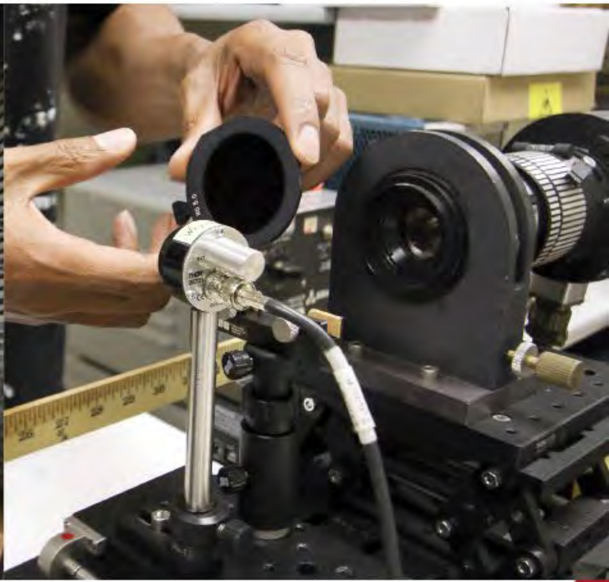
Experimental observations of shock-wave-induced bubble collapse and hot-spot formation in nitromethane liquid explosive



S&T Work-in-Progress Seminar, April 19, 2022

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Background

- One of our jobs is to help the national laboratories make better measurements.
- We develop diagnostics and techniques.
- When we are lucky, we actually help answer important science questions.

Science question: **Do hot spots caused by collapsed voids assist the onset of detonation in high explosives?**

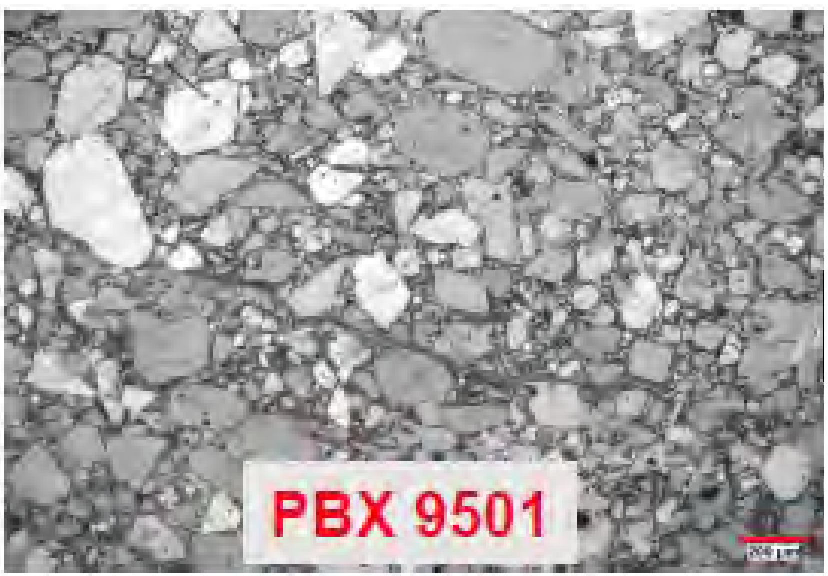
Project goal: **Develop and apply methods to directly measure collapsed voids and their effect on detonation.**

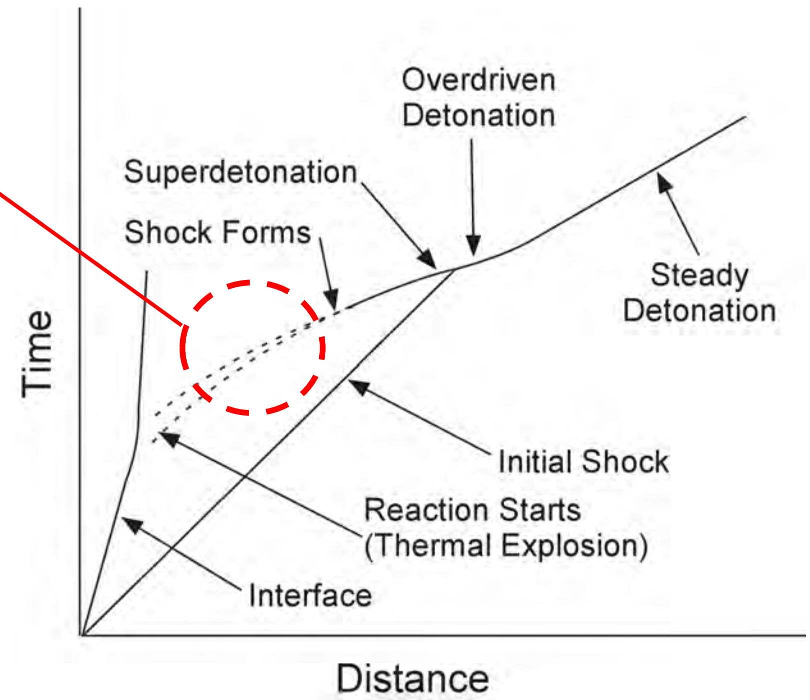
Controlling detonation is critical to performance of high explosives

What controls shock initiation of high explosives?

Two important mechanisms:
Thermal-driven initiation
Hot-spot formation

Hots spots result from porosity, impedance mismatches, grain boundaries, friction, crystal defects, etc.





D. Dattelbaum et al. “Influence of Hot Spot Features on the Initiation Characteristics of Heterogeneous Nitromethane.” Paper presented at the 14th International Detonation Symposium, Coeur d’Alene, ID, April 2010.

Two approaches to modeling explosive performance

Bulk scale

Explosives with different void fractions are characterized experimentally.
Each formulation is treated as a separate explosive with different material properties (density, compressibility) and explosive characteristics (sensitivity, run-to-detonation).

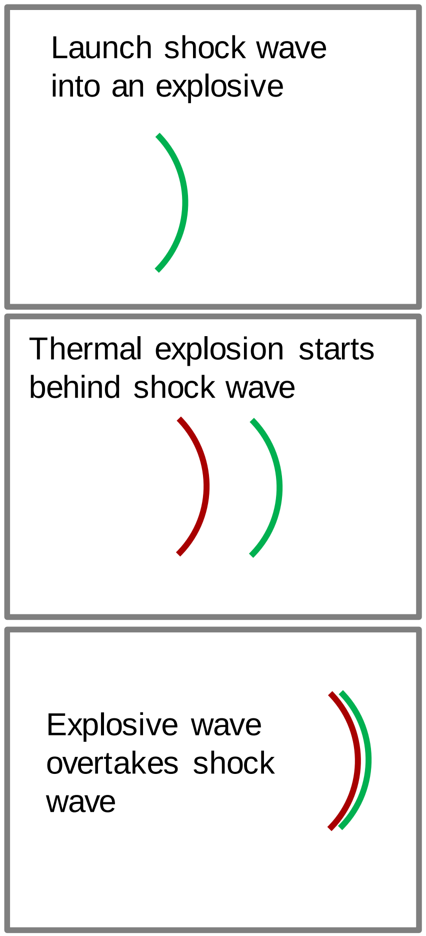
Meso scale

Explosive burn model is not altered for different void fractions.
Void collapse effects are modeled numerically and explicitly included in the simulation.
Void influence on bulk properties is simulated by seeding the model with voids.

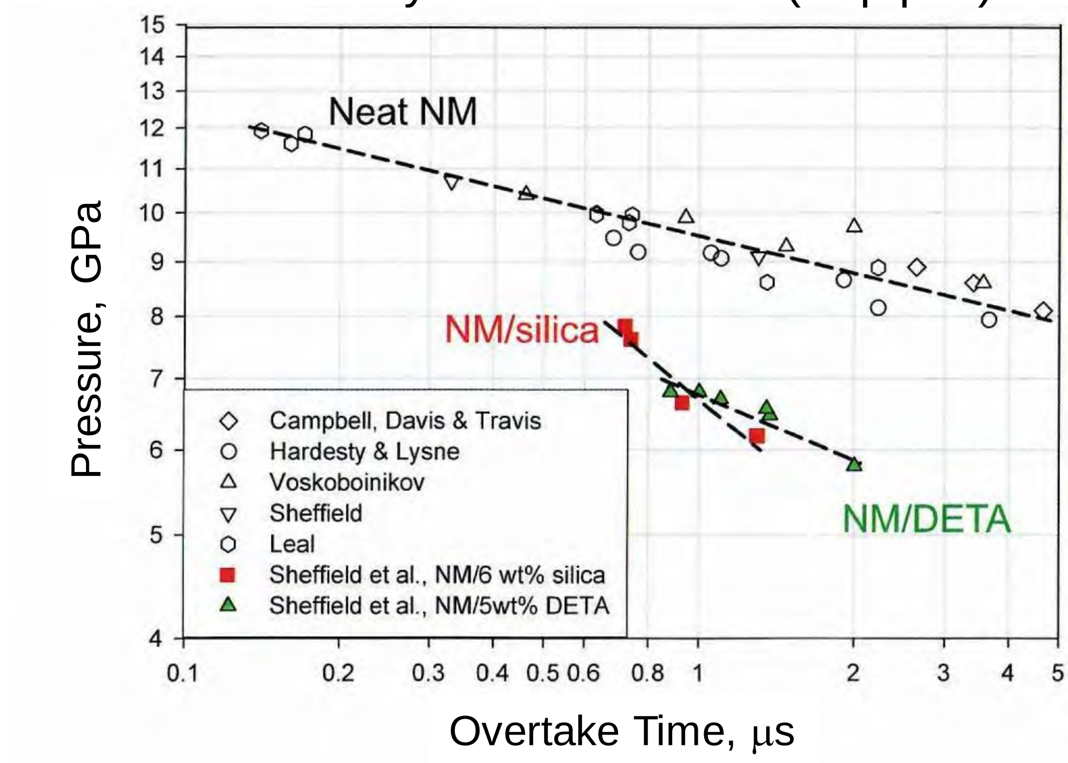
Experimental measurements, especially temperature, are lacking to test these models.

How is explosive performance measured?

Measure the time it takes for explosive wave to overtake shock wave.



Sensitivity of nitromethane (Pop plot)

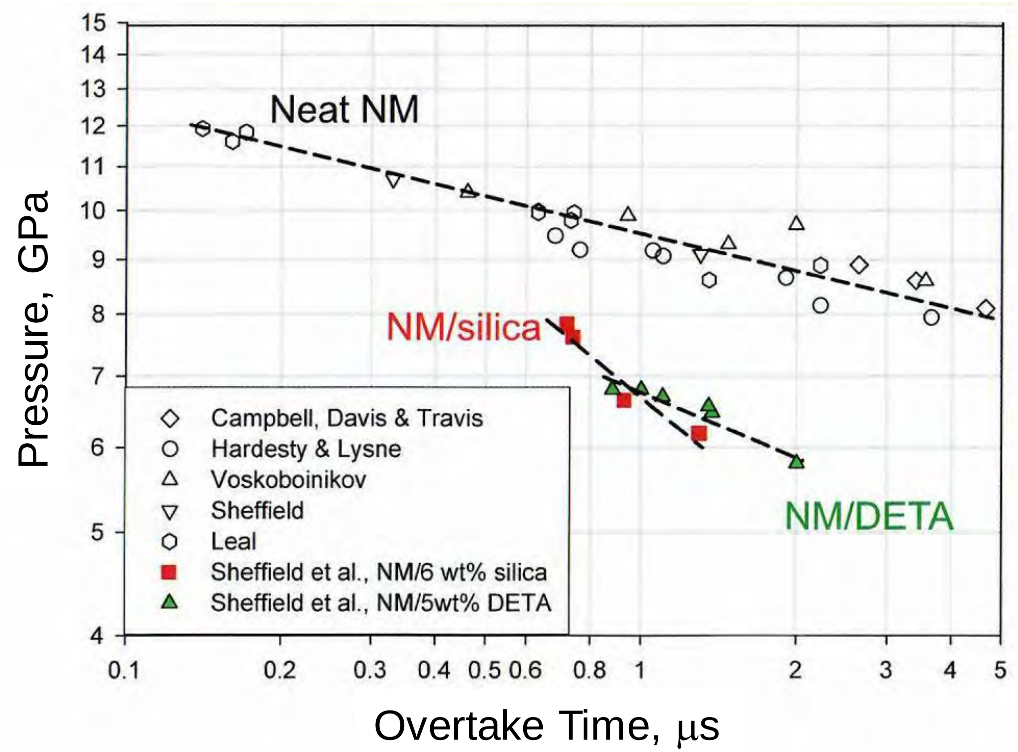


(Dattelbaum et al. 2010)

What does the prior work tell us?

Prior work:

- Imbedded gauges used to detect overtake of shock wave by explosive wave
- Sensitivity is time required for explosive wave to overtake shock wave
- Sensitivity has been shown to be affected by chemical and physical additives



(Dattelbaum et al. 2010)

How did we measure hot spots?

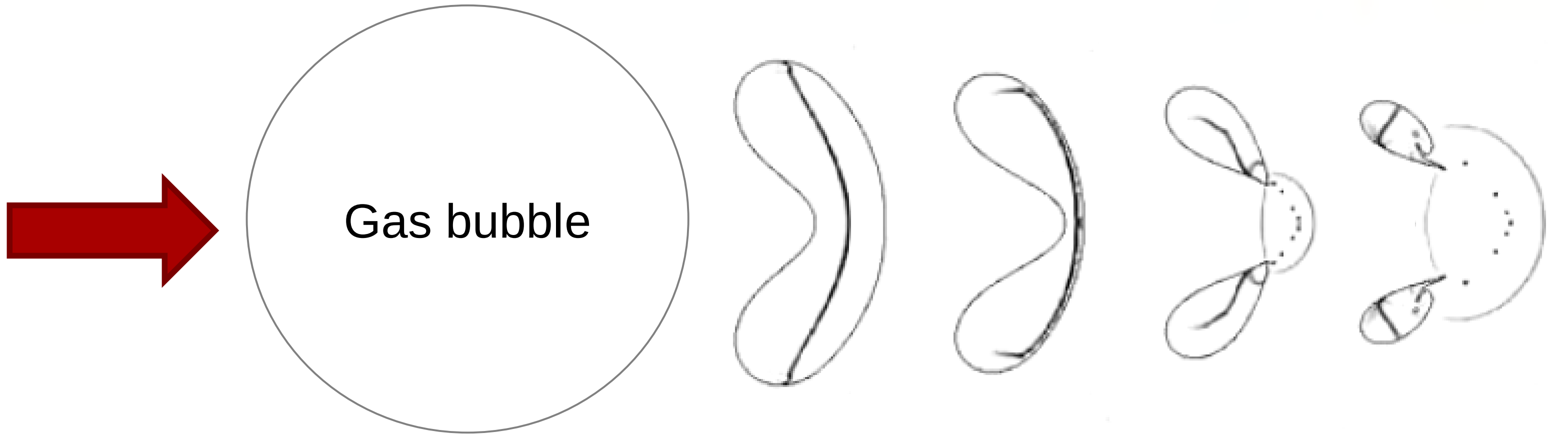
Studied transparent explosive nitromethane (NM, CH_3NO_2). This allows us to use bubbles to control hot-spot formation and optical methods to study the initiation process.

$$CH_3NO_2 \rightarrow CO_x + H_2O + H_2 + NO_x + NH_3 + \text{“soot”}, \quad -709 \text{ kJ/mol}$$

Our approach allows us to address the following questions:

- Does cavity collapse in explosives affect sensitivity?
- Can we relate formation of localized temperature peaks (hot spots) to early stages of ignition?
- Can we use imaging and other diagnostics to study this phenomenon?

What happens when an individual bubble collapses?



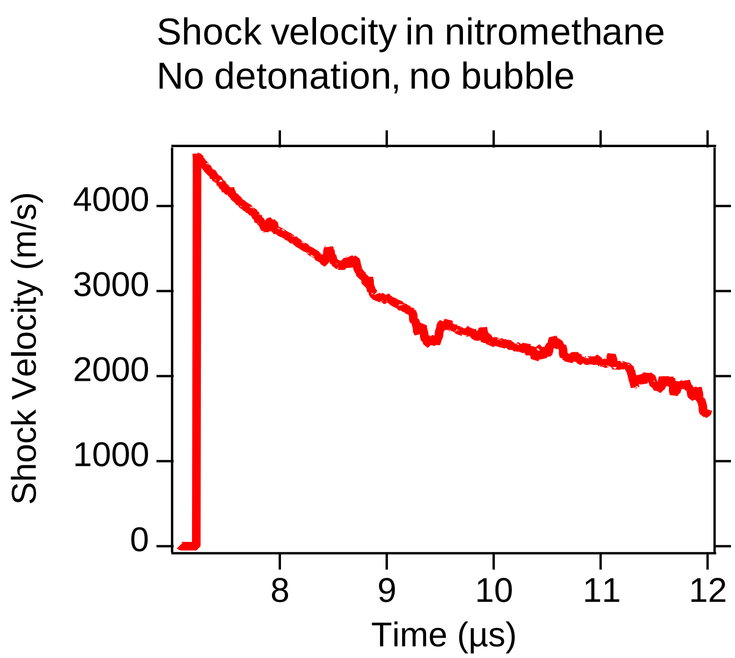
Possible mechanisms for hot-spot formation:

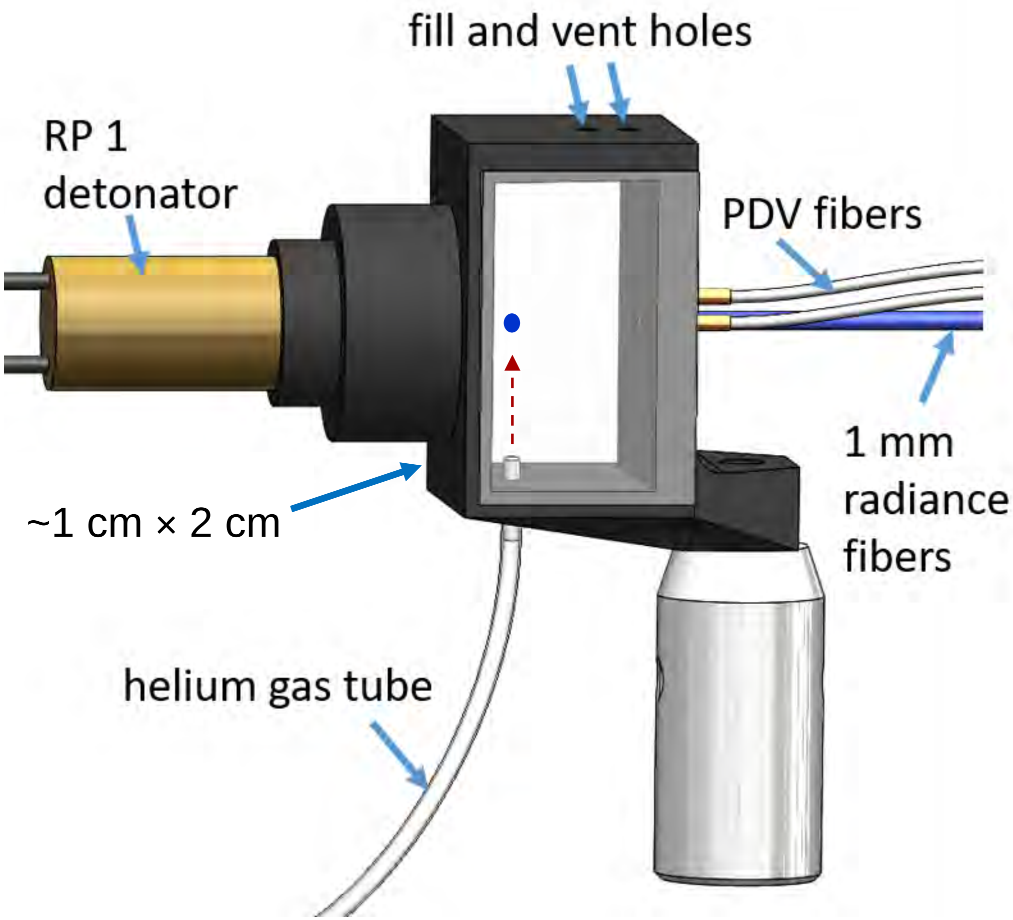
- Deformation at bubble cavity walls
- Rapid compression of gas in bubble
- Impact of jet on back of bubble

N. Bourne and A. Milne. "On Cavity Collapse and Subsequent Ignition." Paper presented at the 12th International Detonation Symposium, San Diego, CA. August 2002.

Technical approach

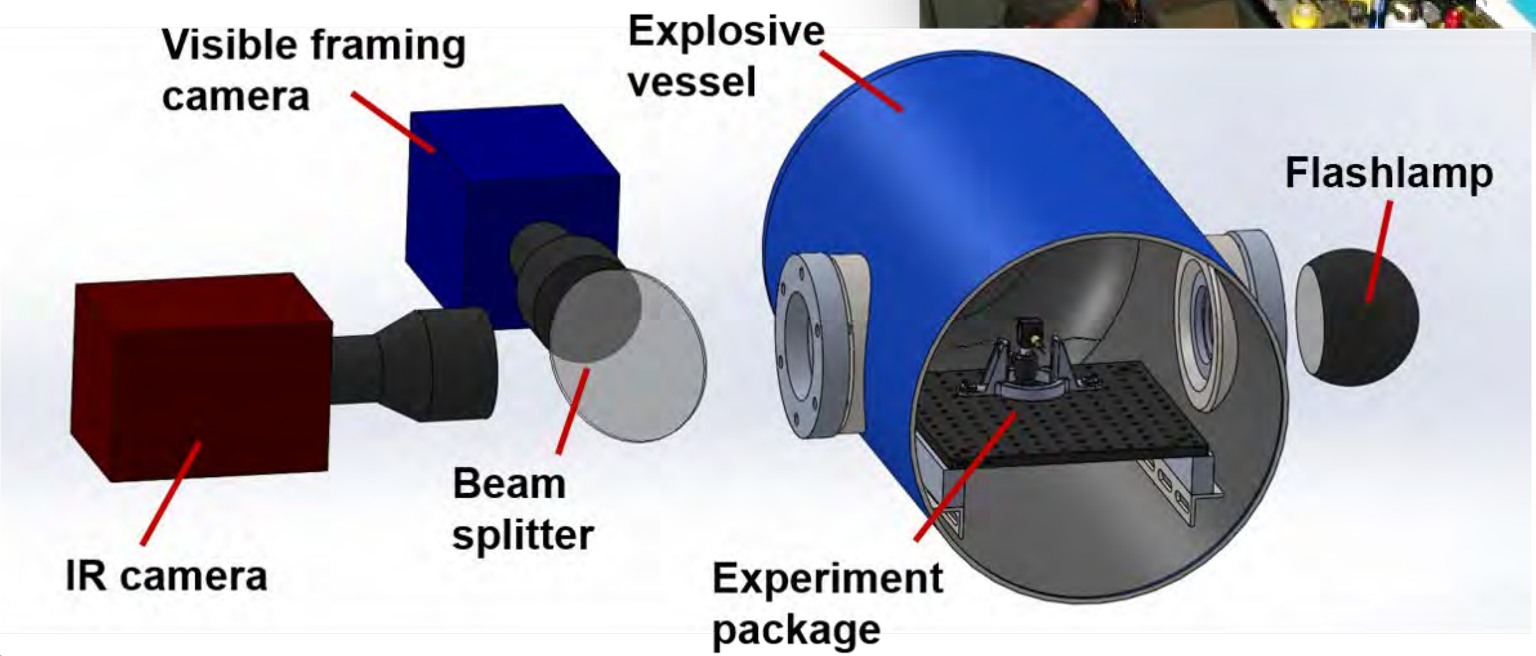
- We used a detonator to create a shock wave to collapse a bubble in nitromethane
- Change package wall thickness to adjust shock wave strength
- Decay of this shock wave in time creates some experiment limits



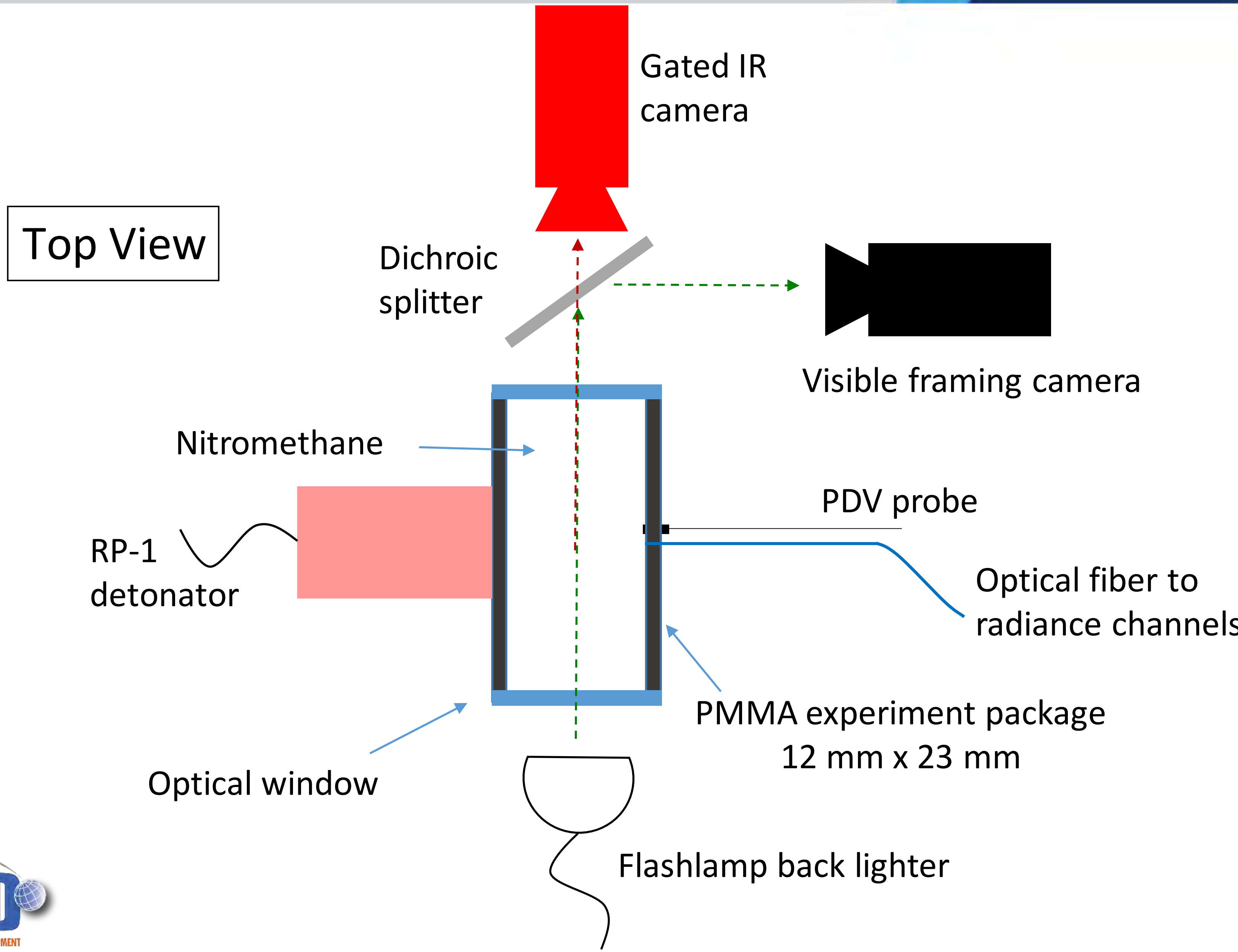


Experiment layout

Experiments were done at NNSS/STL Boom Box

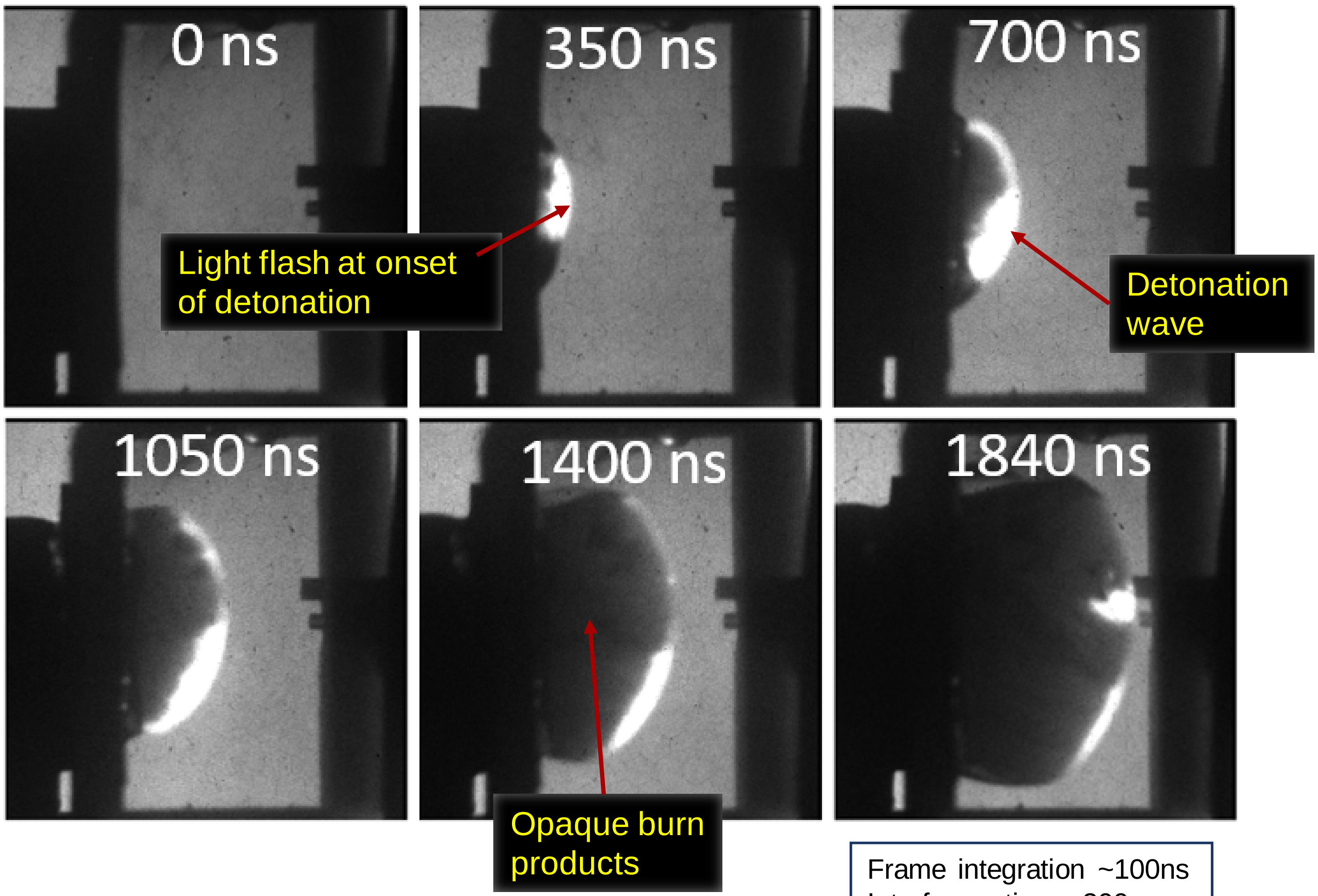


Diagnostics setup



Shocked nitromethane with detonation

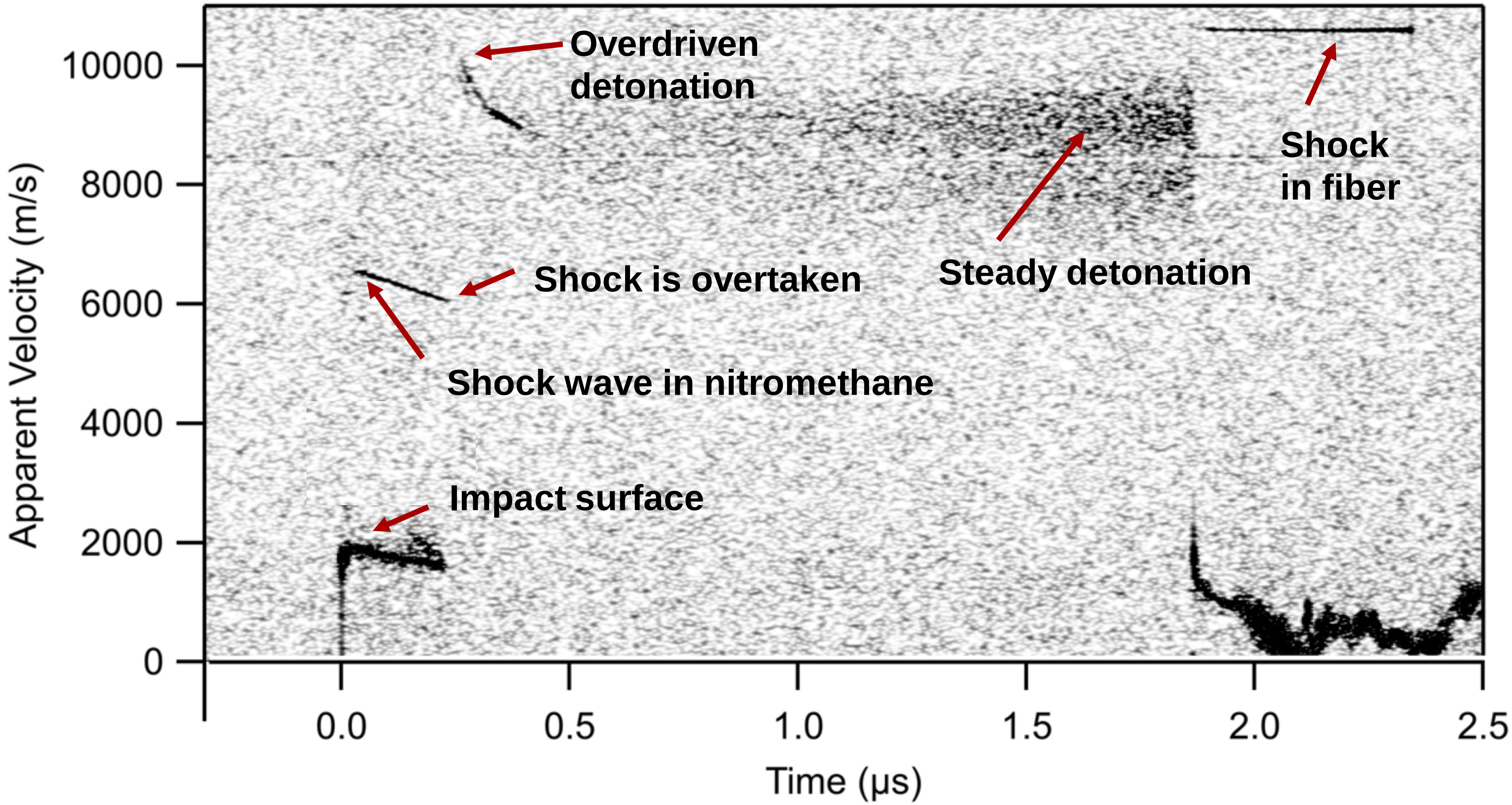
Imaging, velocimetry, pyrometry, and optical spectroscopy used to characterize detonation properties



Frame integration ~100ns
Interframe time ~300ns

Shocked nitromethane with detonation: Velocimetry

Response of nitromethane shocked to ~10 GPa



Shocked nitromethane with detonation: Velocimetry and radiance

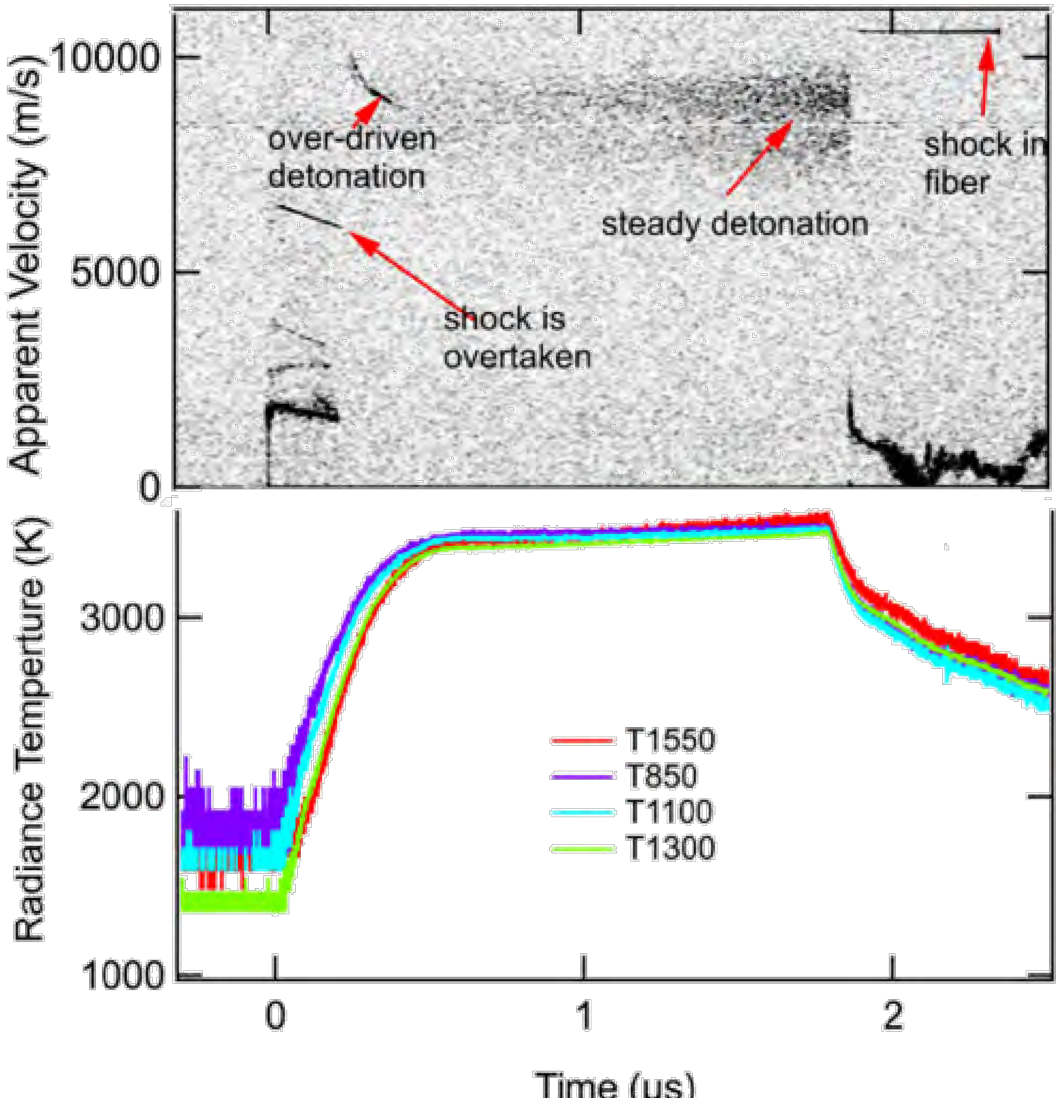
Measured interface velocity, shock and detonation waves

Overtake time ~200 ns

Velocity spread in detonation wave may indicate cellular process

Temperature rise before overtake indicates onset of thermal explosion

Peak radiance T > 3000K consistent with detonation



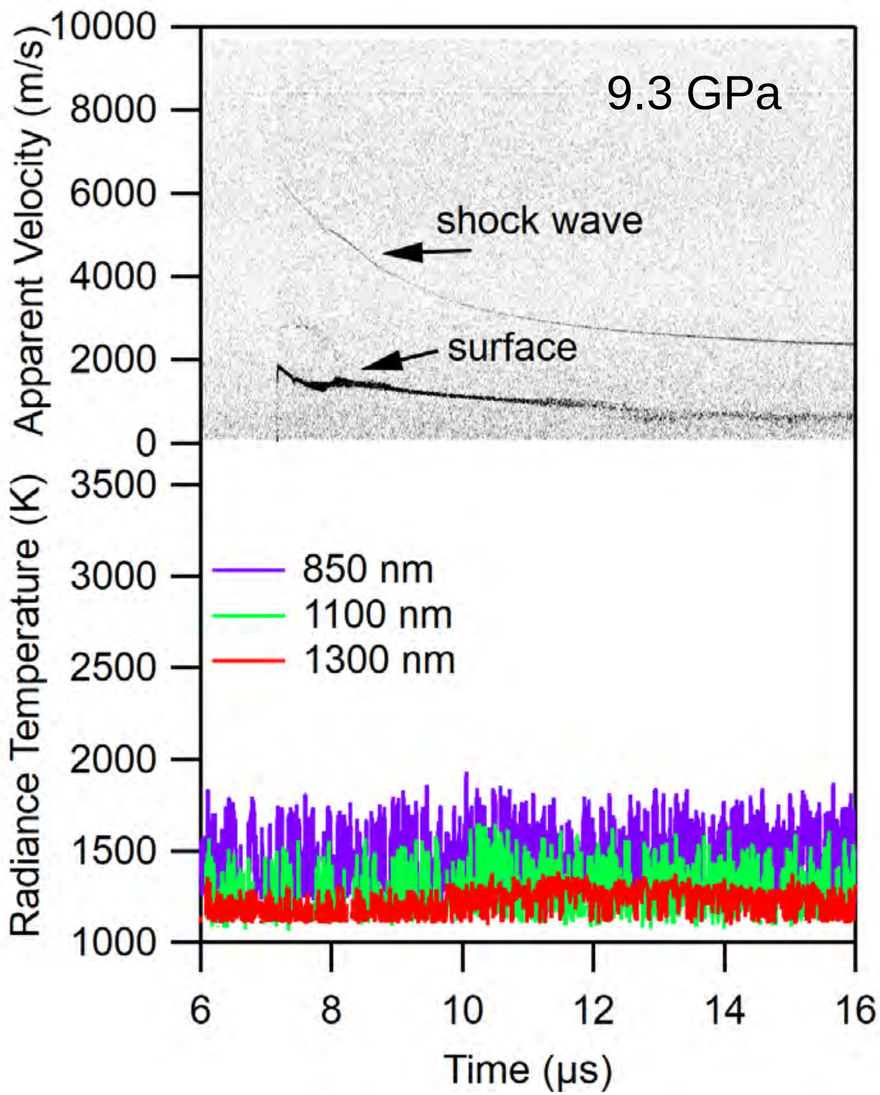
Shocked nitromethane with no detonation: Velocimetry and radiance

Apparent velocities with no bubble and no detonation.

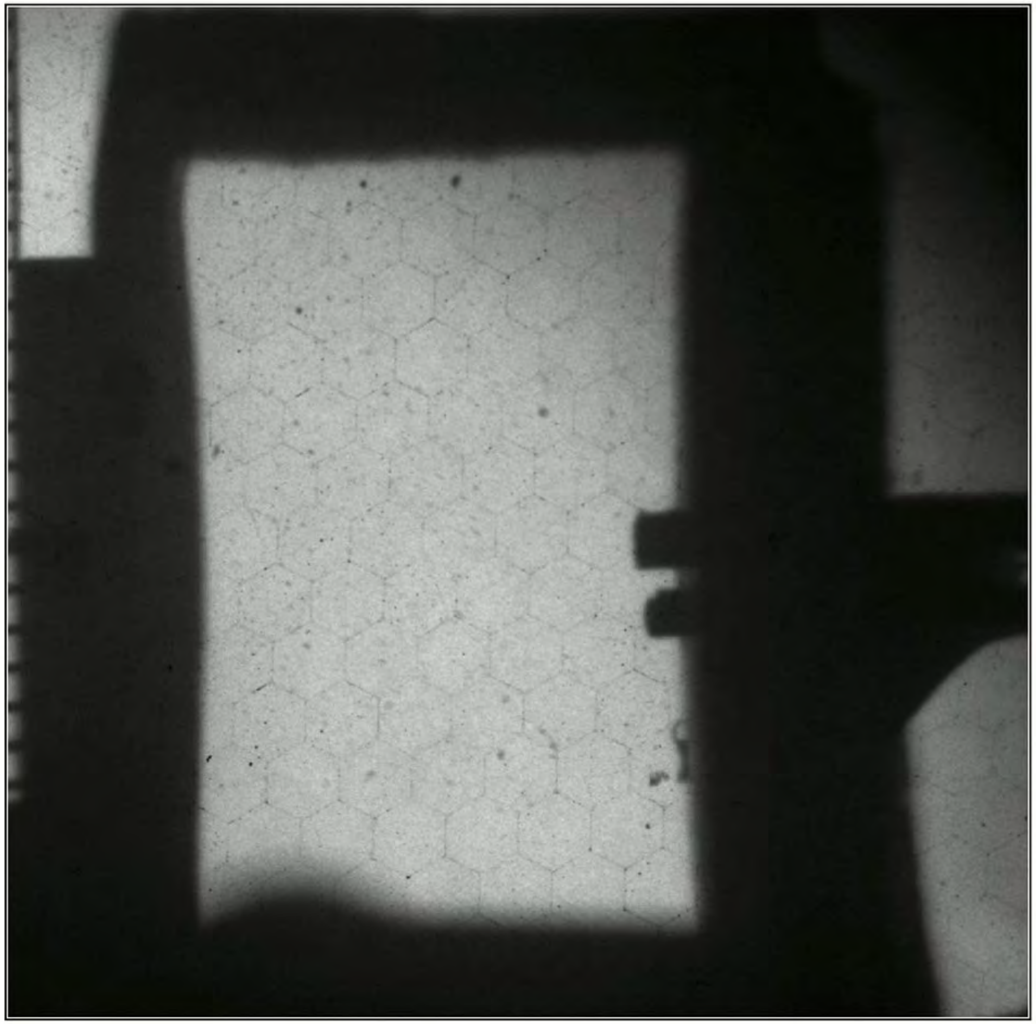
Decaying shock wave in nitromethane and motion of package surface resolved.

Peak shock velocity is 4.57 km/s, consistent with literature.

Radiance temperatures are below the detectability in the three spectral channels.



Bubble collapse movie

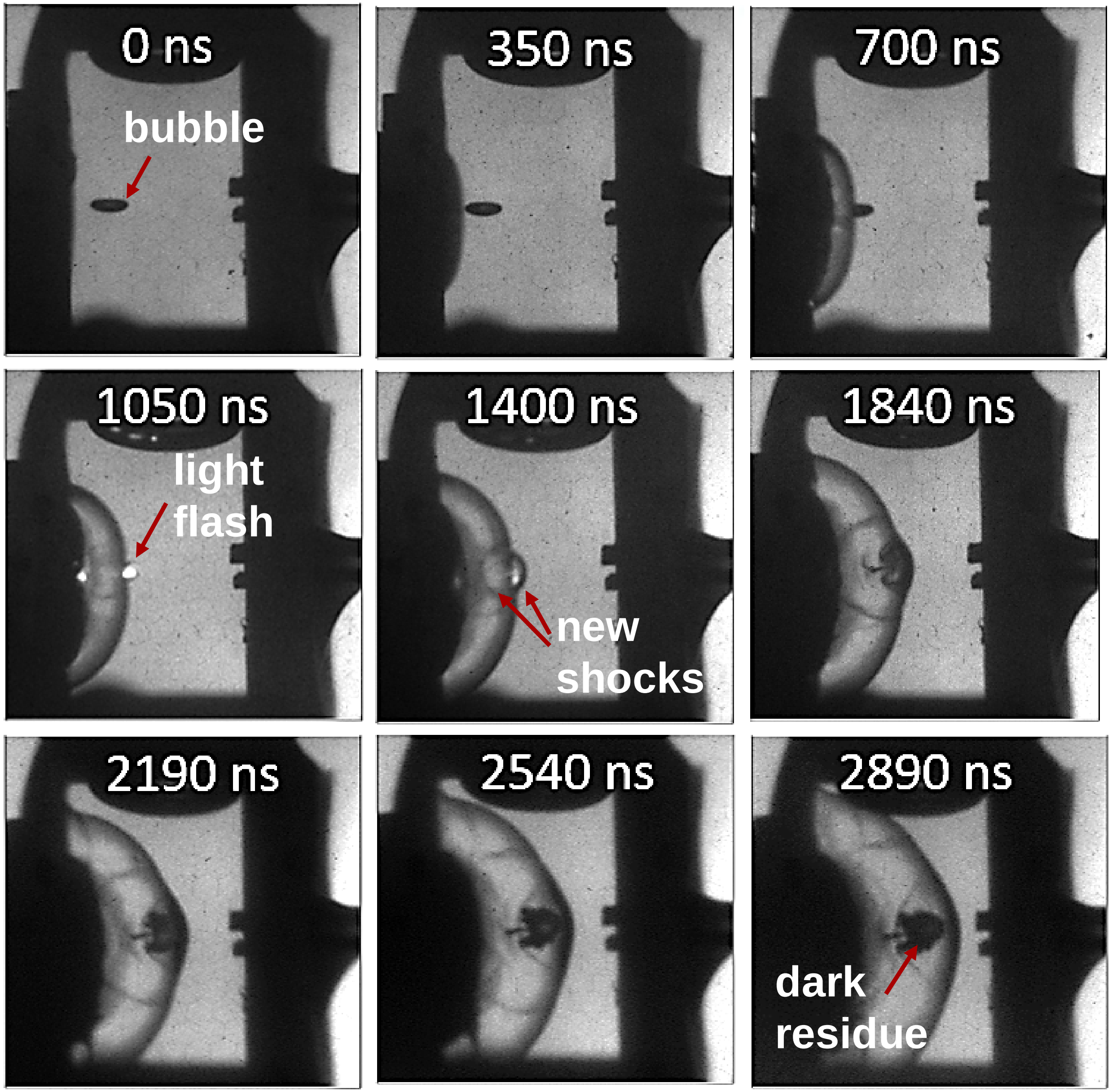


Character of bubble collapse and partial detonation

Light flash at bubble collapse on leading edge of shock wave

Forward collapse and back collapse shock waves

Dark residue after flash



Bubble collapse: Velocimetry and radiance

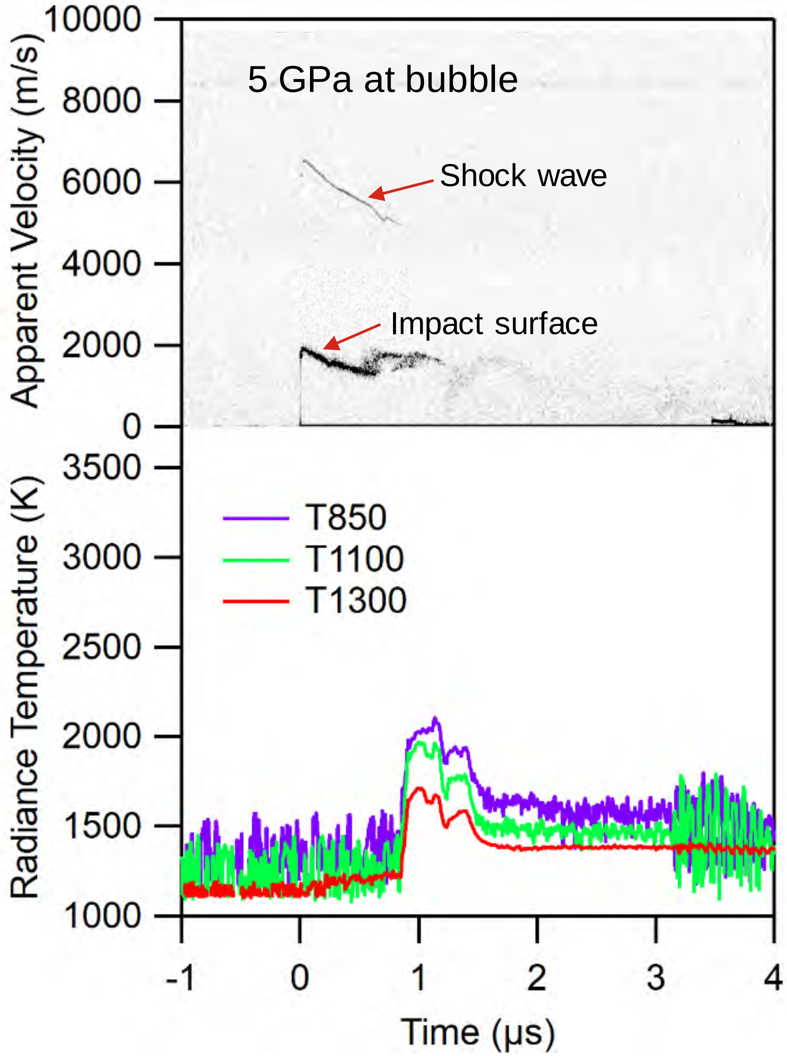
Observed interface motion and shock wave in nitromethane

Signals drop out when wave collapses bubble

Temperature pulse at bubble collapse

Emissivity affected by limited fill of optical fiber

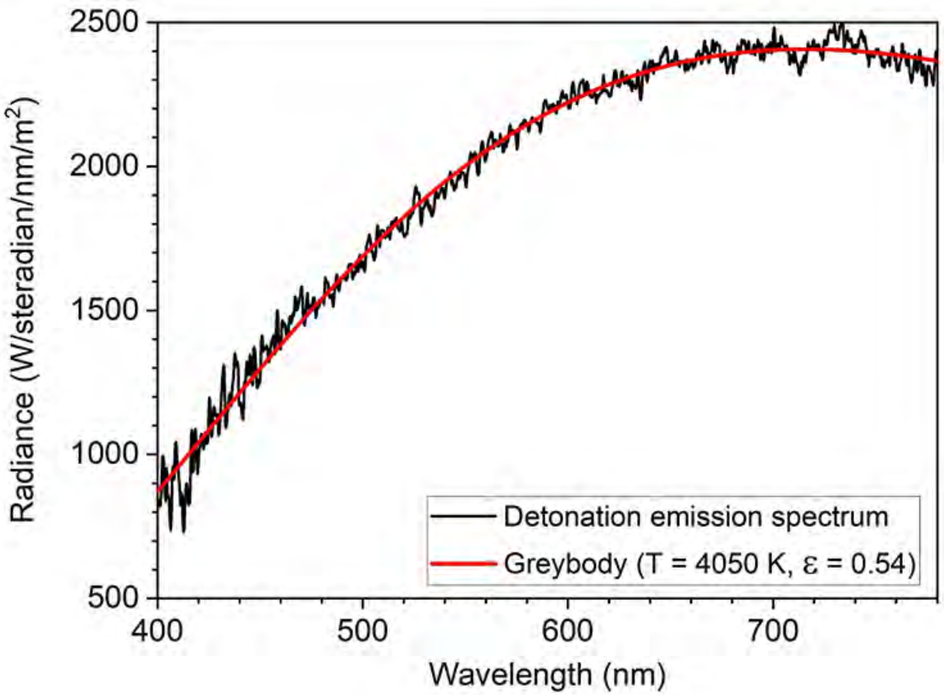
Actual temperatures likely much larger



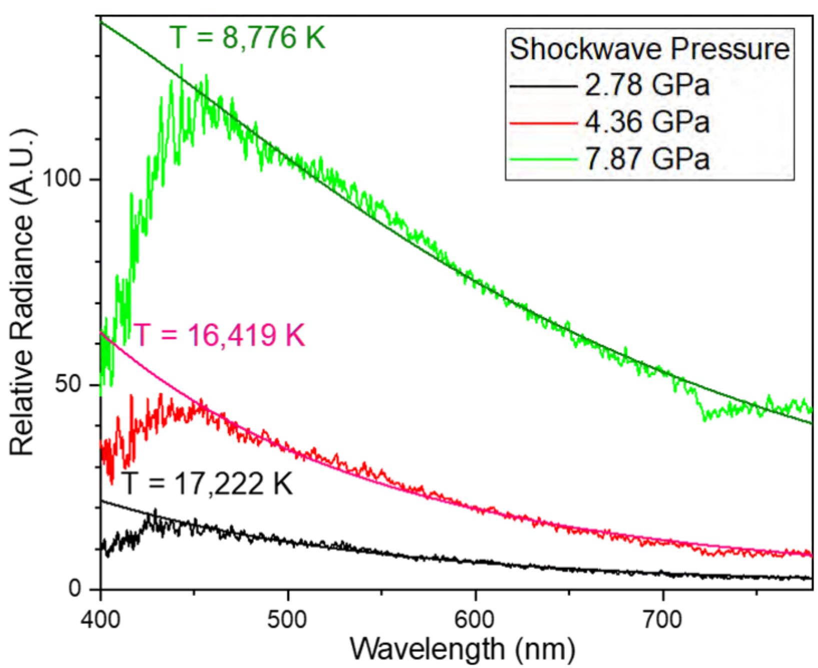
Spectrum of emission from detonation and bubble collapse

- Emission from detonating nitromethane fits well to Planck blackbody temperature function.
- Emission from bubble collapse is complex and probably a combination of nitromethane emission and helium plasma.

Detonation



Bubble collapse no detonation



Spectra are corrected for system response and ambient absorption of nitromethane.

Modeled bubble collapse and extent of explosive reaction

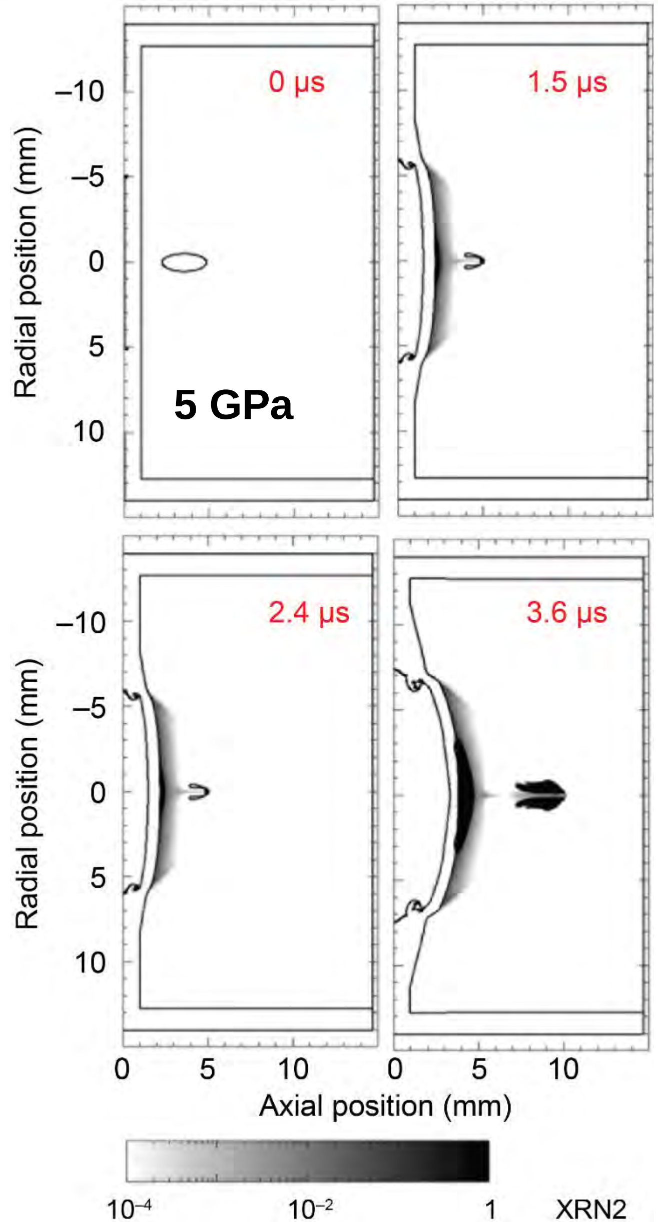
Used Sandia Eulerian code CTH to model general features such as extent of reacted material (XRN)

Assume 2D cylindrically symmetric ellipsoid (vs. oblate spheroid)

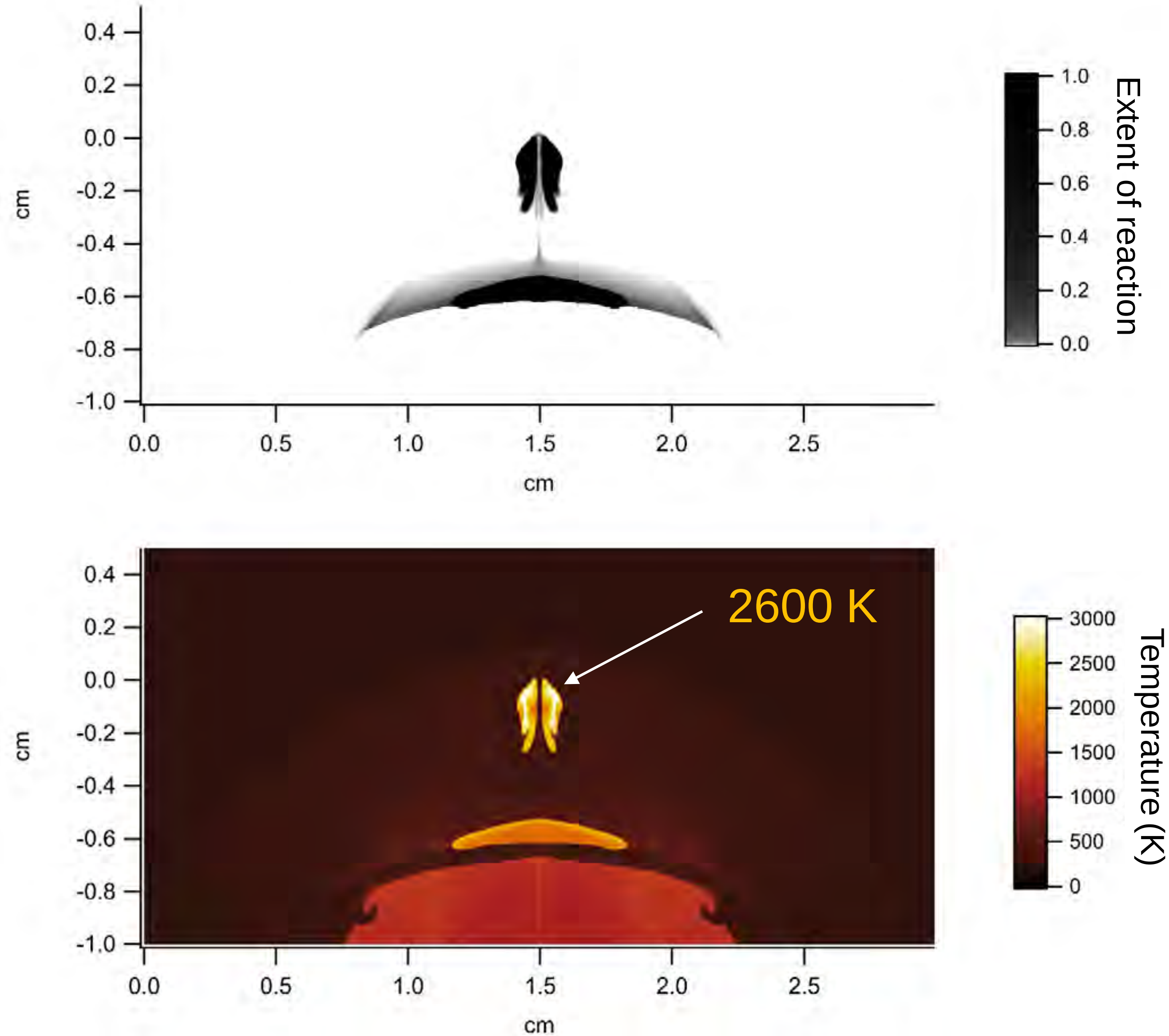
Unreacted nitromethane and detonation products are modeled with Mie-Grüneisen and SESAME EOS models

Arrhenius reactive burn (ARB) used to predict the nitromethane burn

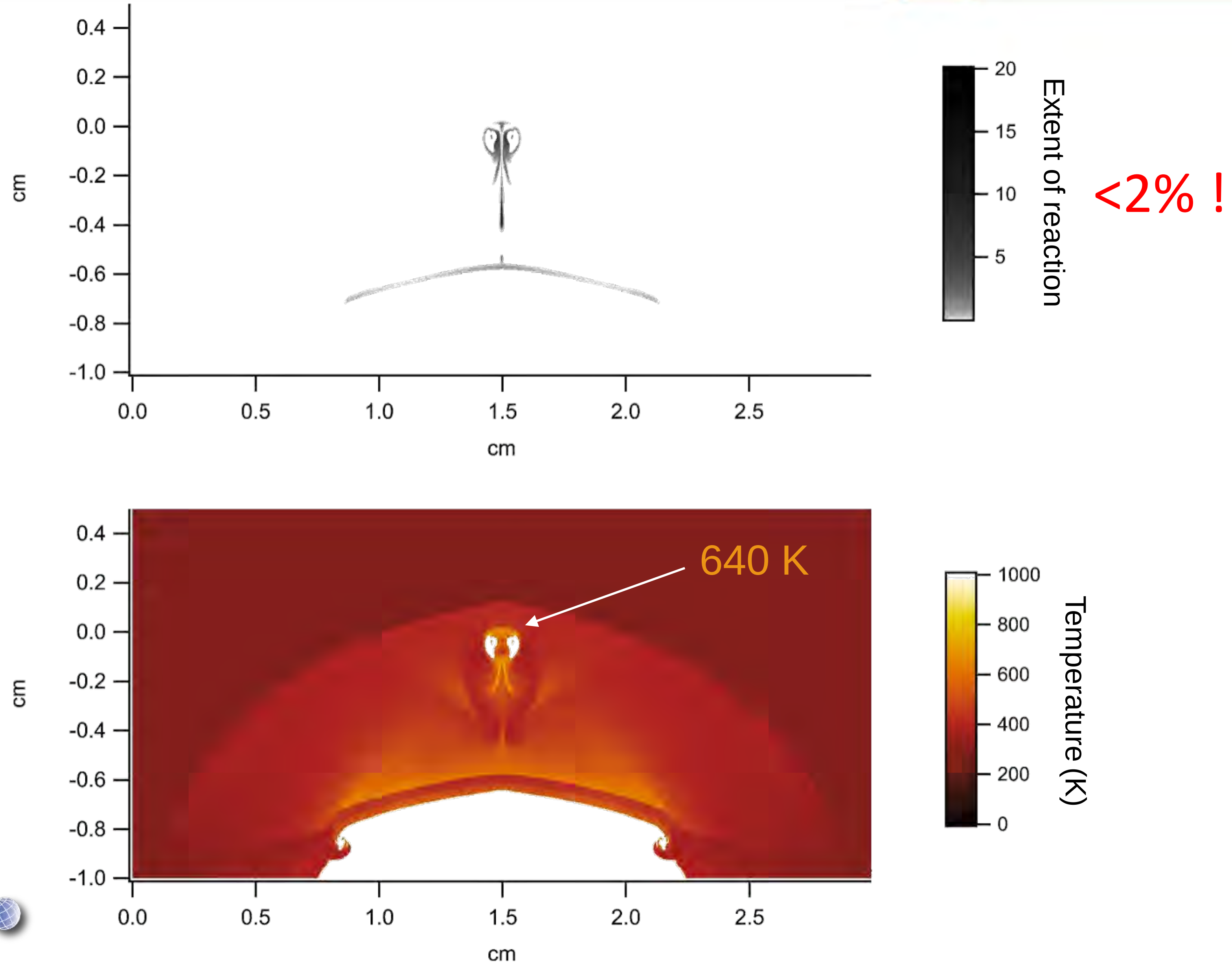
Shape of opaque residue similar to observed shapes in experiment images



Arrhenius reactive burn (ARB) model

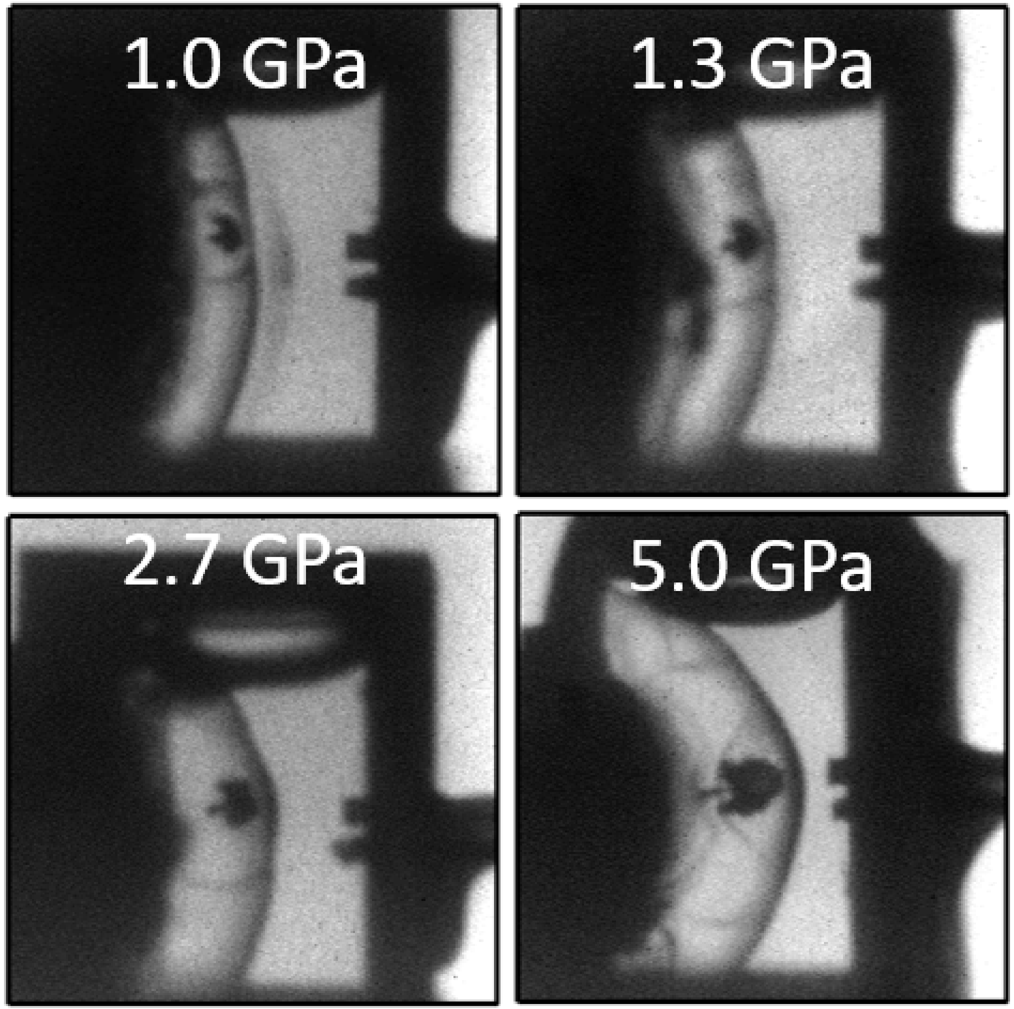


History variable reactive burn (HVRB) model

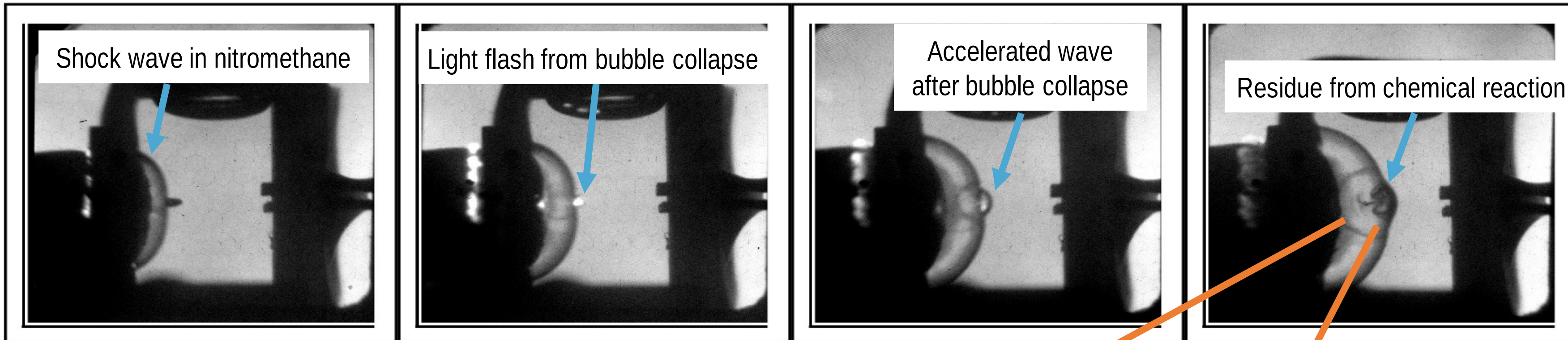


Reaction depends on input stress

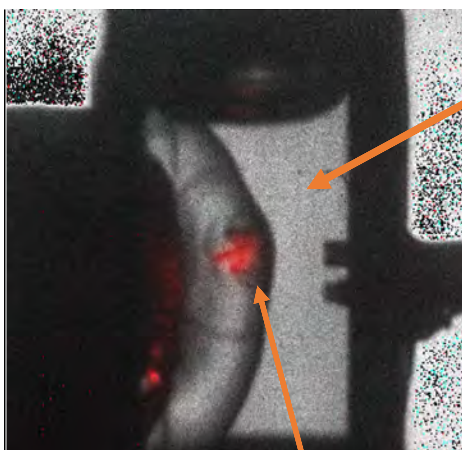
Volume of residue (extent of reaction) increases with input stress at bubble



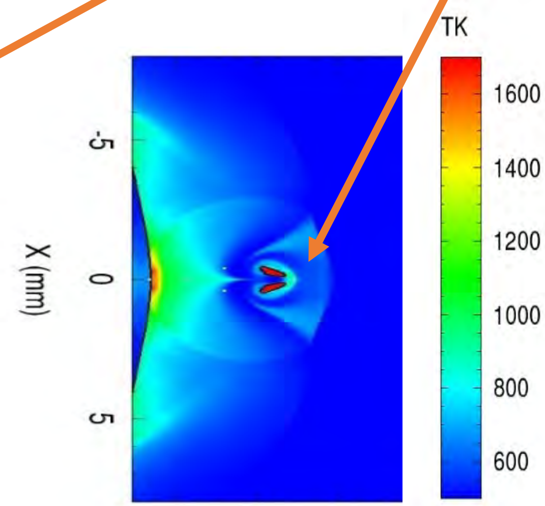
Measurements and modeling help us understand effects of bubble collapse



Overlay of visible and IR images

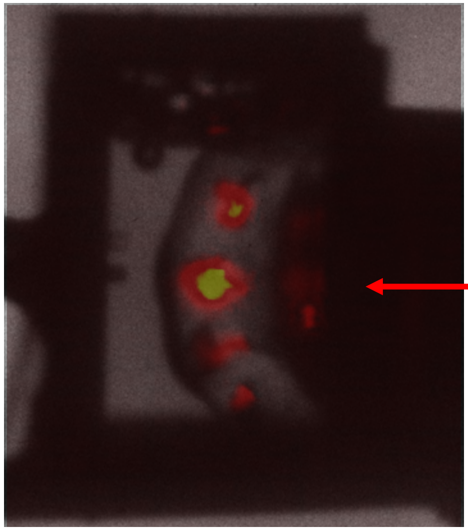


Peak radiance temperature
~1100 K

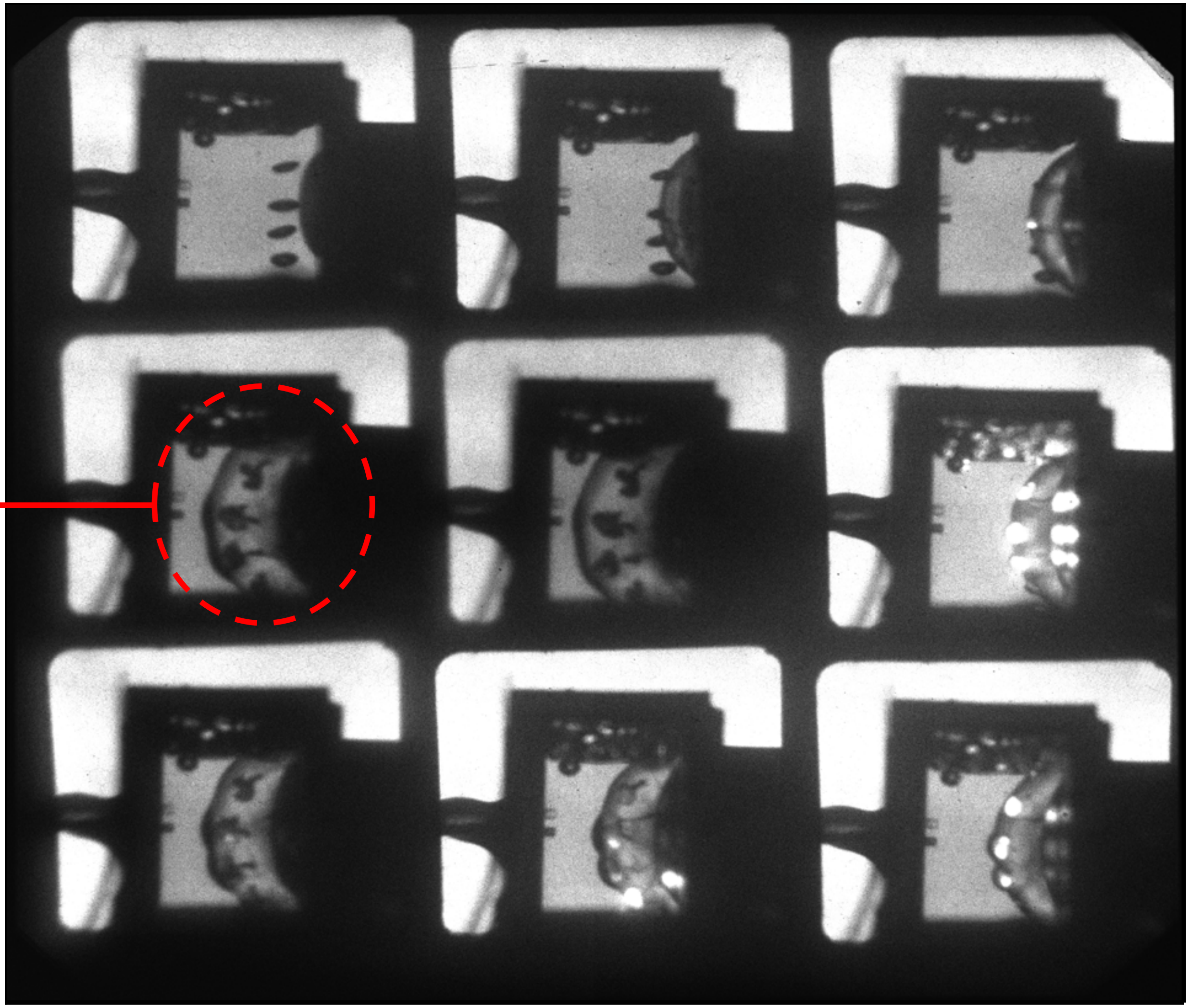


Calculated temperature
from bubble collapse

How do multiple bubbles affect the process?



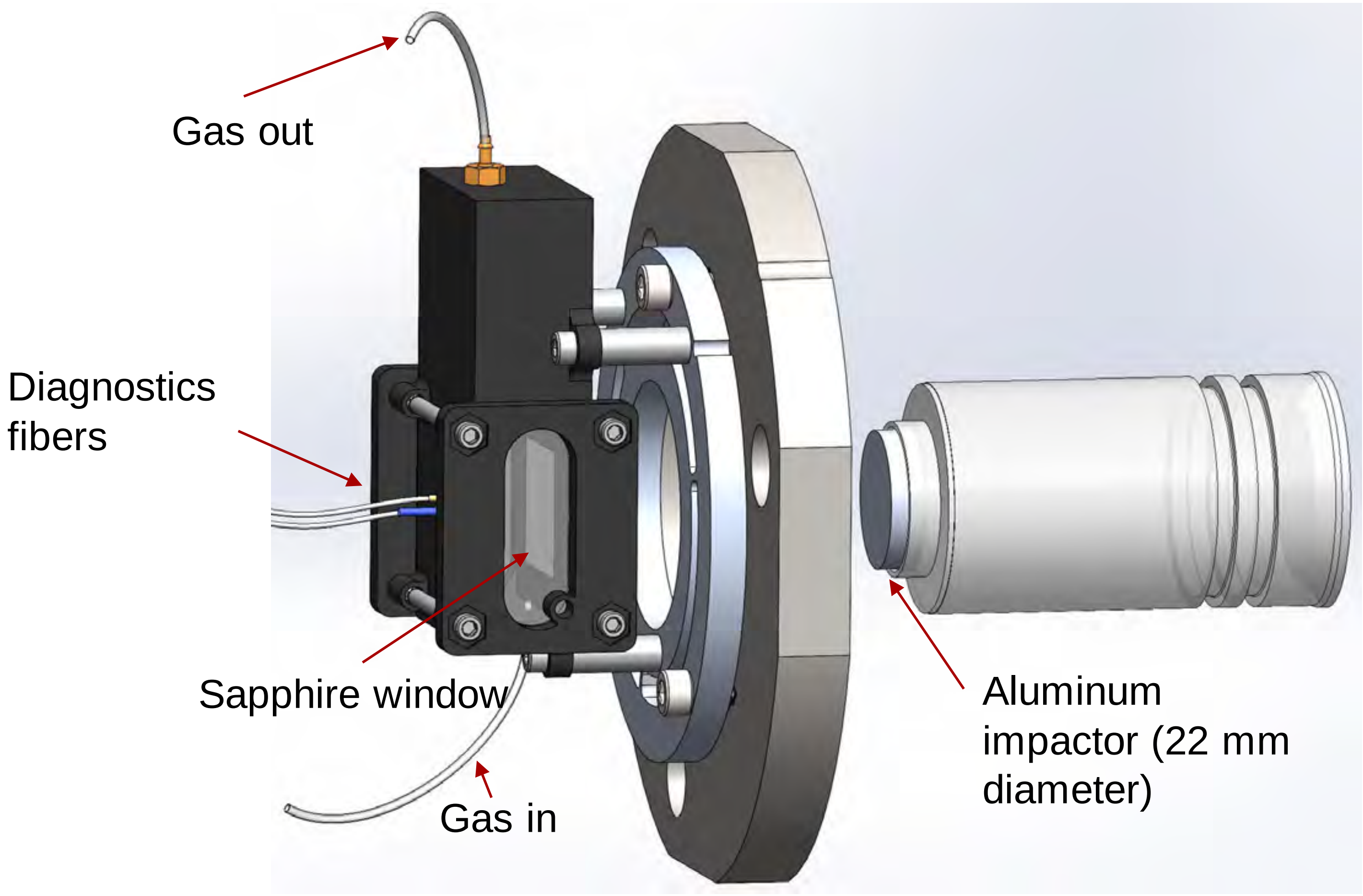
Overlay of IR and visible images



190429_001, 2 mm buffer, 4 bubbles, 1μl DETA

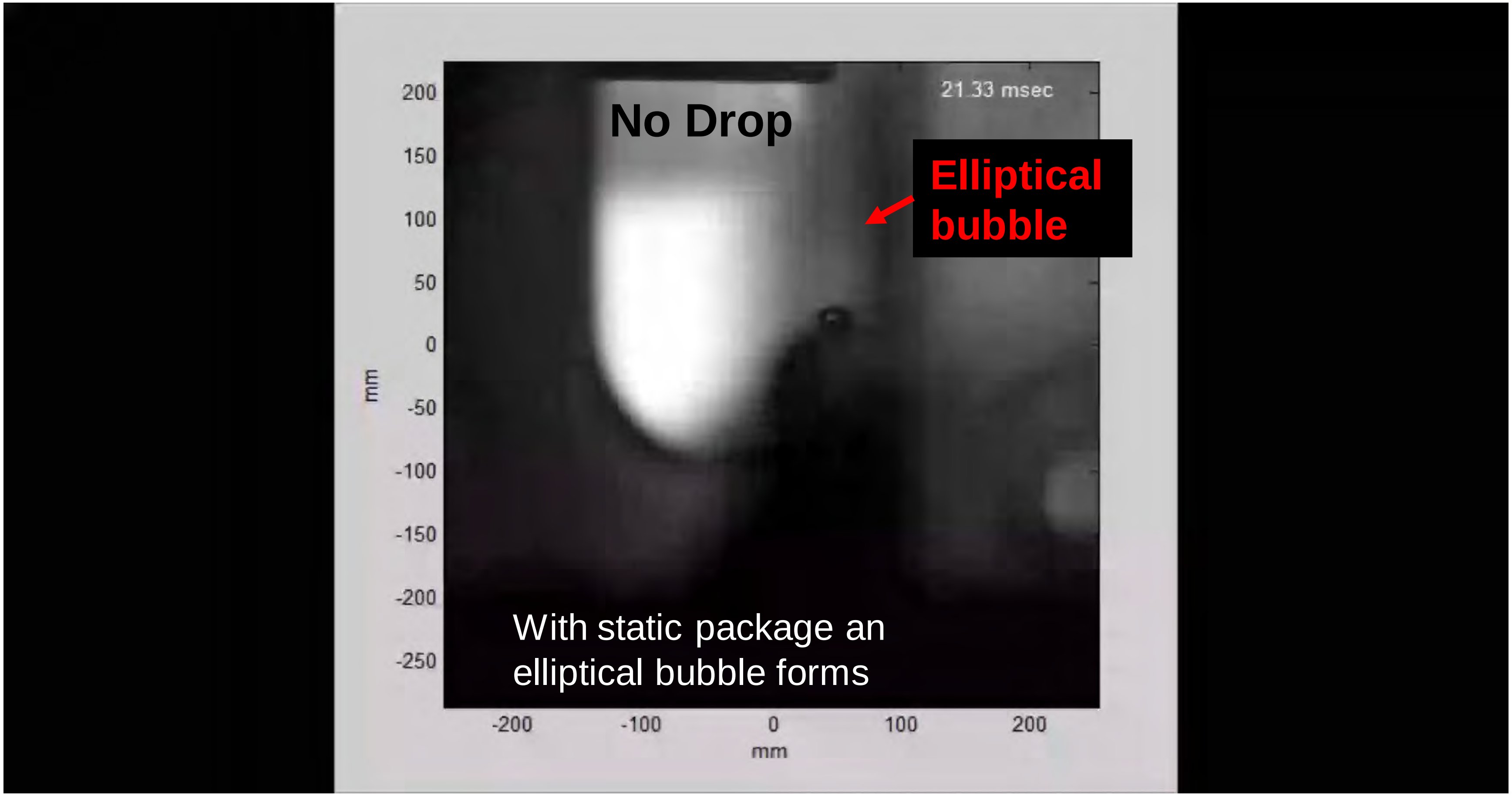
How can we better control bubble effects?

Do supported shock (powder gun) experiments

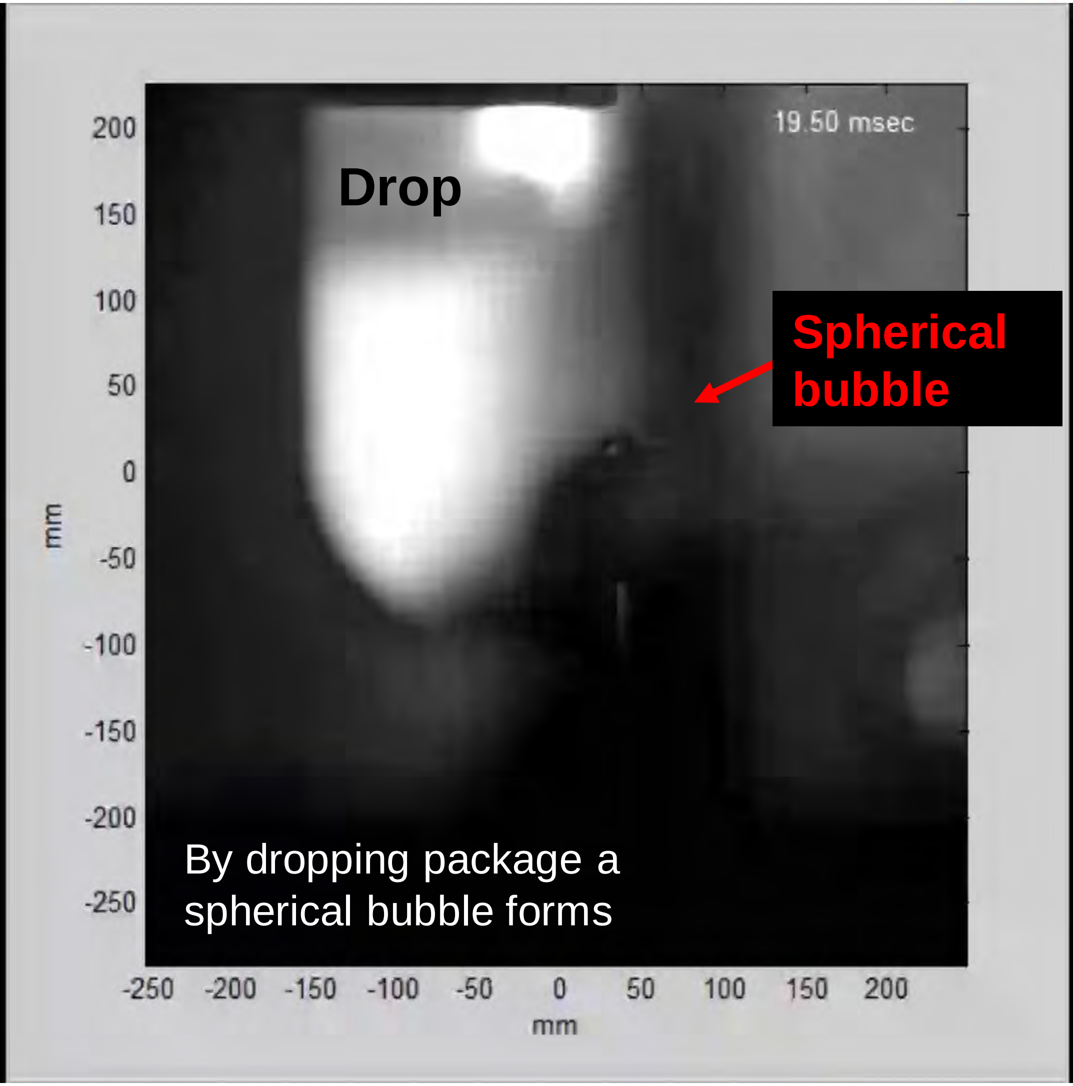


Package for powder gun experiments

How can we create a spherical bubble?

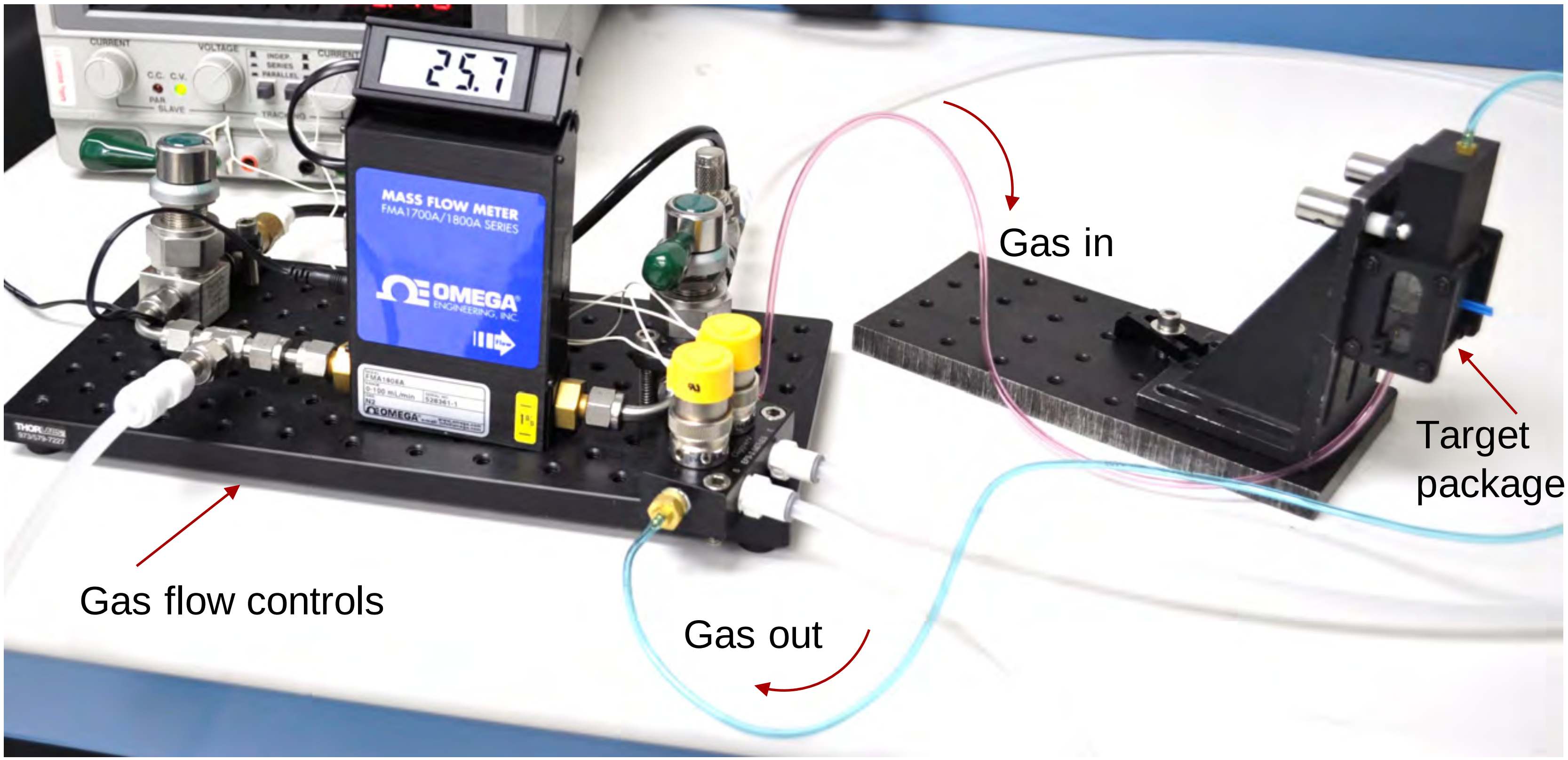


If we “drop” the whole liquid cell, the effects of gravity are minimized and a spherical bubble forms in ~10 milliseconds.



Prototype gun package

- Prototype target package with gas flow system has been assembled and bench tested.
- Next step is to make it work in evacuated gun chamber.



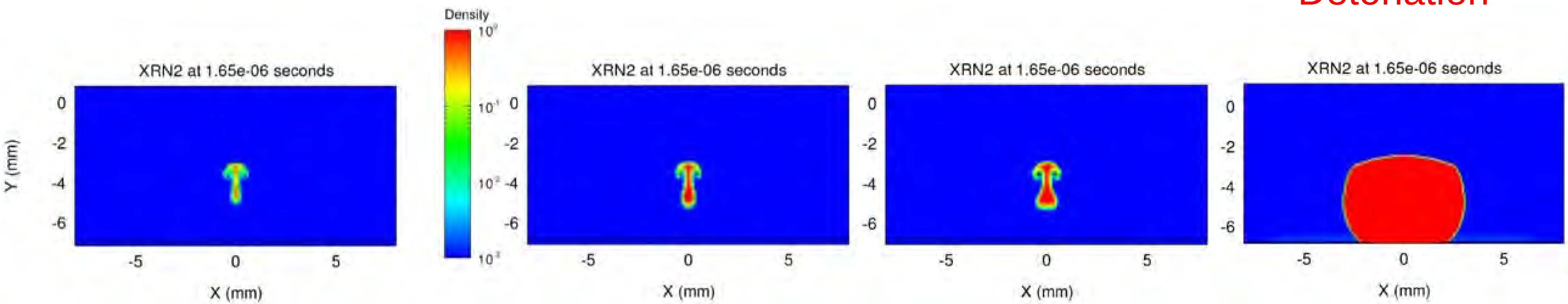
SDRD SITE-DIRECTED RESEARCH & DEVELOPMENT

We did some detonation chemistry simulations

How does bubble collapse contribute to the onset of detonation?
At what stress does the bubble collapse lead to sustained detonation?

CTH calculations

~8 GPa
Detonation



u_{imp} = 2.15 km/s

u_{imp} = 2.20 km/s

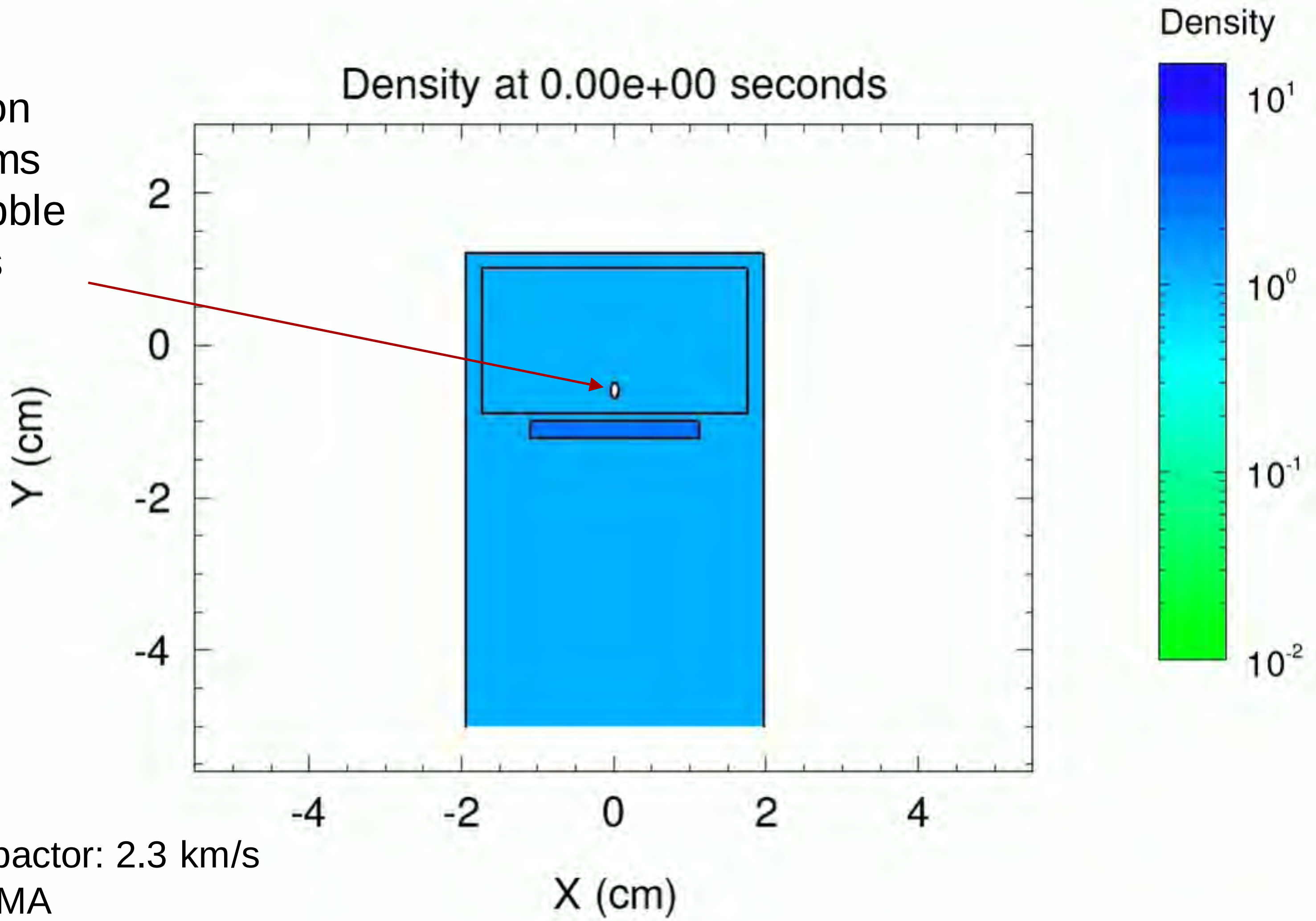
u_{imp} = 2.22 km/s

u_{imp} = 2.25 km/s

Extent of chemical reaction (XRN) in shocked nitromethane

CTH used to model supported shock experiments

Detonation wave forms when bubble collapses



Aluminum impactor: 2.3 km/s
Package: PMMA
Peak stress in NM ~ 8 GPa

SITE-DIRECTED RESEARCH & DEVELOPMENT

Summary of nitromethane experiments

Current status:

- We recently published our results of bubble collapse effects in nitromethane.

> W. D. Turley, B. M. La Lone, J. G. Mance, M. D. Staska, G. D. Stevens, L. R. Veeser, and D. M. Dattelbaum, "Experimental observations of shock-wave-induced bubble collapse and hot-spot formation in nitromethane liquid explosive," *J. Appl. Phys.* **129**, 145102 (2021), https://doi.org/10.1063/5.0039414.

- We designed and assembled prototype package for powder gun experiments.

What's next:

- Demonstrate functional gun package in vacuum chamber.
- Fabricate all components for gun experiments.
- Adapt triggering scheme and other diagnostics for gun shots.