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Effects of Confinement Conditions on the Detonation Properties of Vapor-Deposited Hexanitroazobenzene Films

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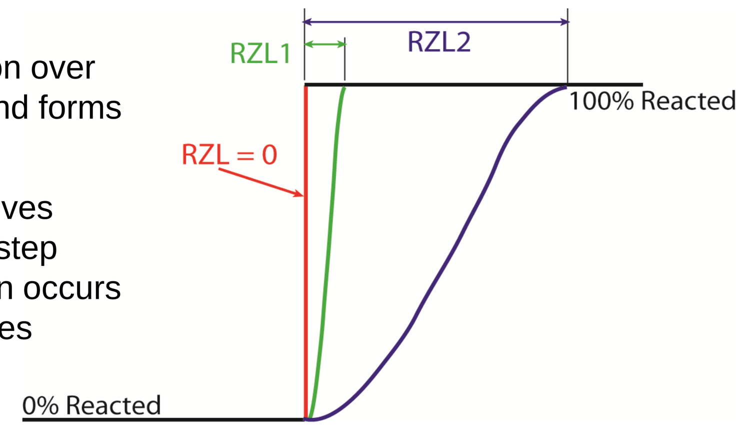
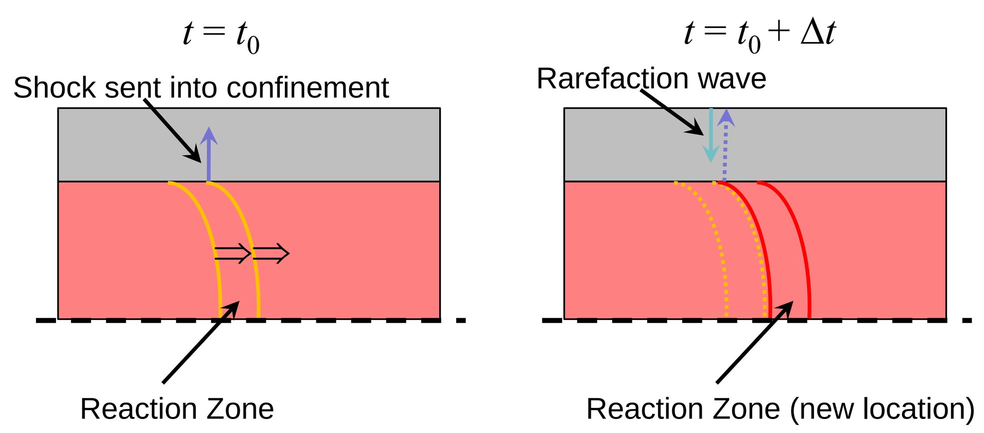
Background: Confinement and the Detonation Reaction Zone

- The detonation reaction zone is the region over which a solid or liquid explosive reacts and forms gaseous products during a detonation
- Current hydrocode simulations of explosives treat the reaction zone (incorrectly) as a step function, assuming that complete reaction occurs immediately as the detonation front passes



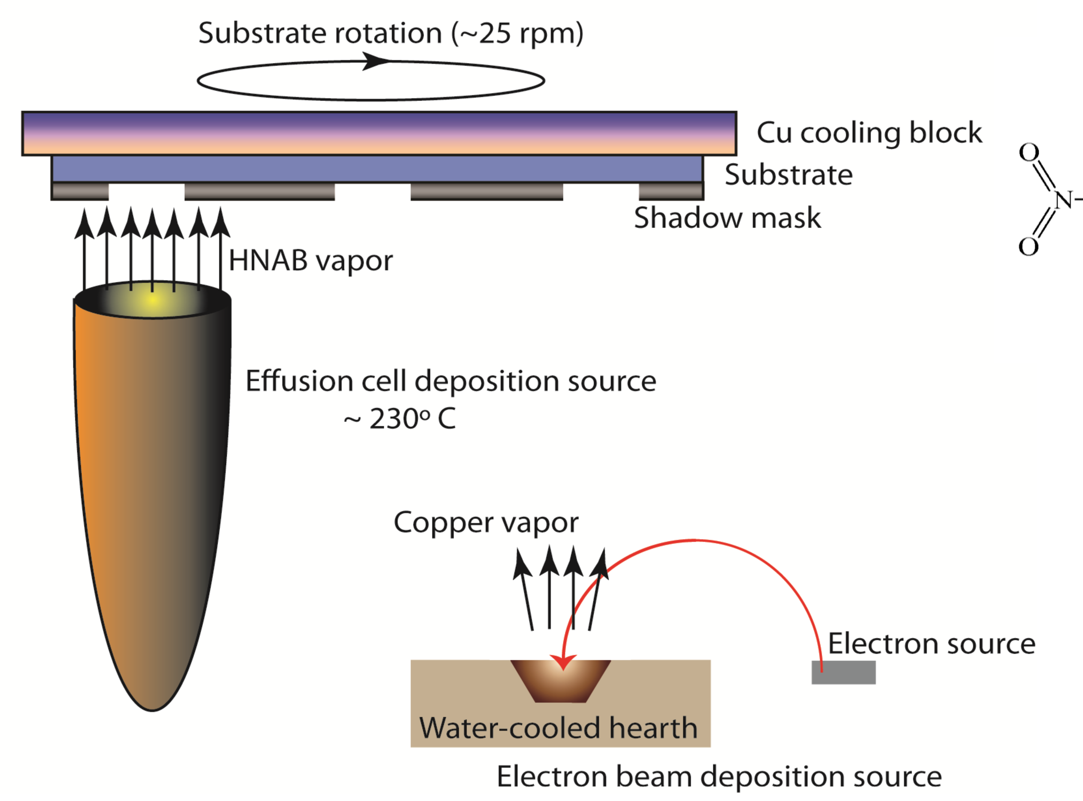
- This assumption typically leads to significant errors in predicting critical detonation output parameters such as pressure, temperature, and detonation velocity
- Current simulations compensate for these errors by adding empirically-determined fitting parameters
- Reaction zone length (RZL) is one of the critical parameters needed to create truly predictive next-generation simulations of explosive behavior



- Confining an explosive is known to have effects on detonation velocity and critical thickness
- If $RZL / D < t_{shock} + t_{rarefaction}$, then confinement should be effectively infinite
- Studying effects of varying confinement thickness may provide information about reaction zone lengths

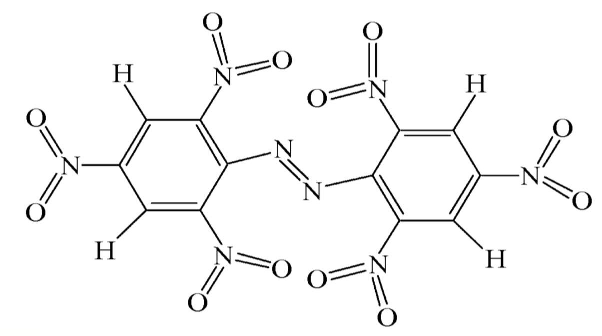
Film Deposition and Microstructure

- Physical vapor deposition used to fabricate both explosive and confinement layers
- On a low-roughness surface, vapor deposition can provide pristine interfaces between explosive and confinement layers



Schematic of the deposition system used to fabricate vapor-deposited confinement/explosive/confinement stacks

- Deposition conducted in a vacuum chamber evacuated to ~ 10^{-6} Torr
- Fast deposition rate (~ 1 μm/min) for HNAB
- Shadow masks used to define deposition geometry
- Deposited onto 1 cm × 3 cm Lexan substrates
  - Good CTE match with HNAB
  - Low shock impedance for minimal effect on confinement
- Vapor-deposited copper confinement requires adhesion layers to avoid delamination

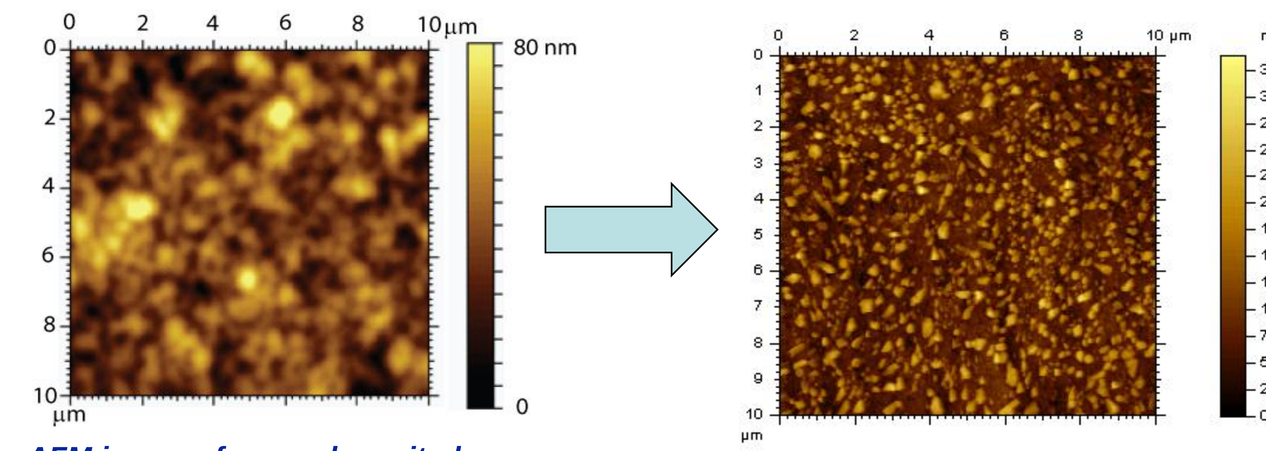


HNAB molecule

- MP = 221ºC
- Chemically stable as melt to ~ 300ºC
- D ~ 7.5 mm/μs
- ρ ~ 1.75-1.80 g/cm³ (dependent on crystal structure)
- Small critical thickness for detonation (< 100 μm)

- HNAB chosen for low as-deposited roughness and consistency of both microstructure and detonation velocity
- Copper chosen as a fairly high shock impedance material that can be deposited without generating a heat flux high enough to decompose the HNAB

Photograph of a 100 μm thick HNAB lines confined by 4 μm copper layers on a 1 cm x 3 cm Lexan substrate. Films are patterned in this geometry for use in detonation experiments

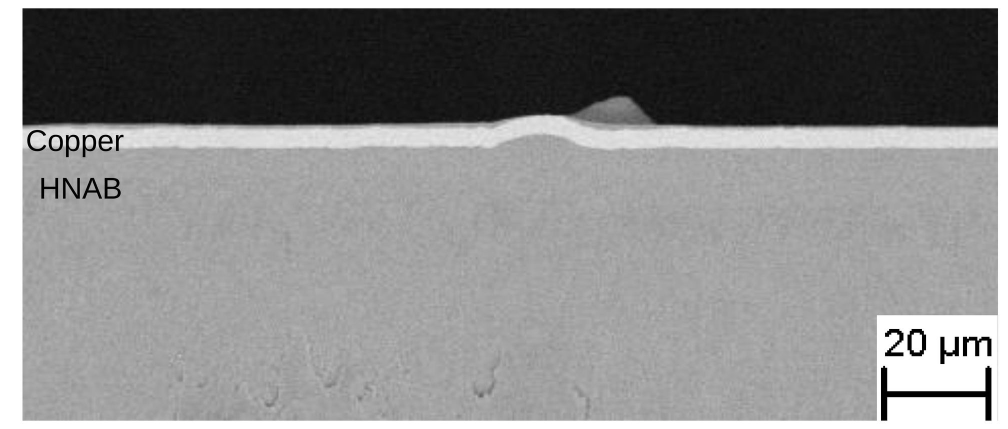


AFM image of an as-deposited amorphous HNAB film

AFM image following crystallization at room temperature

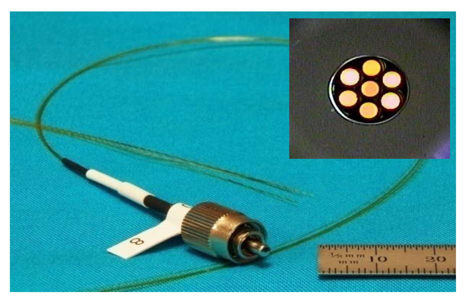
Knepper et al., Propellants, Explosives, Pyrotechnics, 2012 (in press).

- HNAB forms a dense (non-porous) amorphous structure as-deposited with a very low surface roughness (~ 20 nm)
- HNAB films will crystallize over several weeks at room temperature to a structure consisting primarily of the HNAB-II polymorph with very little porosity, a sub-micron grain size, and smooth surface (~ 50 nm roughness)
- These microstructures are very reproducible and vary little with small changes in deposition conditions
- The dense, smooth surface morphology allows high-quality confinement layers to be deposited onto the HNAB with pristine interfaces

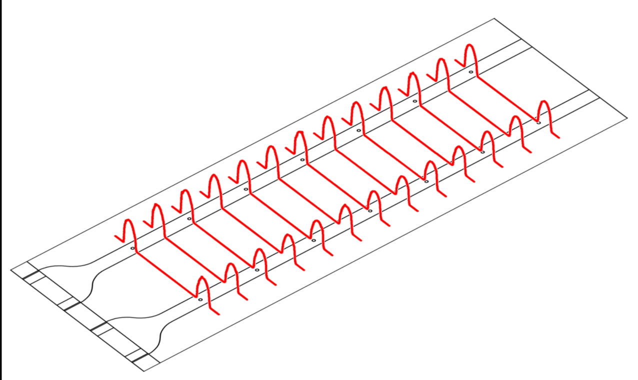


Cross-section SEM image showing the interface between HNAB and copper films

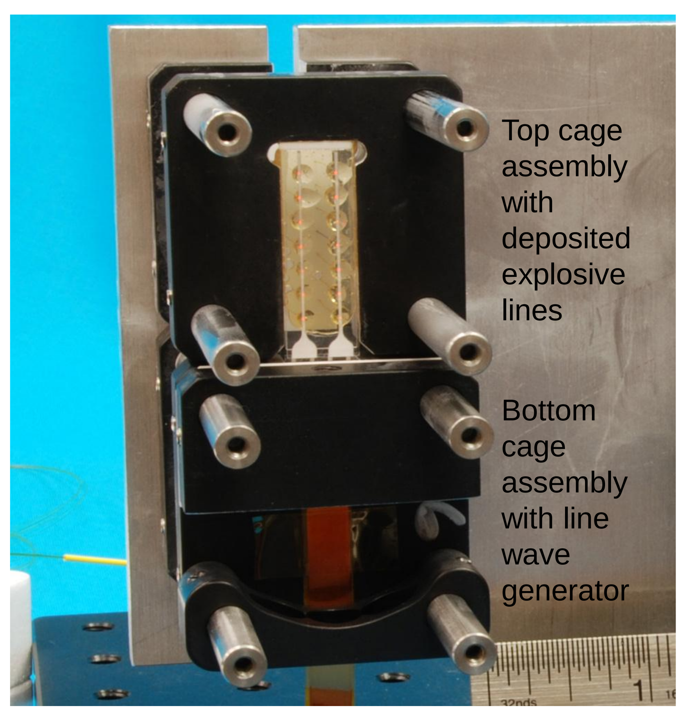
Detonation Experiments



Photograph of optical fiber probe with inset showing six-around-one connector.

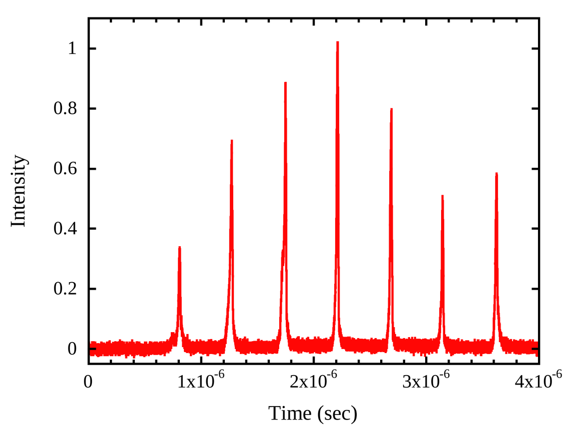


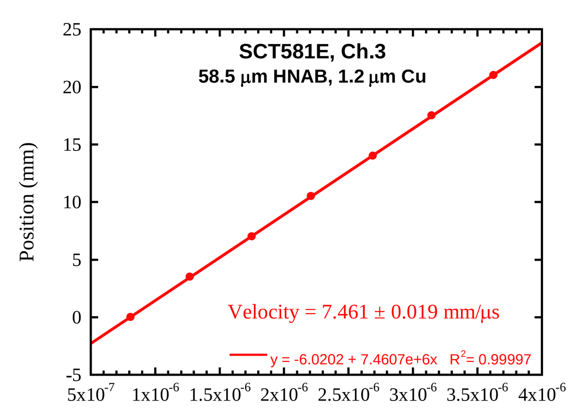
Surface profiler data superimposed on a sketch of deposited explosive material



Detonation velocity/critical thickness experiment

- Detonation train consists of a slapper, a PETN pellet, a four-point line wave generator, and the deposited explosive lines
- Two experiments can be performed simultaneously
- Sample thickness determined from a series of thirteen surface profiler scans across the deposited lines
- Optical fiber probe used to measure detonation velocity
  - Seven fibers placed at 3.5 mm intervals in a laser-machined lid
  - Fibers bundled in a SMA connector and fed into a silicon photodetector
  - Fiber position plotted against time of oscilloscope peaks to determine detonation velocity

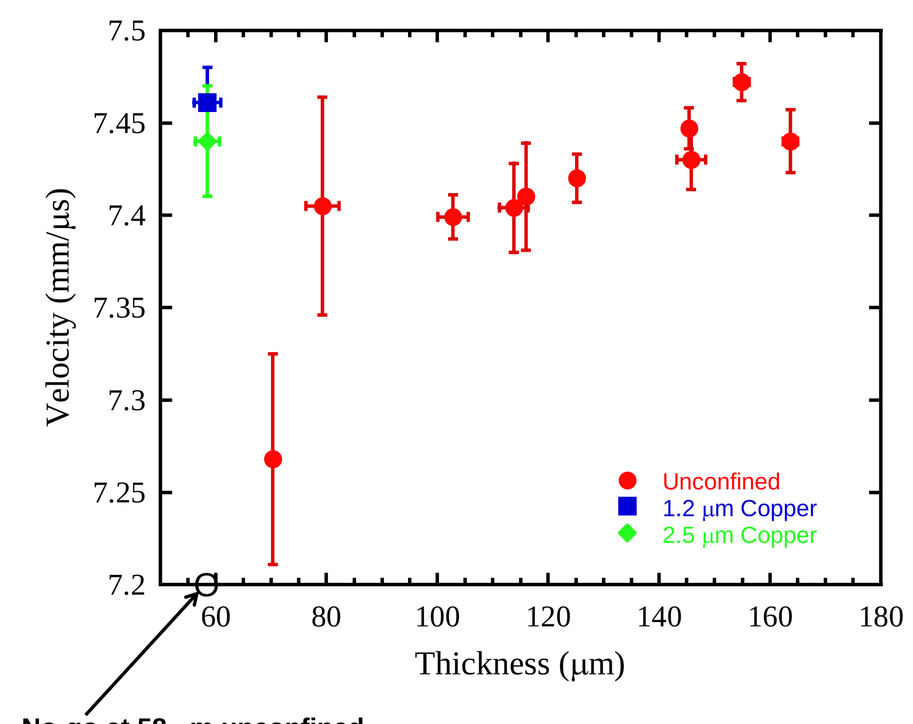




Example of oscilloscope data and resultant position vs time plot to determine detonation velocity

Determining Reaction Zone Lengths

- Determine minimum thickness of confinement necessary to behave as if it was effectively infinite
- Use simulations to determine the amount of time it would take for shock and rarefaction waves to traverse that amount of confinement
- $RZL = D * (t_{shock} + t_{rarefaction})$ [at minimum effectively infinite confinement conditions]
- Functional form of detonation velocity vs. confinement thickness and critical thickness for detonation vs. confinement thickness curves may provide additional insight into the kinetics of the reaction
- Future experiments will examine the effects of confinement shock impedance on RZL



- Initial experiments performed on unconfined HNAB samples and samples with 1.2-8.5 μm thick copper confinement
- Little variation in detonation velocity (D ~ 7.40 – 7.45 mm/μs) in unconfined HNAB until thickness drops below ~ 80 μm
- Critical thickness for detonation (unconfined) < 70 μm
- Copper confinement as thin as 1.2 μm has a substantial effect on detonation behavior, with detonation observed in HNAB films as thin as 58.5 μm
- Difficulties in sample preparation (poor adhesion between HNAB and copper layers, especially with thicker confinement) limited the number of samples of sufficient quality to test and/or complicated data interpretation
  - ⇒ Initial experiments suggest that using chromium adhesion layers at all interfaces will mitigate this problem

Conclusions

- We have developed a method to indirectly determine reaction zone lengths in explosives by measuring the effects of confinement thickness on detonation velocity and critical thickness
- We use physical vapor deposition to fabricate explosive and confinement layers with precise control over both thickness and microstructure to study effects of confinement on explosive properties
- HNAB and copper provide an ideal model system for studying this effect
- Critical thickness for unconfined HNAB < 70 μm
- Copper confinement as thin as 1.2 μm has a substantial effect on critical thickness and detonation velocity
- Knowledge of reaction zone lengths (and reaction times) for various explosives under different confinement conditions (pressures) will greatly enhance the predictive capabilities of next generation computer simulations
- These data will also allow one to engineer confinement conditions to produce desired detonation velocities and reduce the amount of explosive needed, providing enhanced reliability, reduced cost, and limiting collateral damage in devices

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