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MESOSCALE REACTIVE BURN MODELS OF SHOCK INITIATION IN VAPOR-DEPOSITED PETN FILMS

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APS Shock Compression of Condensed Matter Conference

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MOTIVATION

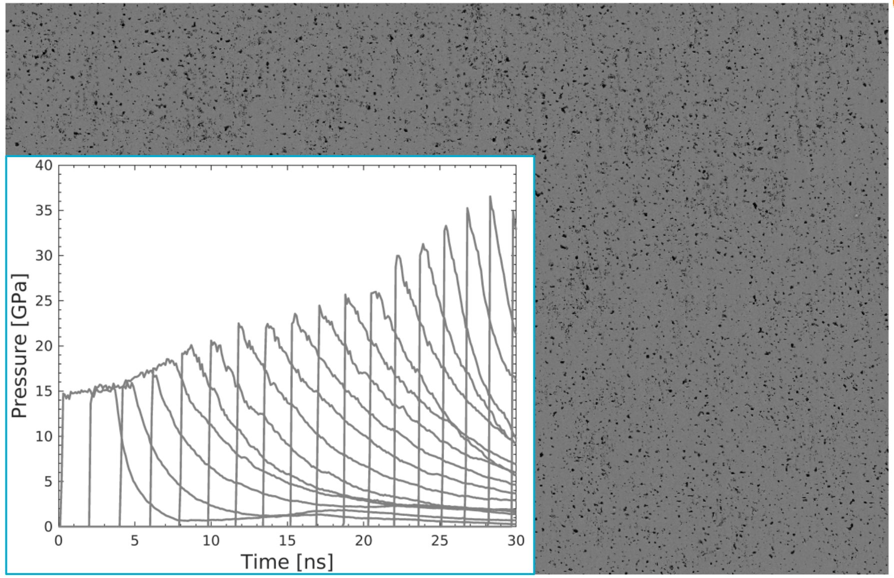
Microstructure of an explosive influences the shock-to-detonation behavior

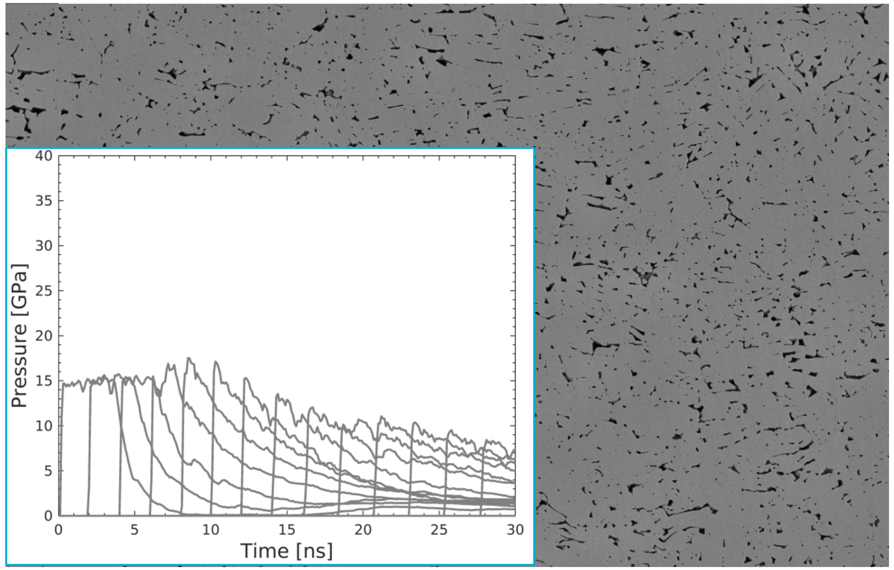
Aging and thermal environments have the potential to affect microstructure through:

- Grain coarsening
- Grain sintering
- Changes in porosity distribution

Objective: Develop hydrocode models to predict effects of aging on initiation thresholds and growth to detonation observed in PETN experiments

- ➢ Joe Monti: Phase-Field Modeling of Aging of Energetic Thin Films *(E06 - Monday 2:15 pm)*
- ➢ Rob Knepper: Effect of Accelerated Aging on Microstructure and Initiation of Vapor-Deposited PETN Films *(V03 – Thursday 10:30 am)*





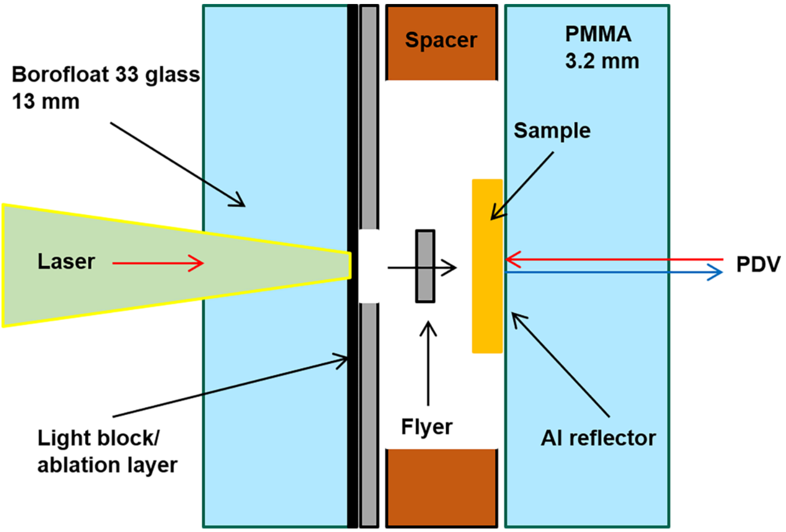
Pressed explosive with different grain sizes. Simulations following flyer impact at the same velocity.

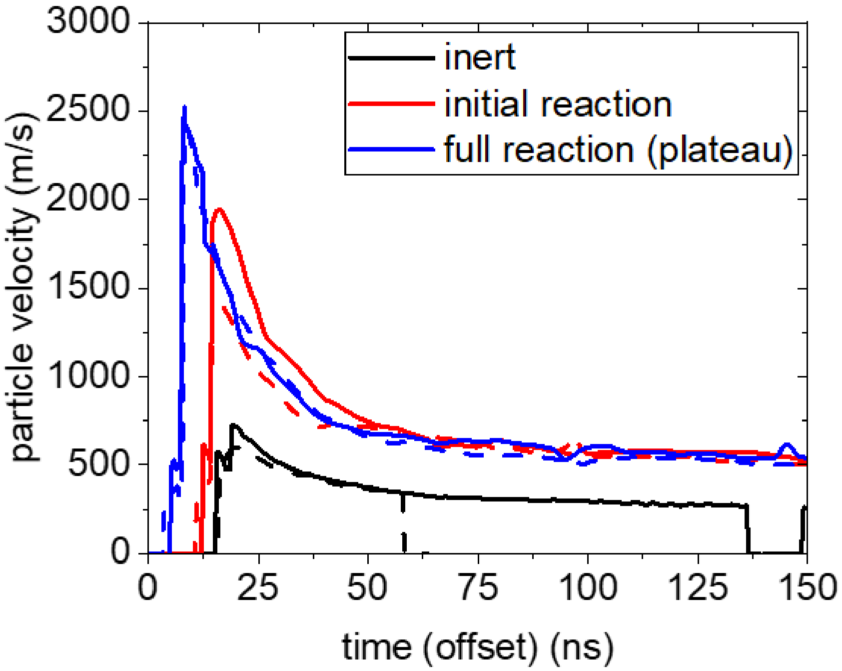
HIGH-THROUGHPUT INITIATION (HTI) EXPERIMENTS

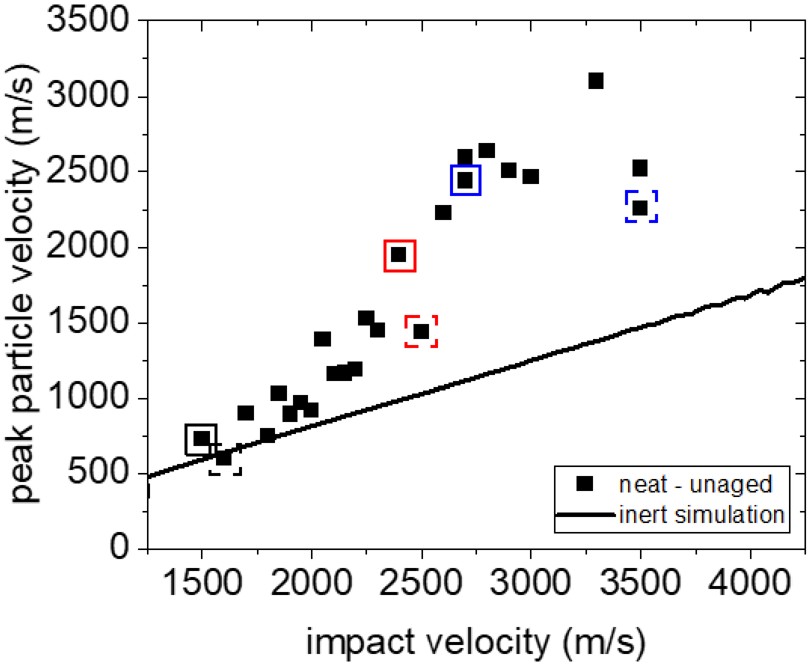
Flyer characteristics define impact shock parameters

- Flyer material (Parylene C) and impact velocity define pressure
- Flyer thickness (25 μm) defines shock pulse width

Transmitted shock wave provides evidence of reaction in sample

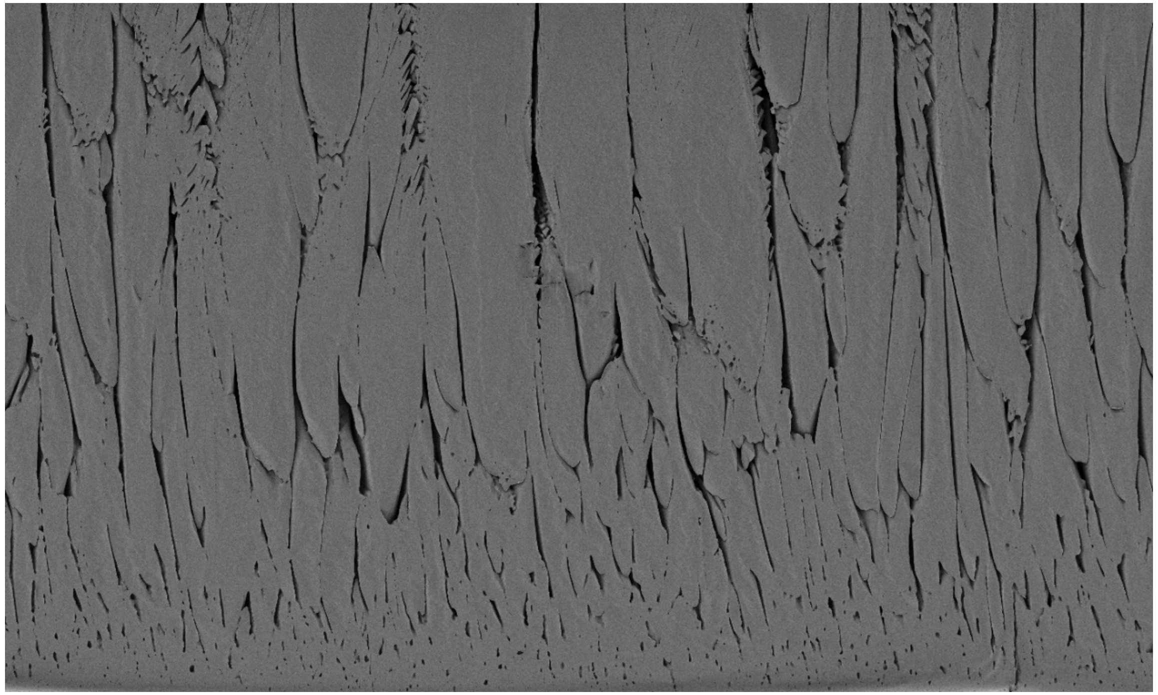




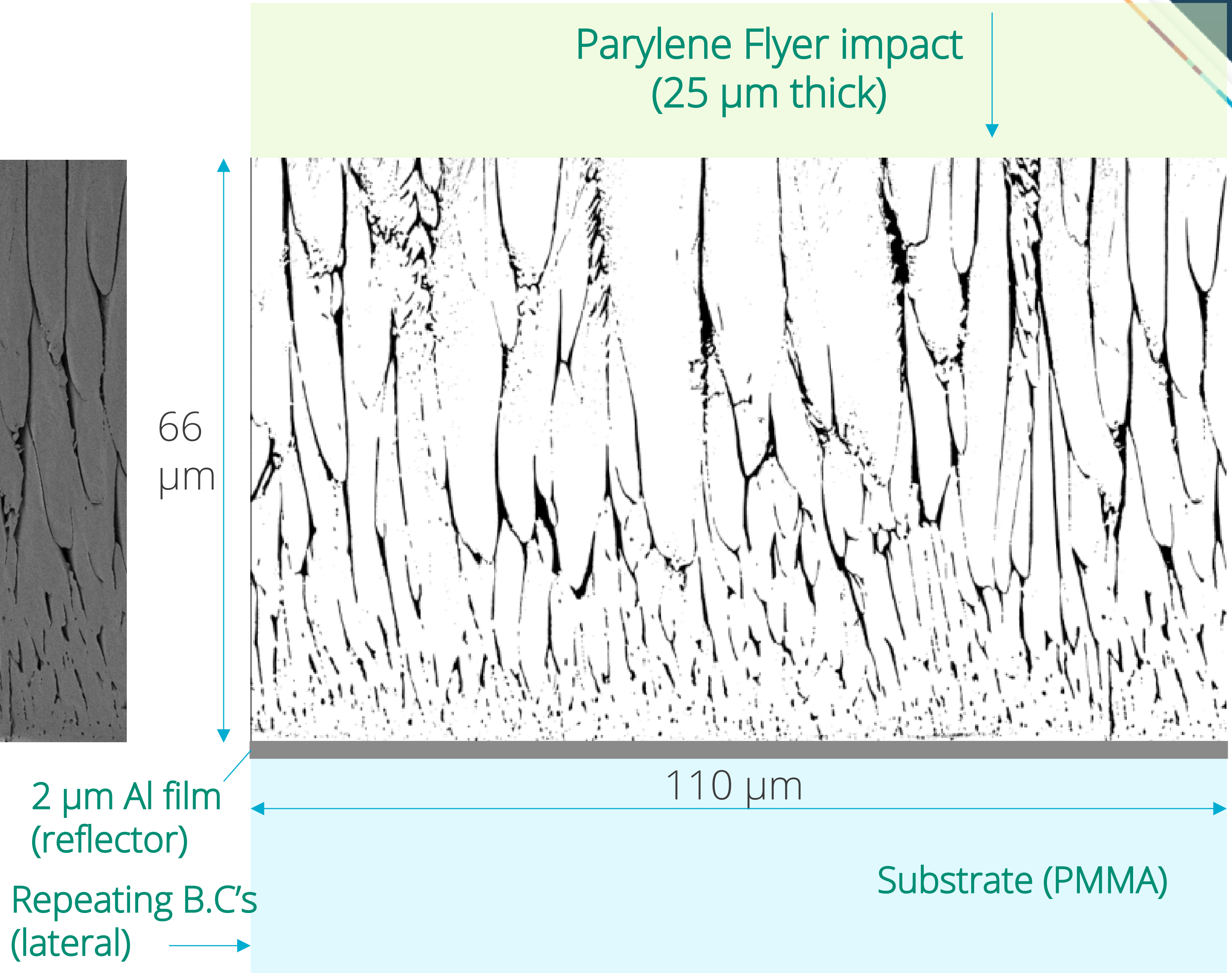


See Rob Knepper's talk on HTI experiments and microstructure characterization of PETN samples (V03: Thurs. 10:30 am)

MODEL DESCRIPTION - MICROSTRUCTURE



Ion-polished cross-section of PETN film (110 μm FOV)



Binarized image is imported into CTH hydrocode model (20 nm mesh resolution)

MODEL DESCRIPTION – MATERIAL PROPERTIES FOR PETN

Equations of State:

- Unreacted solid (UR):
  - Sesame table with temperature-dependent specific heat as described by [1]
- Reaction Products (RP):
  - Sesame table calculated by TIGER [1]

The rate of conversion of unreacted solid to high pressure reaction products is governed by **temperature dependent kinetics**:

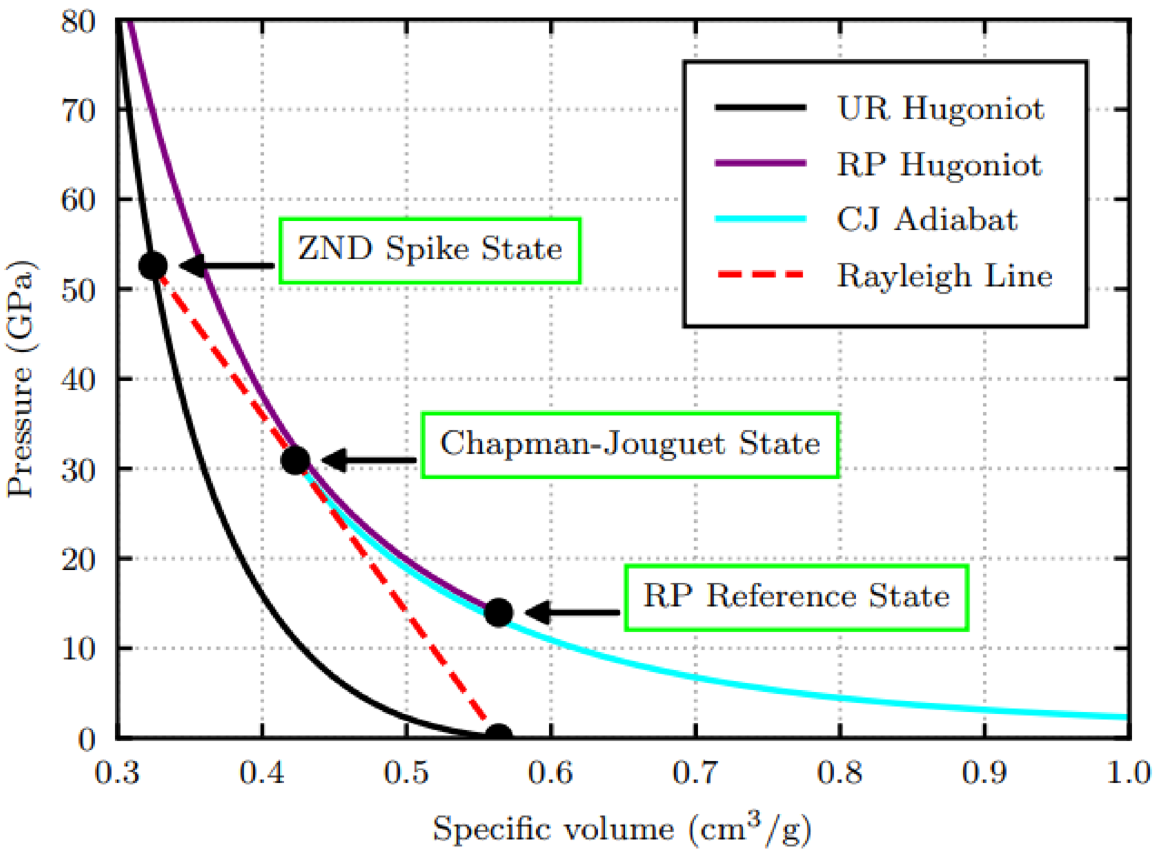
- Global reaction kinetics for PETN derived from physical chemistry and experimental data by Bryan Henson (LANL)

$$k = A \exp(-E/RT)$$

Material strength:

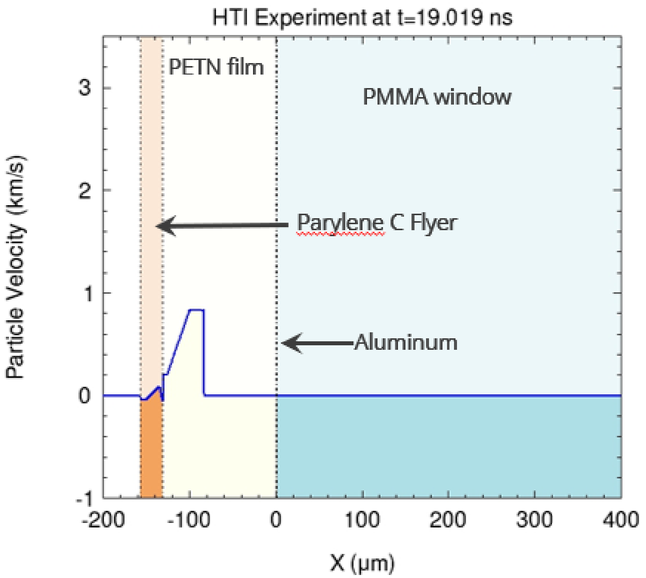
- Elastic-plastic model with yield strength of 1 GPa

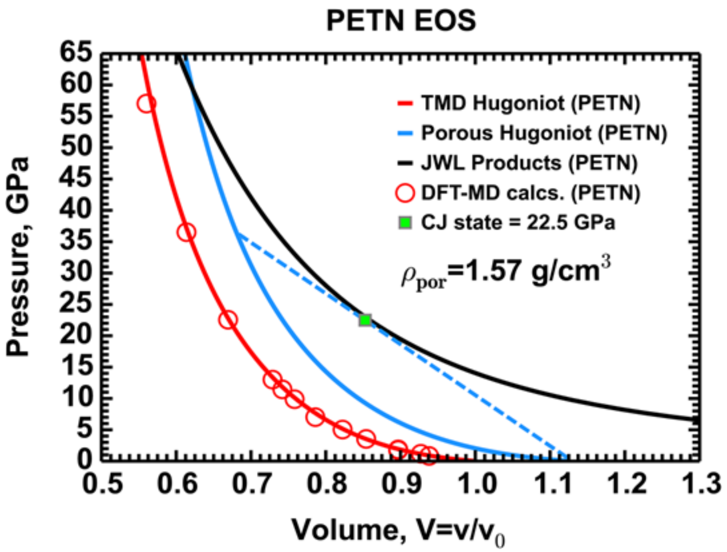
1. Kittell, et al., J. Appl. Phys. 131, 154902 (2022)



P-v diagram of Hugoniots of fully dense PETN and reaction products.
(CJ Pressure = 30.9 GPa; V_N Pressure = 52.6 GPa)

INERT RESPONSE (NO REACTION)





1-d **inert** simulations as described previously [1]

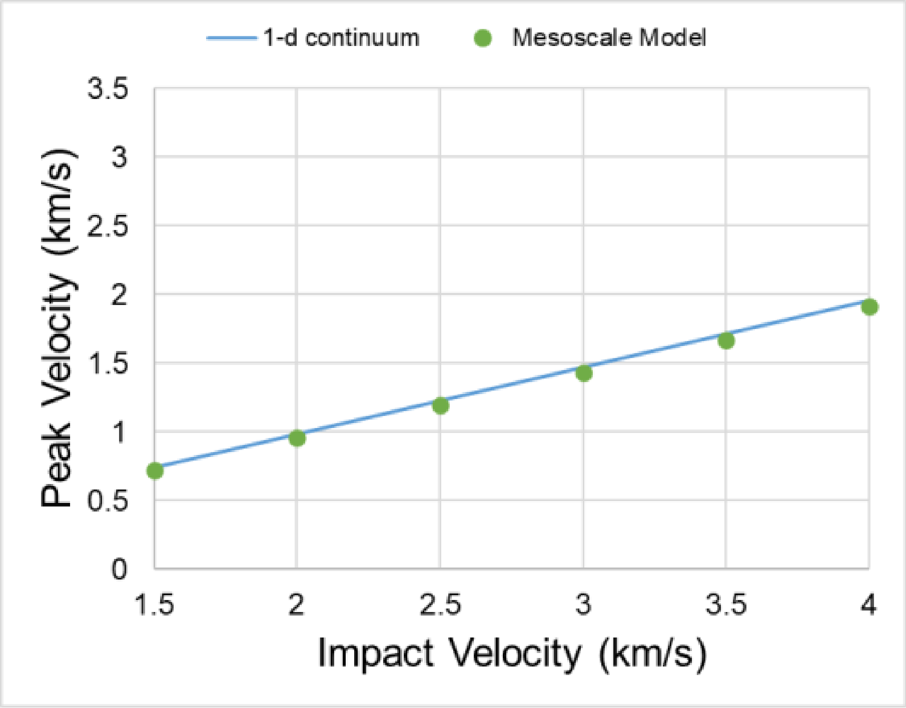
- Continuum model (no microstructure)
- Porous Hugoniot from *p-alpha* model
- Flyer L/D ~40

Thinnest films (30, 67 μm) have similar inert response

- Impact shock reaches the Al / PMMA interface before the release wave

Thickest film (125 μm) has lower transmitted shock wave

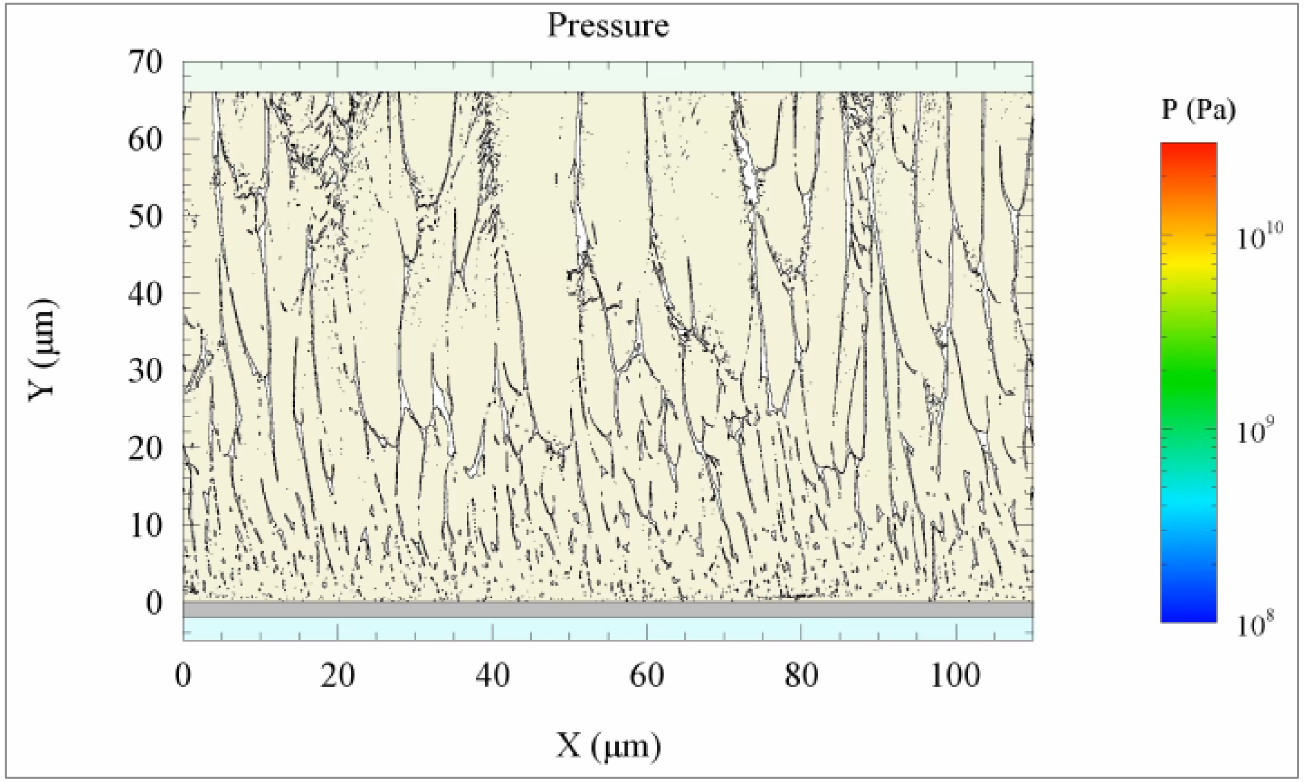
- Release wave reaches the shock front and reduces the shock strength before it is measured at the interface

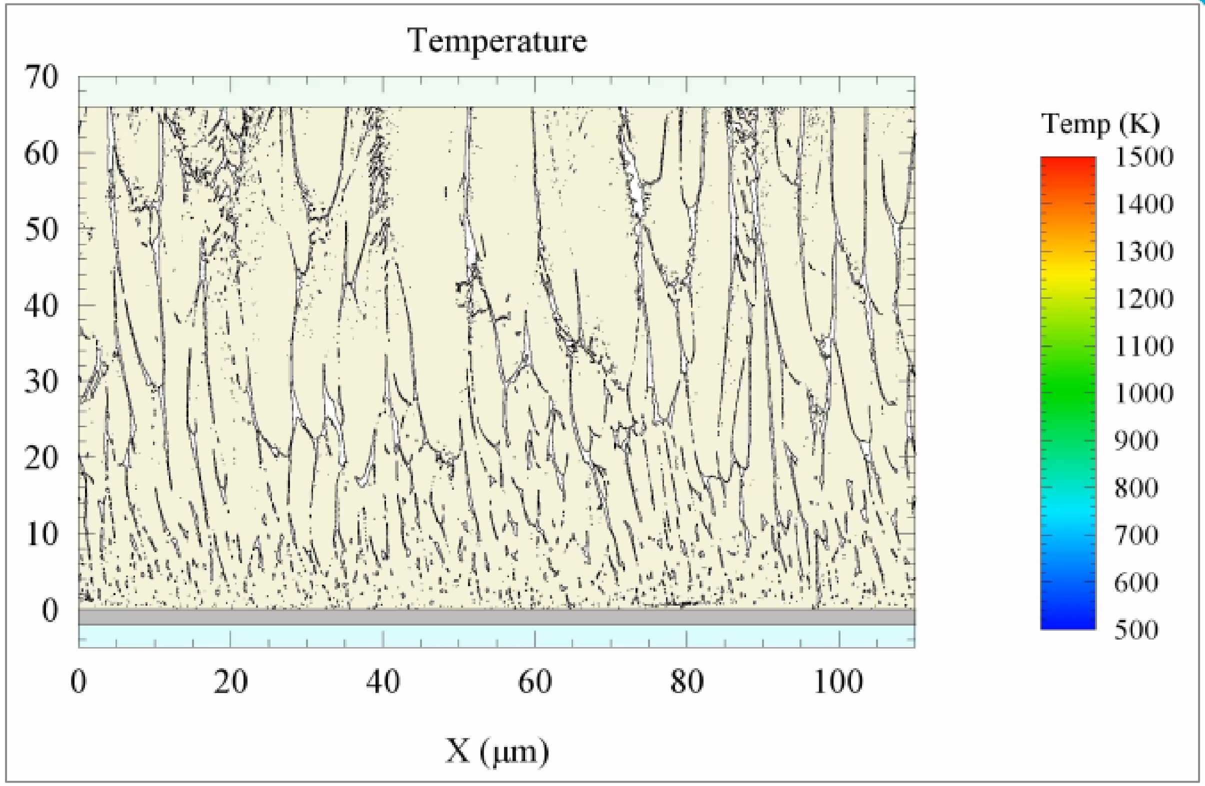


Mesoscale simulations of inert film agree with continuum calculations.

1. Kittell, et al., J. Appl. Phys. 131, 154902 (2022)

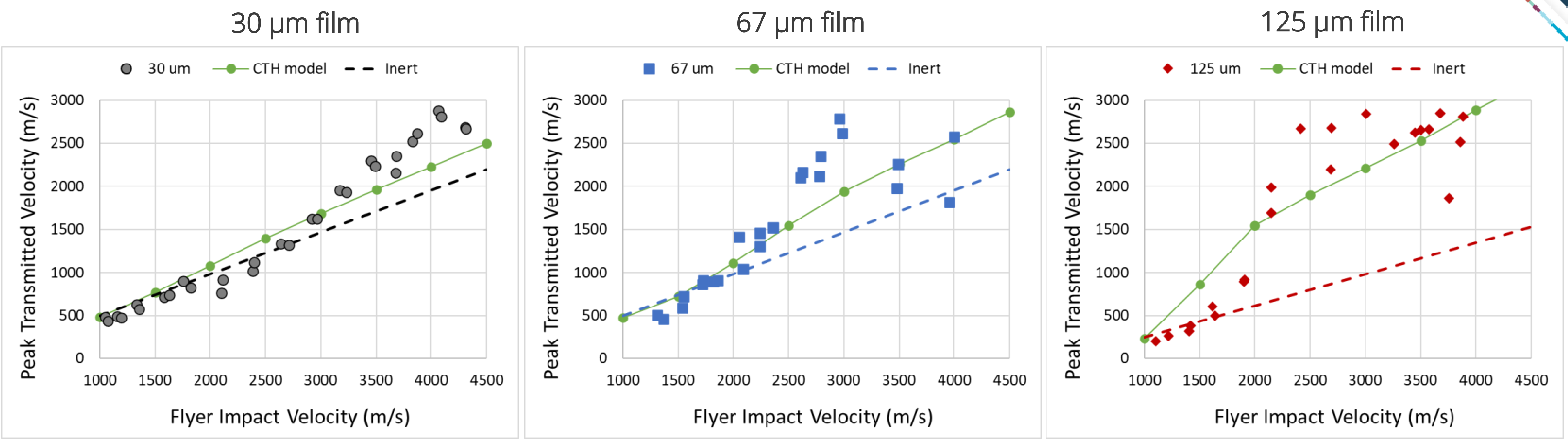
MESOSCALE MODEL – SIMULATION AT 2 KM/S (WITH REACTION)





- Voids and defects at grain boundaries create hotspots that initiate the reaction chemistry
- Tracers at the Al / PMMA interface record the particle velocity history; averaged for comparison to PDV data
- Simulations ran with various flyer impact velocity and film thickness

MODEL VS. EXPERIMENTS – UNAGED FILMS



Preliminary model results:

- No tuning of material parameters or reaction rate
- Simulations and experiments [2] show increasing reactivity with sample thickness (longer run distance)
- Other metrics for comparison include onset of reaction, and growth to detonation

Further development:

- Strength model for PETN crystals
- Multi-step reaction rates or P,T-dependent burn models

2. Knepper, et al., J. Appl. Phys. 131, 155901 (2022)

CONCLUDING REMARKS

A mesoscale model for shock initiation of PETN films has been developed

- Microstructures from ion-polished films are explicitly modeled
- Equations of state for solid crystal PETN and reaction products
- Global reaction kinetics (temperature-dependent)

Preliminary results show reasonable agreement with experimental trends

Additional refinement of material models may be required

Concurrent/Future work:

- Can mesoscale hydrocode simulations capture the observed shifts in initiation threshold due to ageing?
  - Informed by binarized images of ion-polished cross-sections that can be imported to the simulations
- Can phase field models capture the observed trends in microstructure evolution?
  - Predict age-induced changes in microstructure
- Additional experiments at various temperatures, and additional microscopy of PETN films