
VELOCE samples assembled with Sylgard® 527, low-viscosity silicone.

1. Graeber, E.J. and Morosin, B., "The crystal structures of 2,2',4,4',6,6'-hexanitroazobenzene (HNAB), forms I and II," *Acta Crystallographica Section B,* vol. 30, no. 2, pp. 310-317, 1974.
2. Tappan, A.S., Wixom, R.R., and Knepper, R., "Geometry effects on detonation in vapor-deposited hexanitroazobenzene (HNAB)," *AIP Conference Proceedings,* vol. 1793, no. 1, p. 030036, 2017/01/13, 2015.
3. Knepper, R., unpublished data, Sandia National Laboratories, 2017.

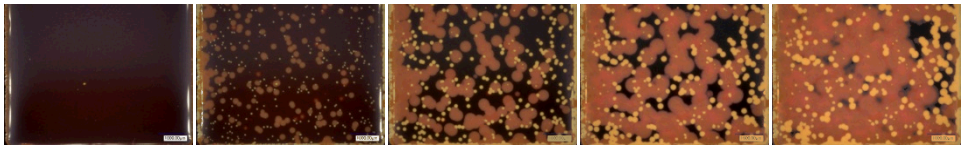
HNAB crystallization

- Amorphous HNAB films crystallize over time
- Pronounced difference in crystallization above glass transition temperature (T_g, ~70 °C)





DSC data from an amorphous HNAB film heated from 40–250 °C at 5 °C/min.



Time-lapse of HNAB crystallization, 65 °C, 24 min./image.

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," *Propellants, Explosives, Pyrotechnics,* vol. 37, pp. 459 – 467, 2012.