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EFFECT OF ACCELERATED AGING ON MICROSTRUCTURE AND INITIATION OF VAPOR-DEPOSITED PETN FILMS

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APS Shock Compression of Condensed Matter Conference

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MOTIVATION

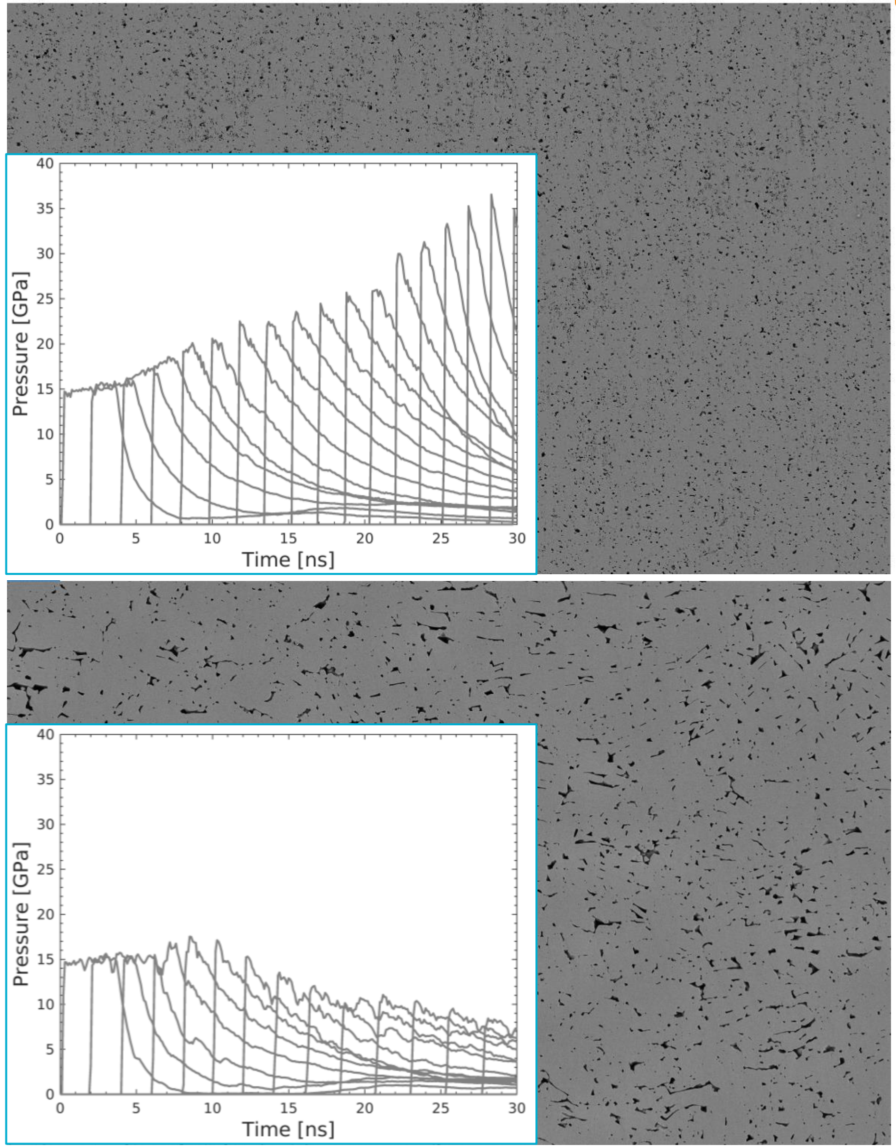
Microstructure of an explosive can have a significant impact on performance

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

- Grain coarsening
- Grain sintering
- Changes in porosity distribution

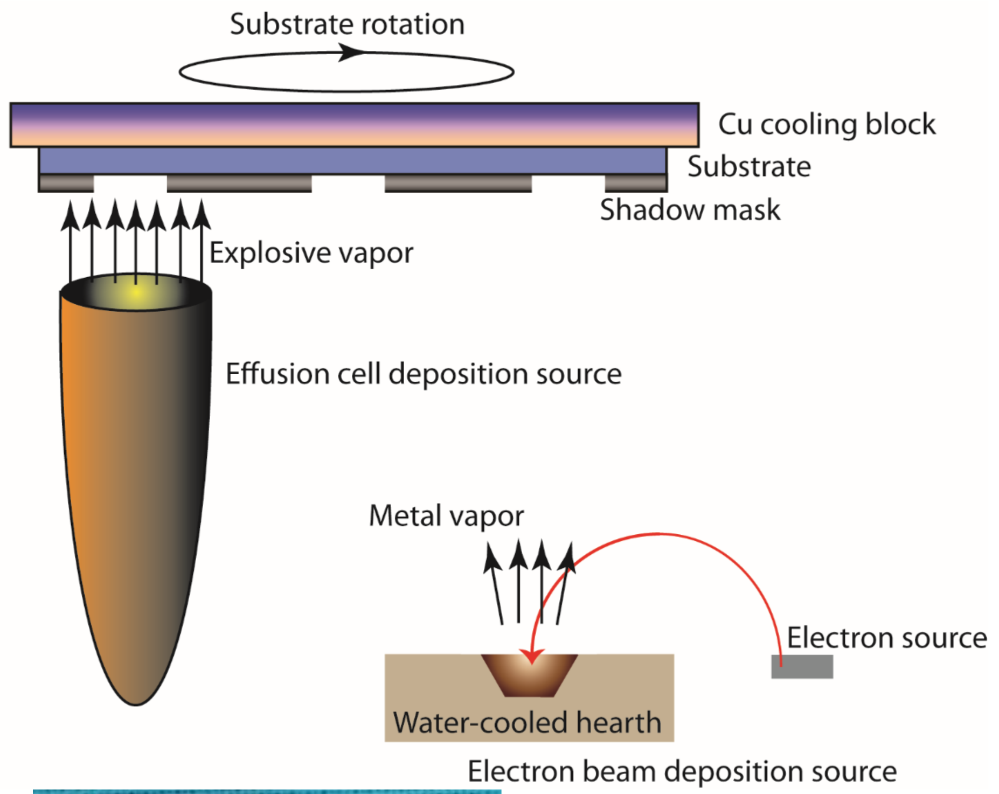
Experiments are needed to support model development for predicting effects of aging on microstructure evolution and growth to detonation

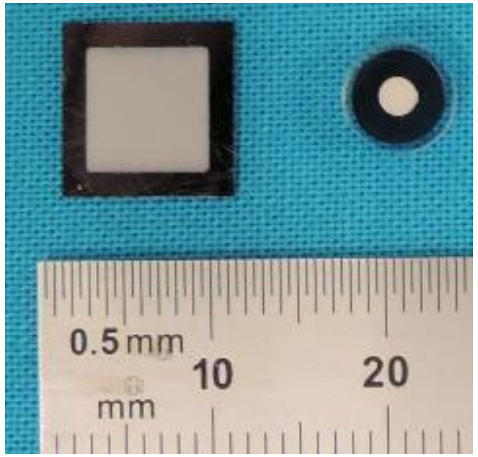
- ➢ Joe Monti: Phase-Field Modeling of Aging of Energetic Thin Films *(E06 - Monday 2:15 pm)*
- ➢ David Damm: Mesoscale Reactive Burn Modeling of Shock Initiation in Vapor-Deposited PETN Films *(F03 – Monday 4:30 pm)*



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

VAPOR-DEPOSITED PETN AS A MODEL SYSTEM





Sketch of Sandia's deposition system for energetic materials (top) and a photograph of PETN films on a 10 mm silicon substrate and a 6.35 mm PMMA substrate (left).

PETN films are a good model system to investigate the effects of aging

- Can induce significant changes in microstructure at moderate time/temperature conditions
- Can be used with Sandia's High-Throughput Initiation (HTI) experiment to rapidly characterize growth to detonation

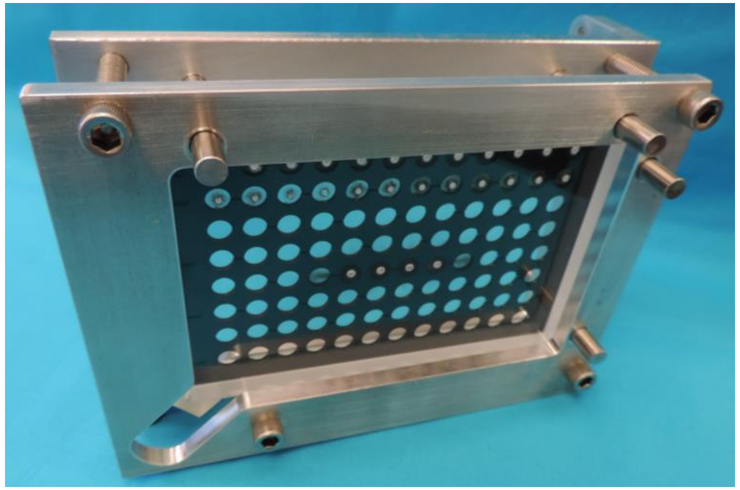
PETN films deposited in two different geometries

- 100 μm thick films on PMMA for HTI experiments
- 80 – 120 μm thick films on silicon for microstructure characterization
- All films deposit at ~90% TMD

Accelerated aging conditions investigated to date:

- As-deposited
- 4 hours @ 60°C
- 1 day @ 60°C
- 1 week @ 60°C
- 2 weeks @ 60°C
- 1 month @ 70°C

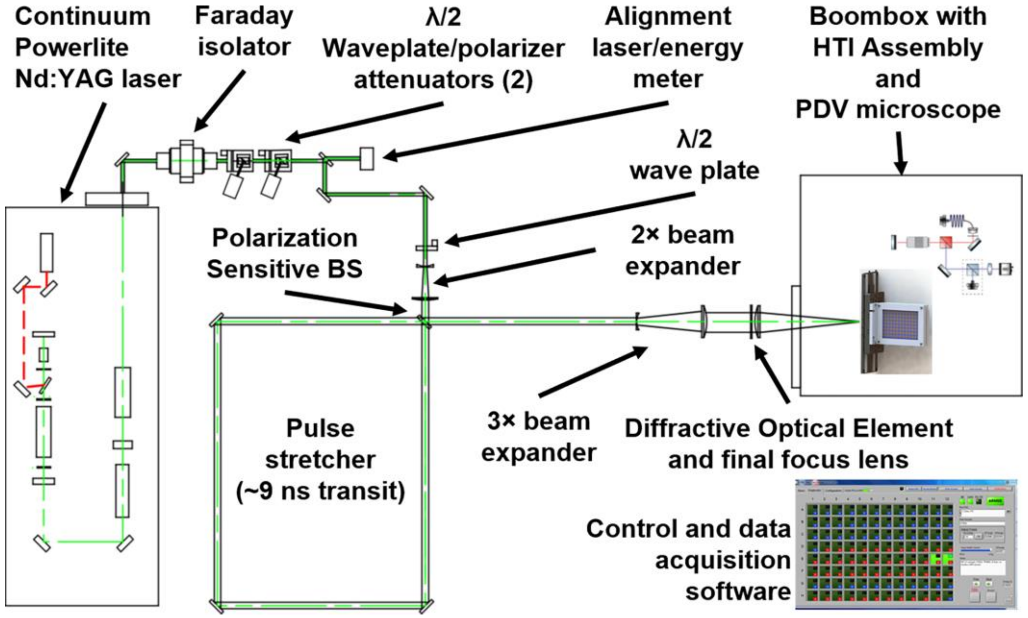
HIGH-THROUGHPUT INITIATION (HTI) EXPERIMENT



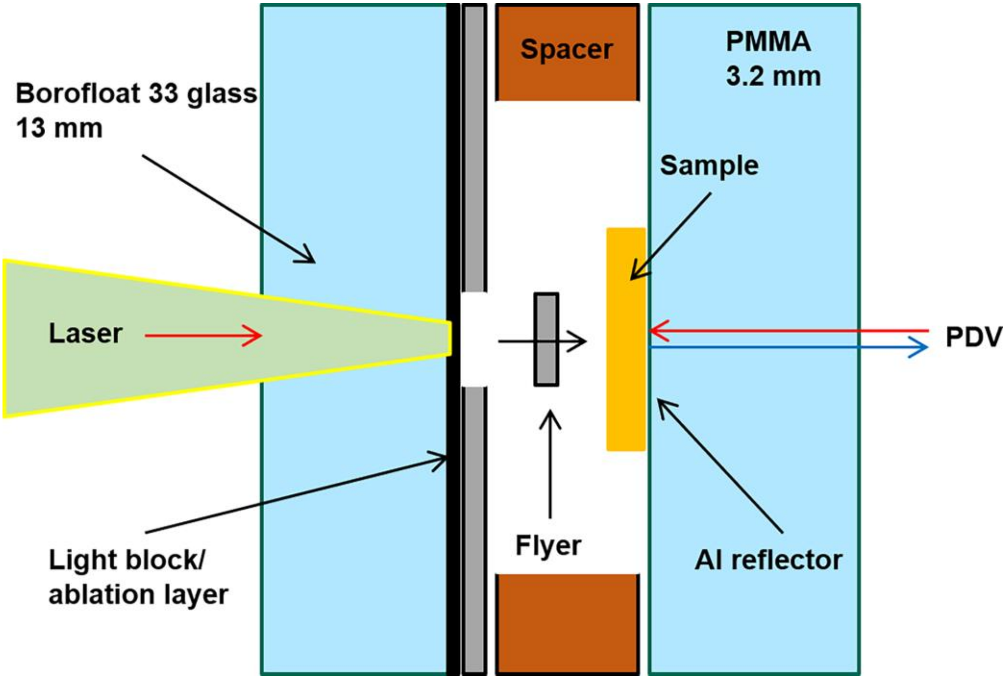
Laser-driven flyer based on work in Dana Dlott's group (UIUC)

Flyer characteristics define shock parameters

- Flyer material (Parylene C) and laser fluence define pressure
- Flyer material and thickness (25 μm) defines shock pulse width
- Laser profile defines flyer diameter/spot size (~1.1 mm)

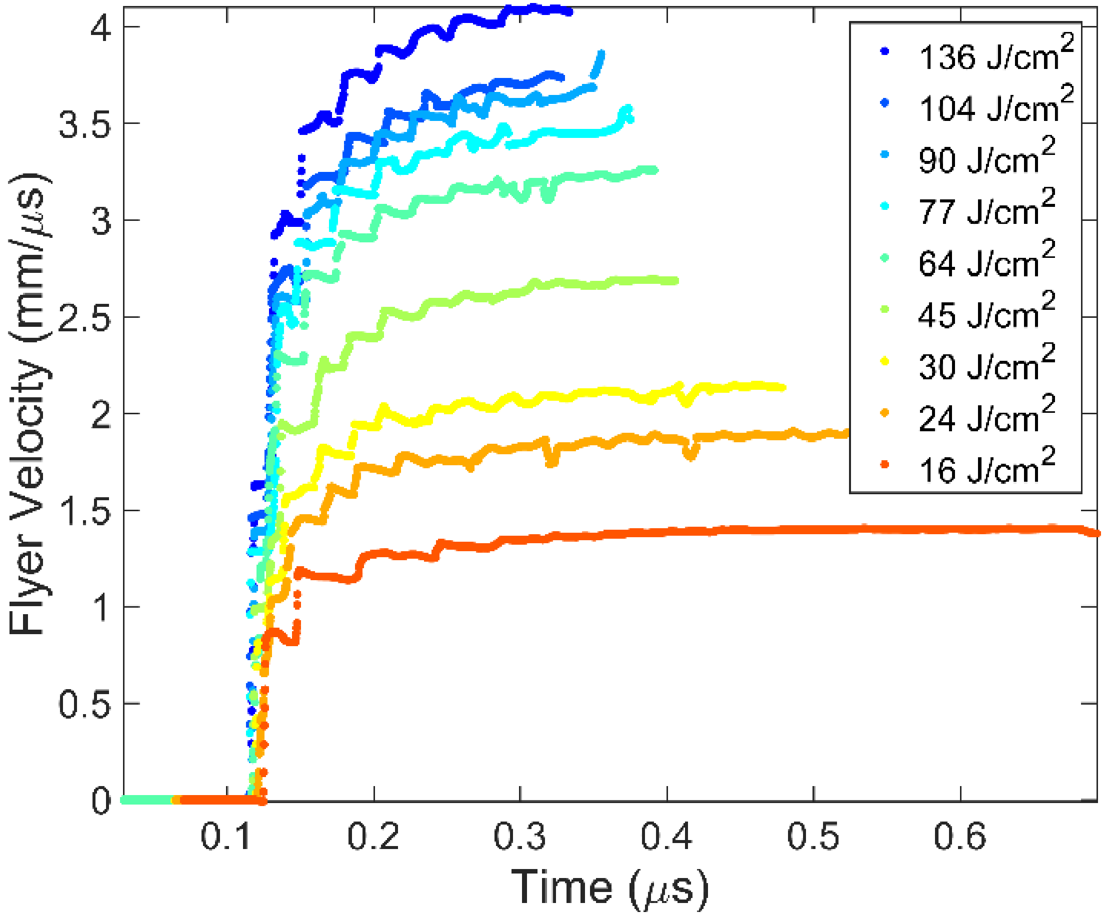


Knepper *et al*, J. Appl. Phys., **131**, 155901 (2022).

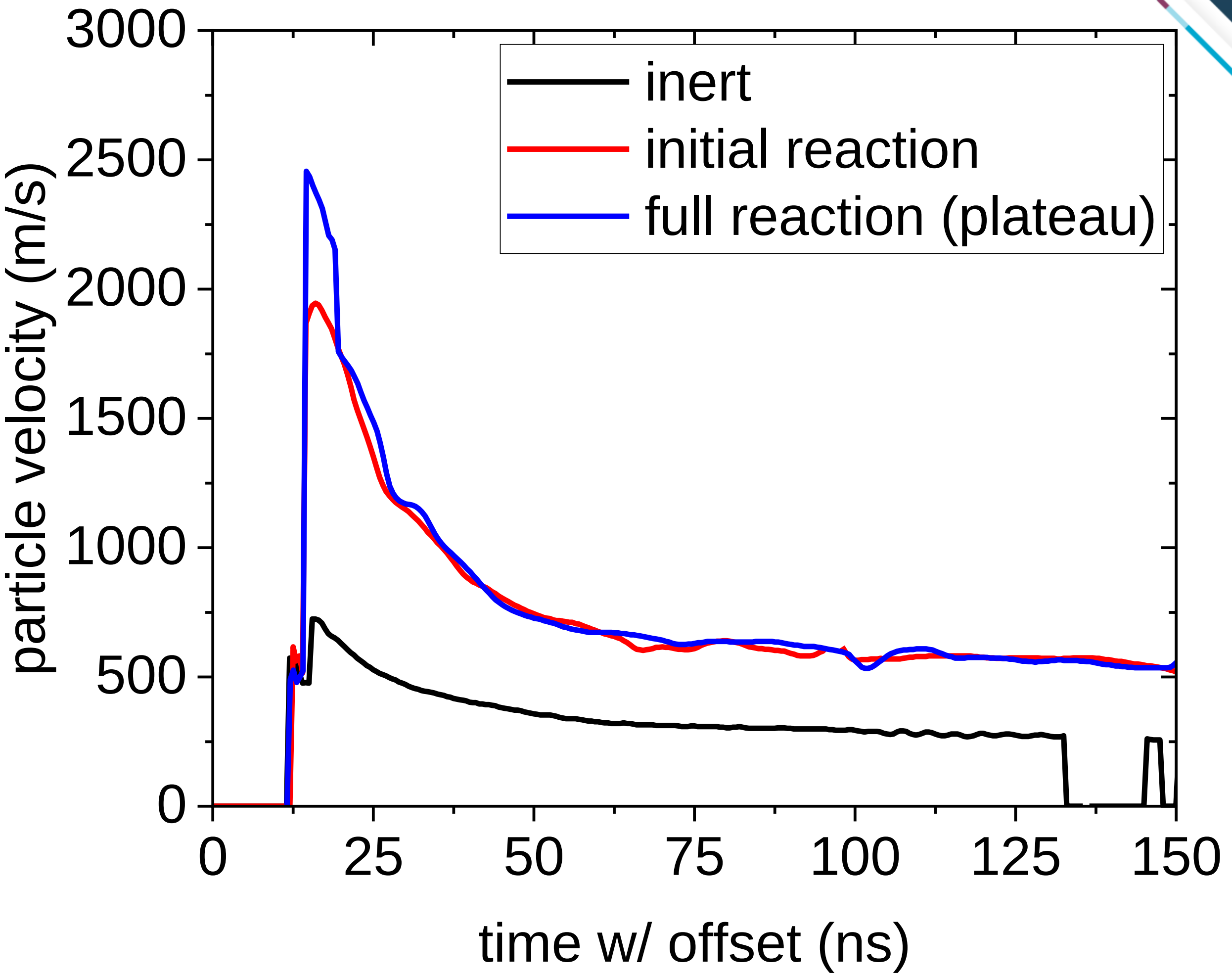


Sandia's High-Throughput Initiation experiment and photograph of the 96-well sample geometry.

PHOTONIC DOPPLER VELOCIMETRY (PDV) DIAGNOSTICS IN HTI

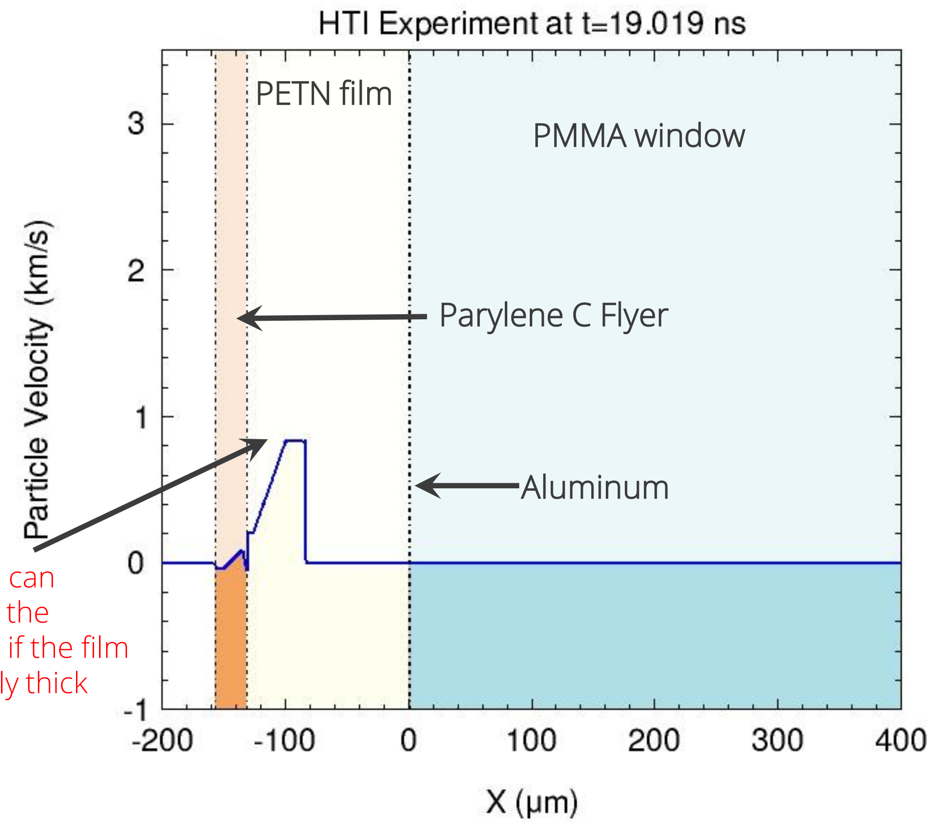


PDV traces of Parylene C flyers launched at various laser fluences.

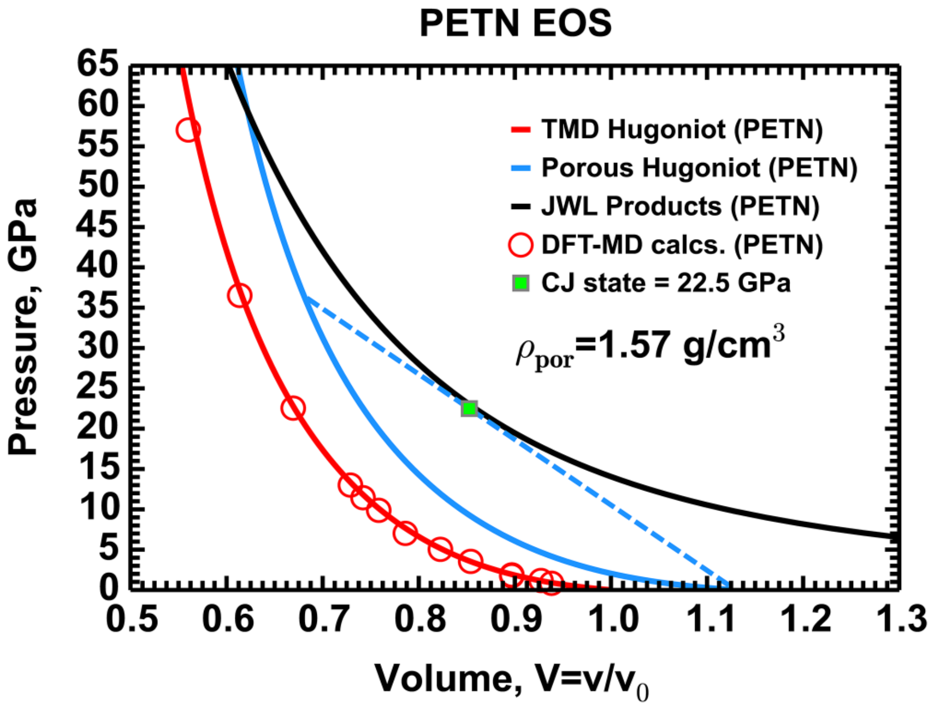


PDV traces of explosive sample response at various stages of reaction.

ONE-DIMENSIONAL CTH SIMULATIONS SHOW PREDICTED INERT RESPONSE



Rarefaction can catch up to the shock front if the film is sufficiently thick

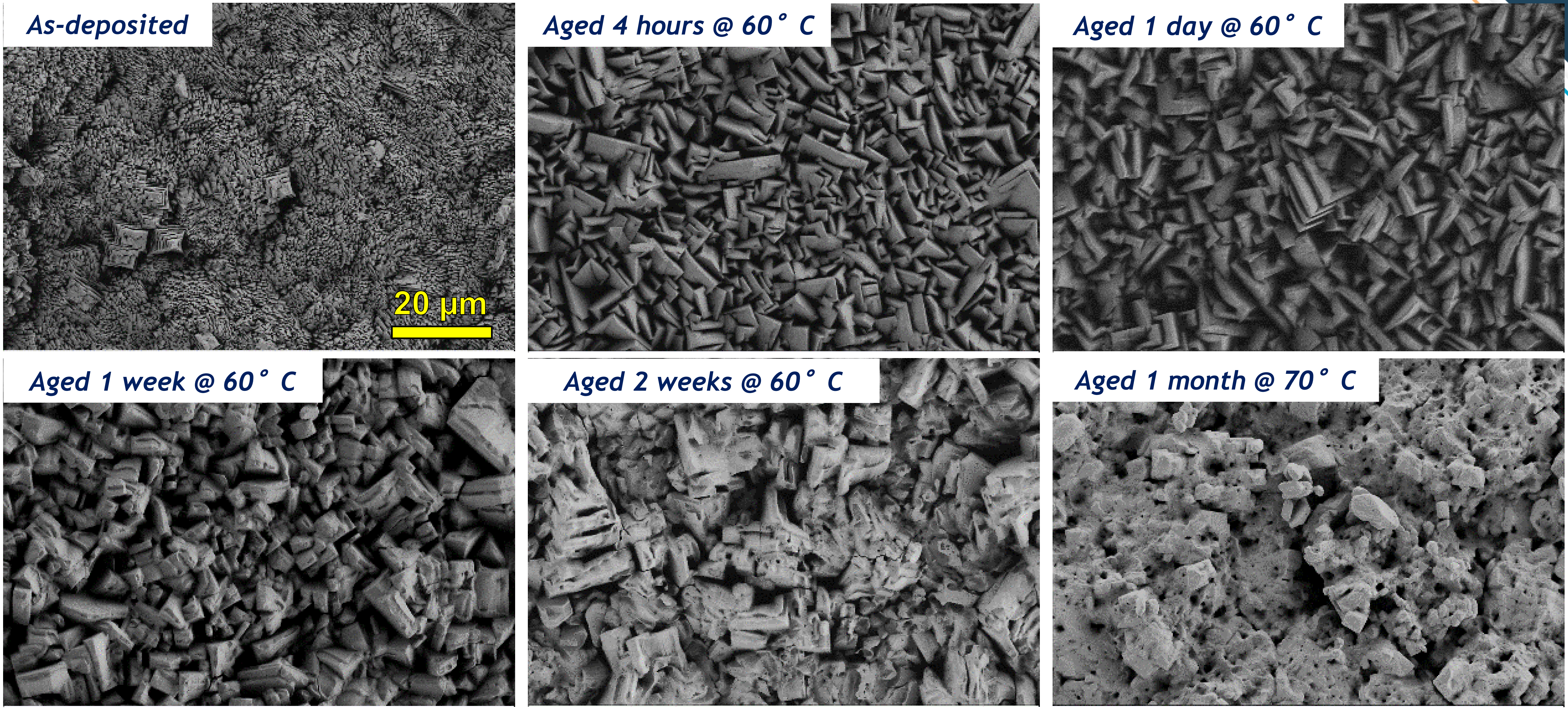


1D simulation of a shock wave traveling through a PETN film (left) and a plot showing EOS data for a PETN film with a density of 1.57 g/cm^3 (right).

Mesh resolution is 3 zones/μm (well-resolved), simulations run with reactions disabled

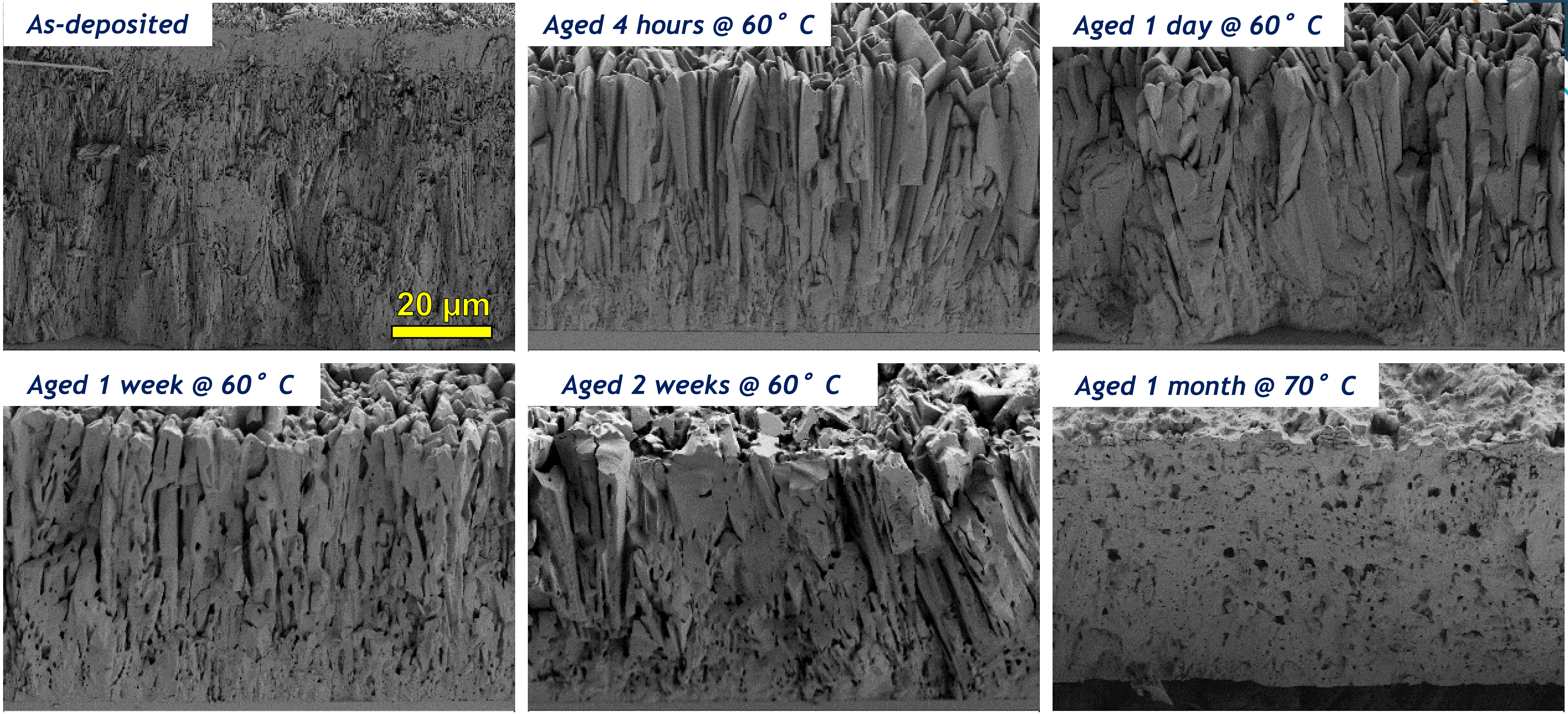
Deviation of experimental data from the predicted inert response indicates where chemical reactions begin to impact performance

EVOLUTION OF TOP SURFACE MORPHOLOGY



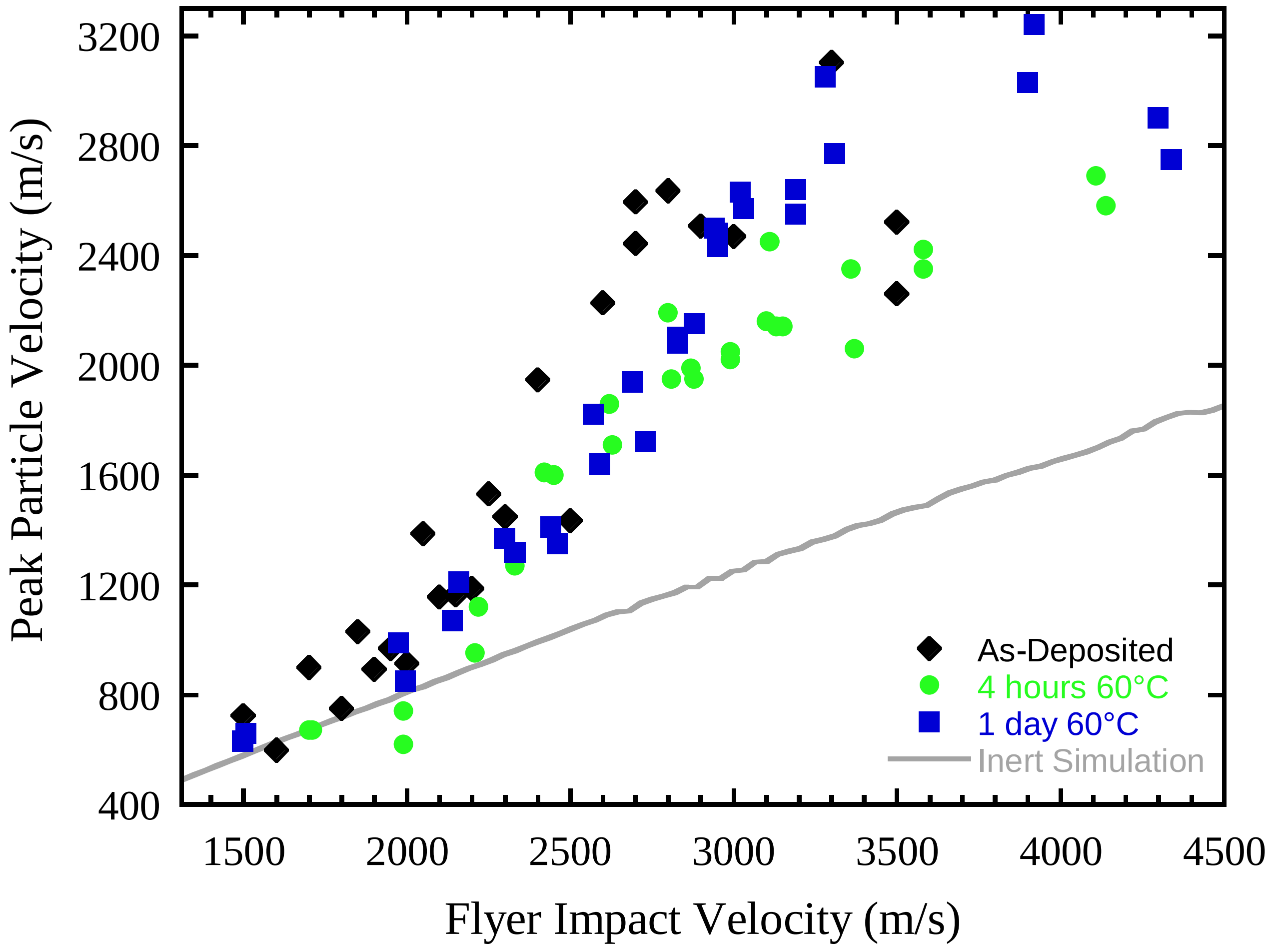
Top surface SEM images of as-deposited and aged PETN films.

EVOLUTION OF FRACTURE CROSS-SECTION MORPHOLOGY

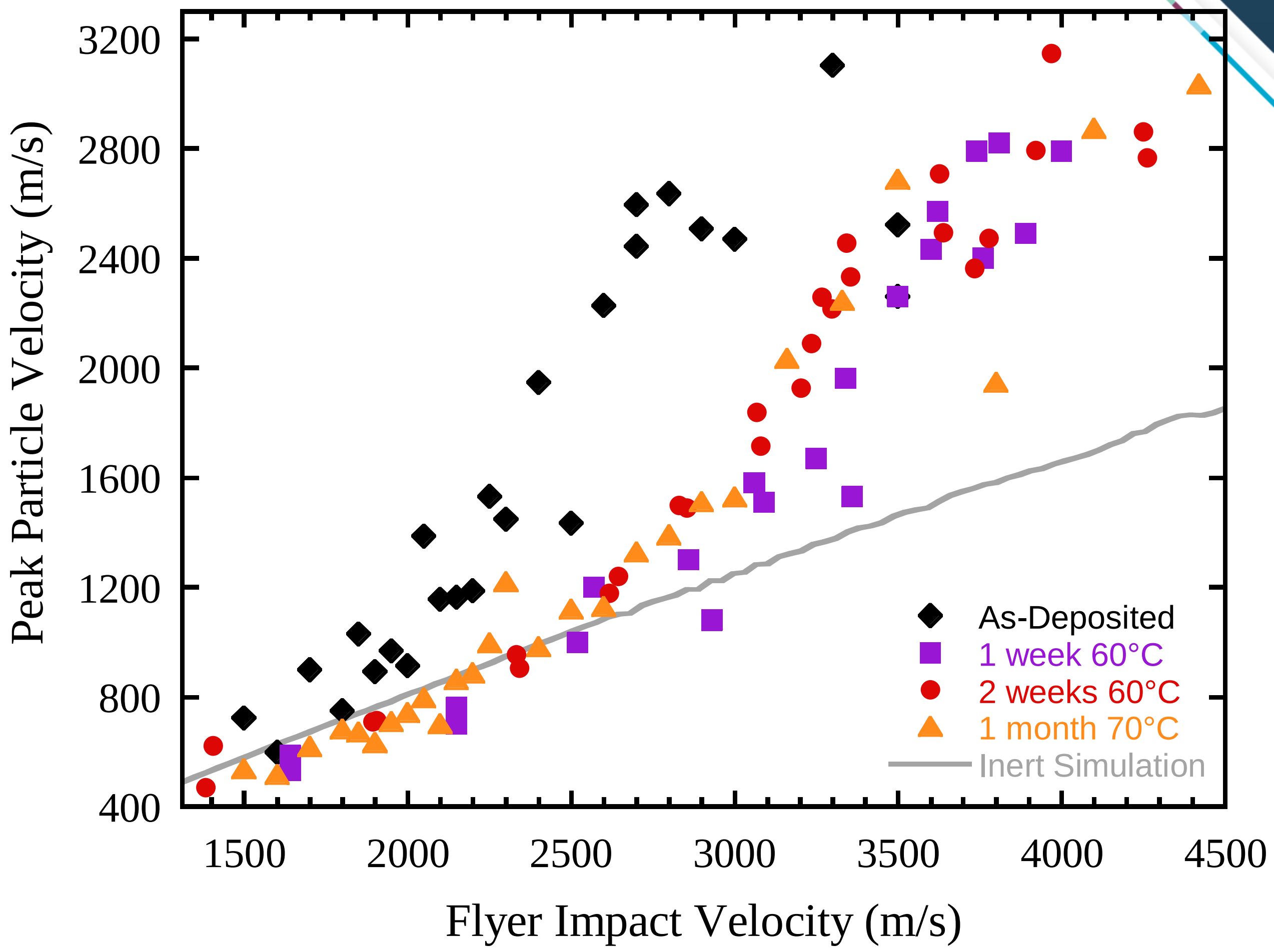


Fracture cross-section SEM images of as-deposited and aged PETN films.

AGING EFFECTS ON INITIATION THRESHOLD

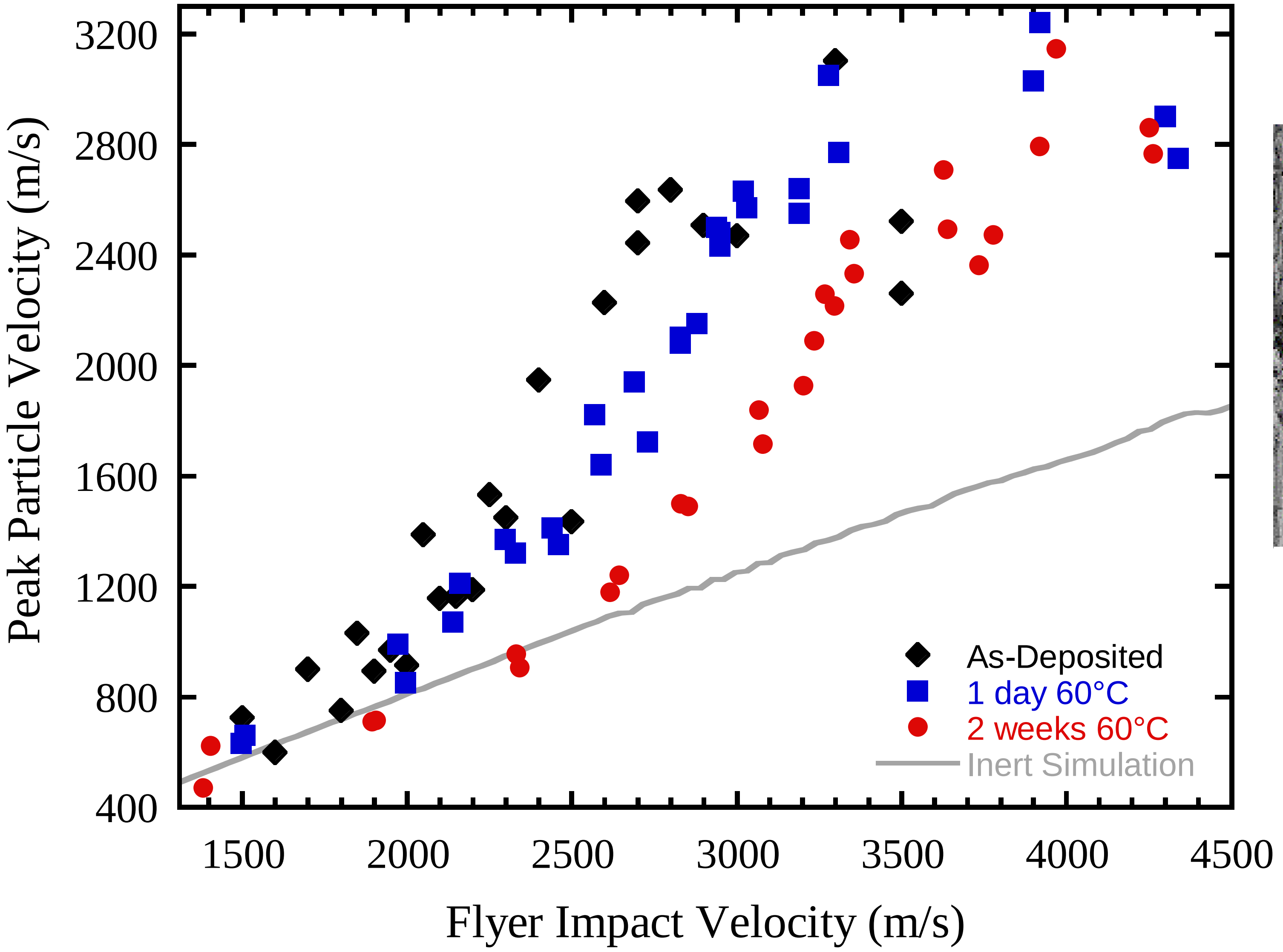


Comparison of as-deposited with 4 hours - 1 day thermally aged data.



Comparison of as-deposited with 1 week - 1 month thermally aged data.

AGING EFFECTS ON INITIATION THRESHOLD



As-deposited

1 day 60° C

2 weeks 60° C

Comparison of the three distinct stages of aging in HTI data on 100 μm thick PETN samples.

CONCLUDING REMARKS

PETN films show rapid grain coarsening at elevated temperature, porosity appears to take somewhat longer to coarsen

HTI can enable rapid quantification of initiation thresholds and run distances in materials that grow to detonation at sub-millimeter length scales

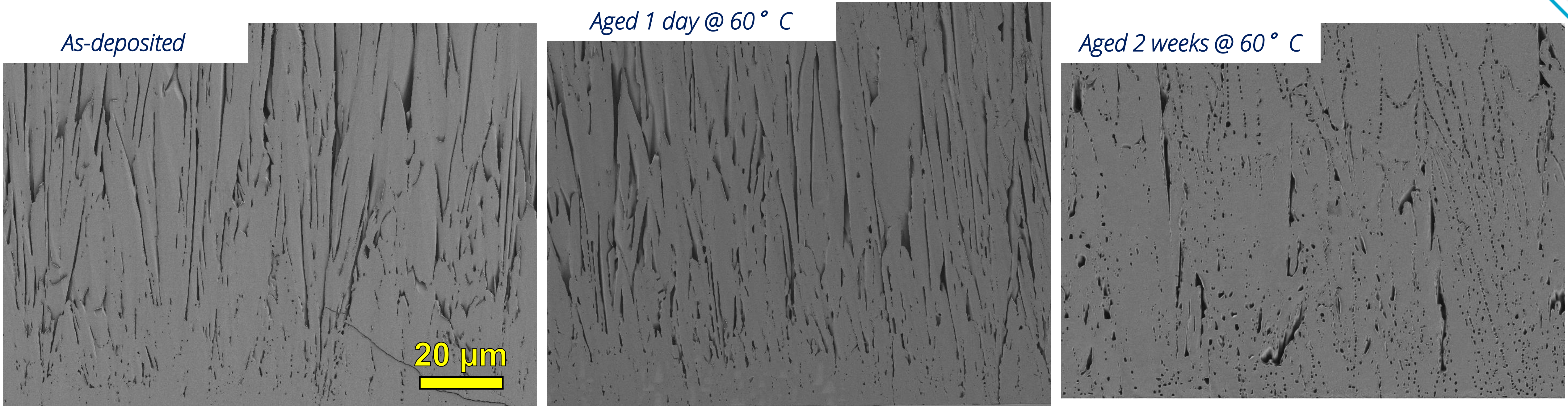
Initiation threshold and onset of reaction shift rapidly when samples are exposed to elevated temperatures but level off after some amount of time

Concurrent/Future work:

- Can phase field models capture the observed trends in microstructure evolution?
- Can mesoscale hydrocode simulations capture the observed shifts in initiation threshold?
  - Informed by binarized images of ion-polished cross-sections that can be imported to the simulations
- Experiments on samples aged at lower temperatures
  - Do grains coarsen as quickly? Can we capture the coarsening process as it occurs?
  - Do we see similar trends in initiation threshold following aging?

BACKUP SLIDES

ION-POLISHED CROSS-SECTIONS



SEM images of ion-polished cross-sections in as-deposited and aged PETN films.

Can threshold/binarize ion-polished images for quantitative analysis and import to CTH

Similar distributions of porosity in as-deposited and aged 1 day structures; slightly less porosity and less anisotropy in the aged 2-weeks structure