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Phase-Field Modeling of Aging of Energetic Thin Films

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Sandia National Laboratories

APS SCCM 23

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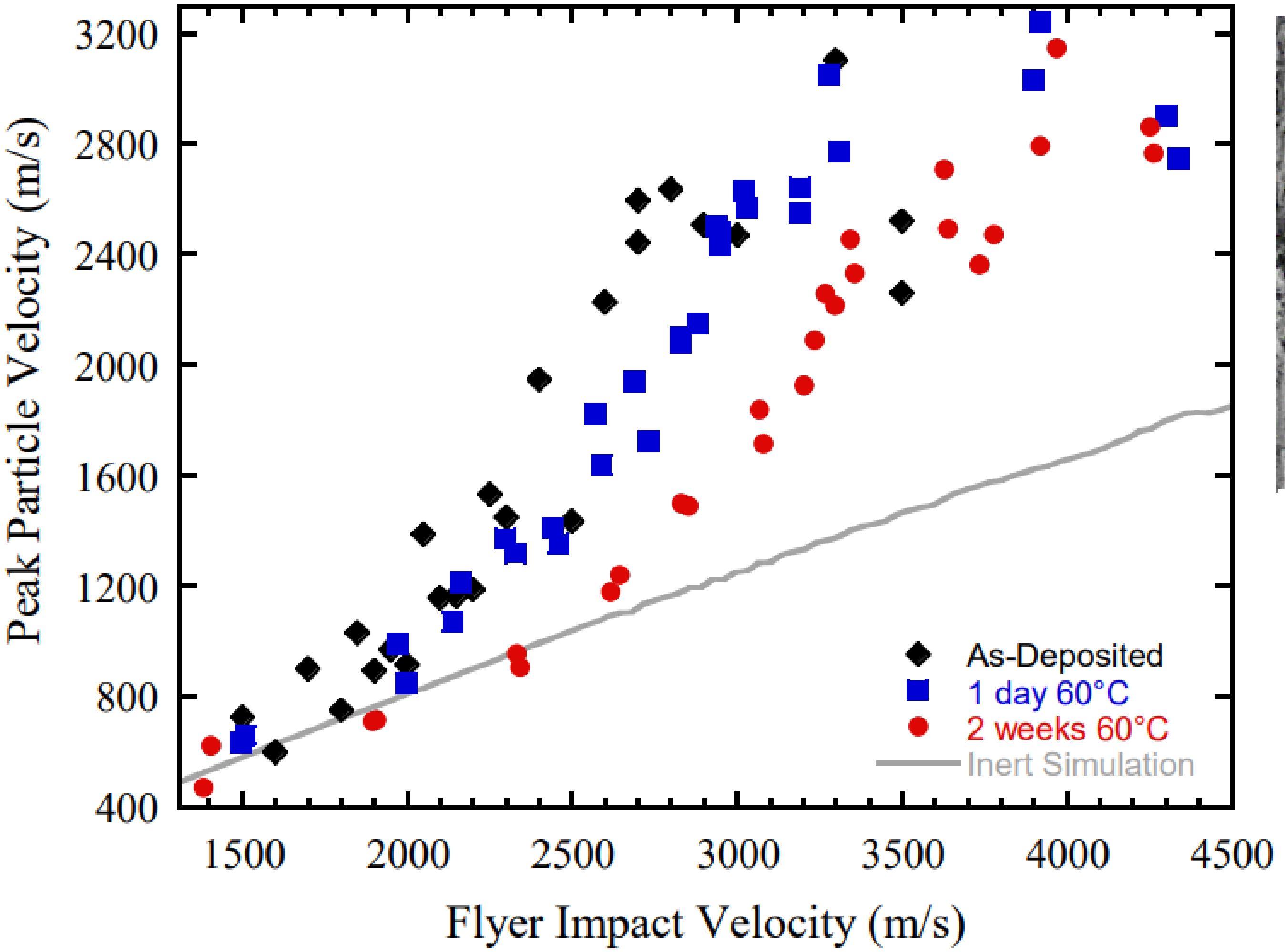
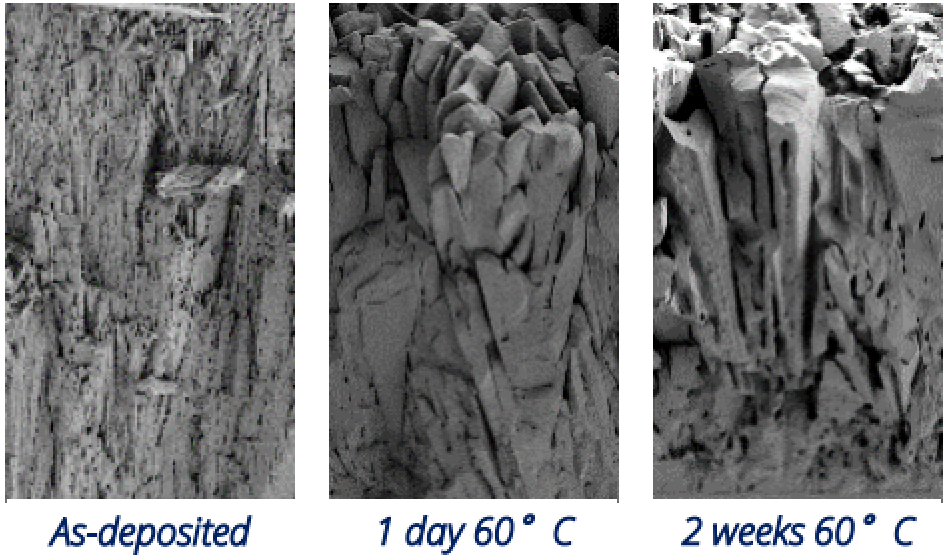
Ageing Effects on Initiation Threshold and Microstructure



PETN thin films

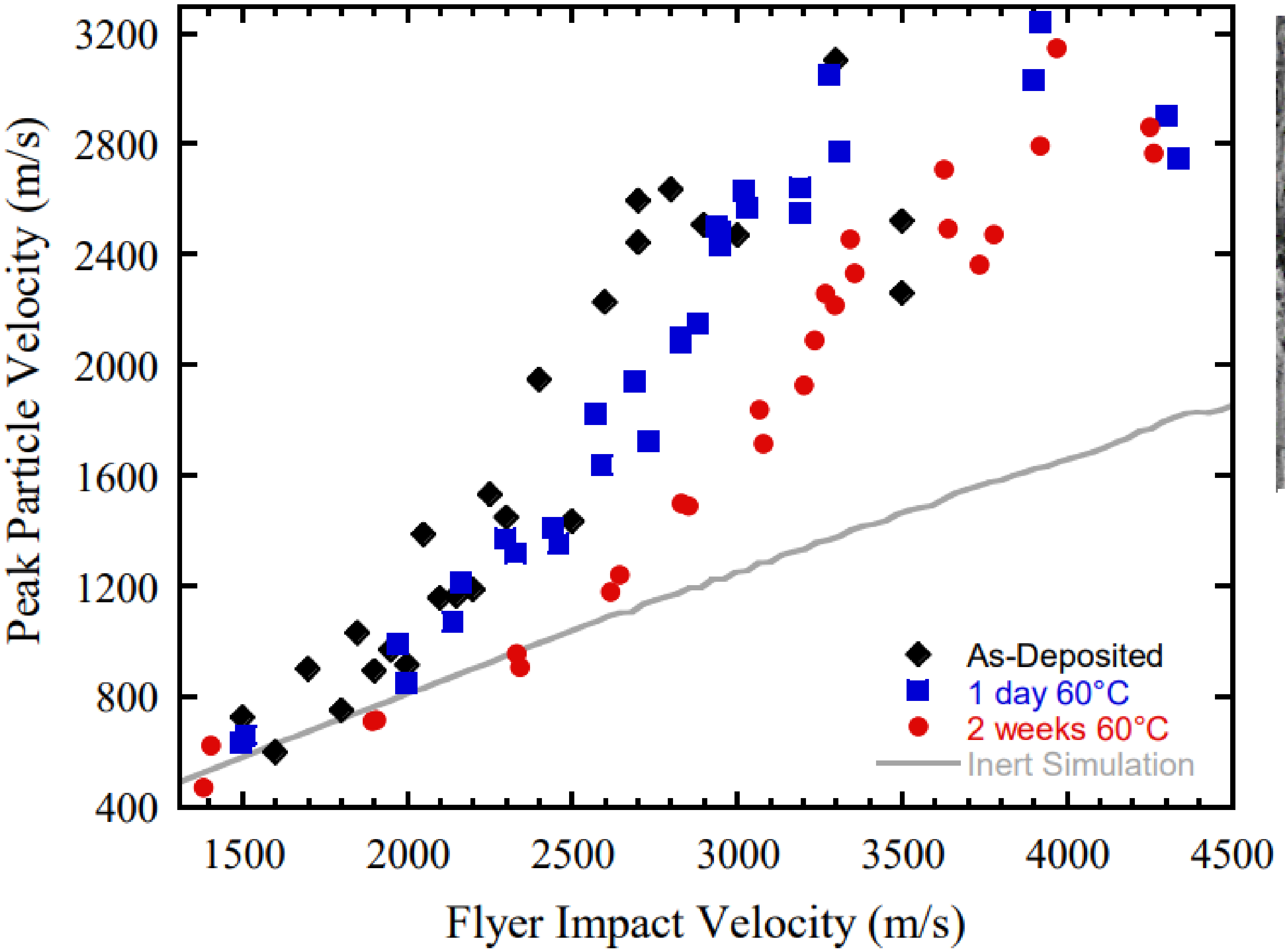


Goal is to predict microstructure evolution using Phase-Field modeling

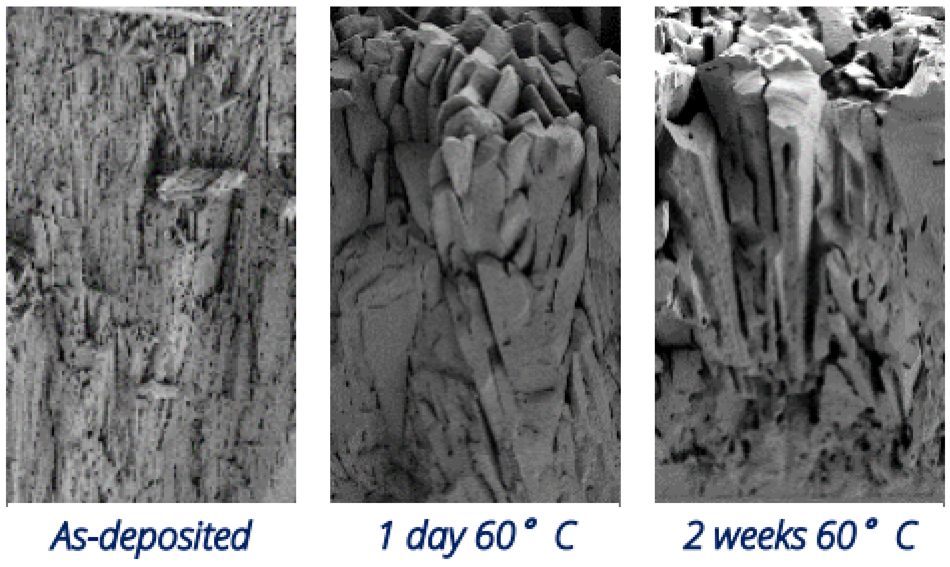
Developing a mesoscale shock initiation model of HTI experiments

Comparison of three distinct stages of ageing in High Throughput Initiation (HTI) data on 100 μm thick samples of PETN

Ageing Effects on Initiation Threshold and Microstructure



PETN thin films



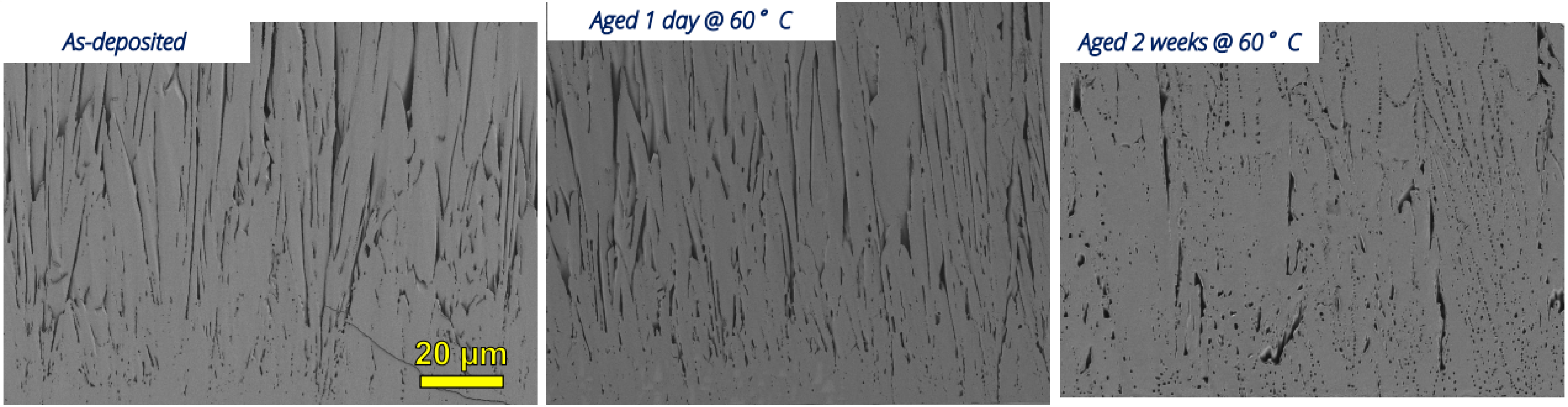
Mesoscale shock modeling: F03.00004
Monday, 4:30-4:45PM by David Damm

Experimental component: V03.00005
Thursday, 10:30-10:45AM by Rob Knepper

Comparison of three distinct stages of ageing in High Throughput Initiation (HTI) data on 100 μm thick samples of PETN

Microstructural Ageing of PETN films

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



Top surface morphologies

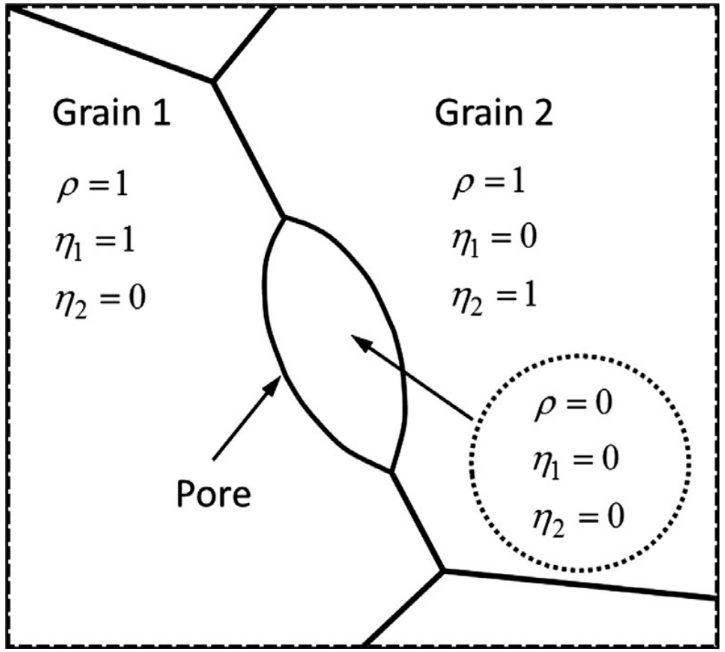
Phase-field porous microstructure model

- Model produces coupled evolution of grains and pores
- Key feature: diffuse interfaces between phases

Formulate free-energy functional $\boldsymbol{F}$:

ρ: pore-matrix order paramet

$\vec{\eta}$: grain order parameters



Allen-Cahn Eqn. → Non-Conserved

$$\frac{\partial \eta_j}{\partial t} = -L_{ij}\frac{\delta F}{\delta \eta_i}$$

Cahn-Hilliard Eqn. → Conserved

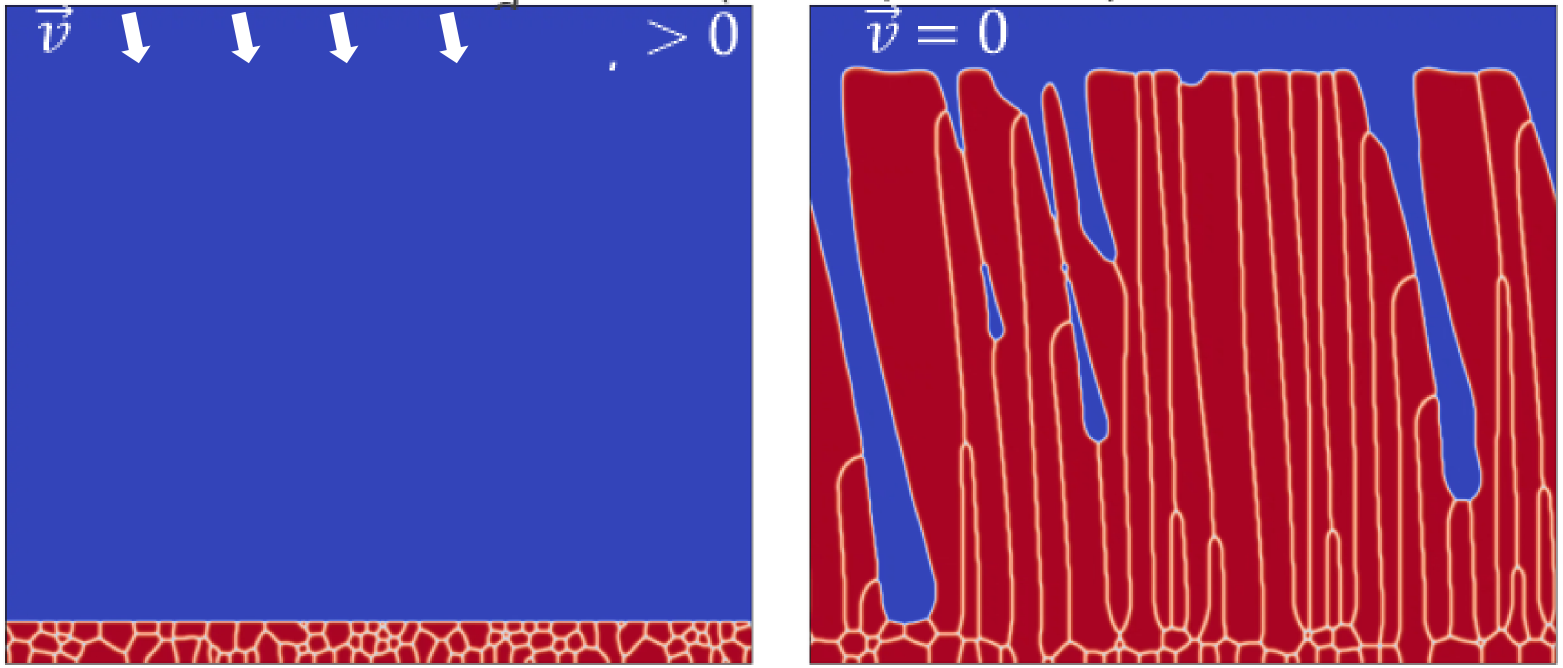
$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(M\nabla\frac{\delta F}{\delta \rho}\right)$$

Ahmed, K., Yablinsky, C. A., Schulte, A., Allen, T., & El-Azab, A. (2013). *Mod. Sim. Mat. Sci. Eng., 21*.
Ahmed, K., Pakarinen, J., Allen, T., & El-Azab, A. (2014). *J. Nuc. Mat., 446*.

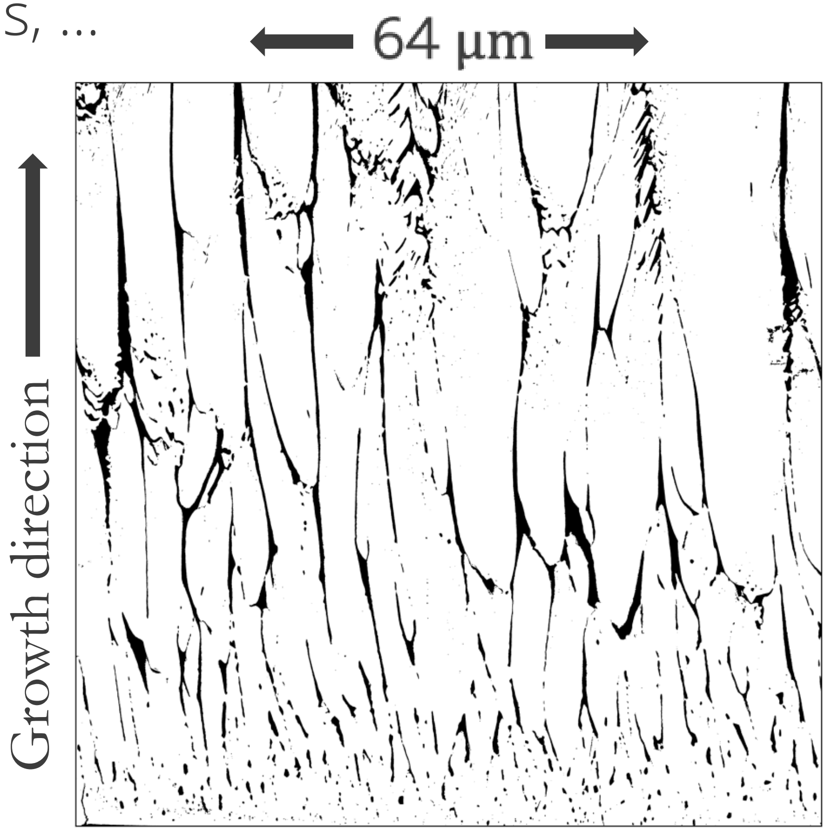
Coupled thin-film growth and porous microstructure evolution models

Film microstructure depends on: chamber pressure, deposition incidence angle and rate, substrate properties, …

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta \rho} \right) + S(\rho, \phi, \vec{v})$$



Typical numerical discretization size ~ 10 nm



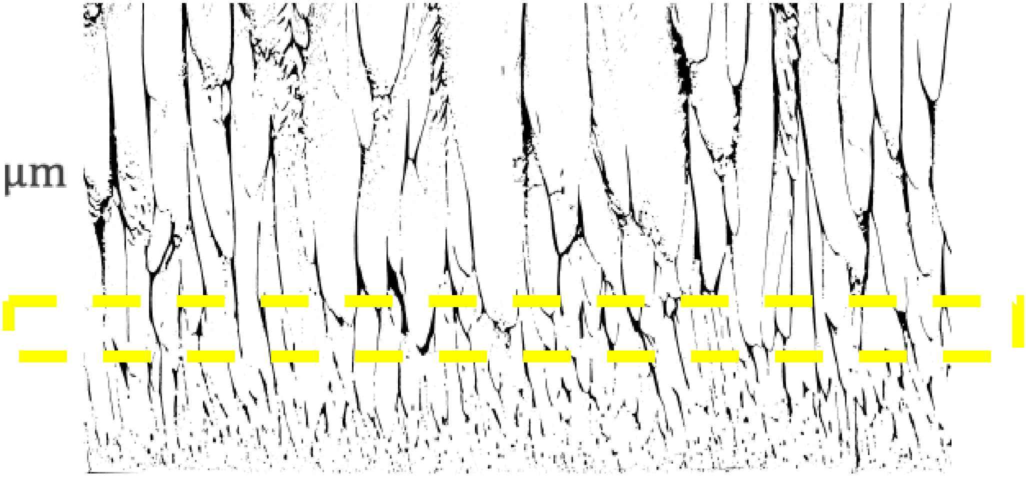
As-deposited PETN cross-section

Monti, J. M., Stewart, J. A., Custer, J. O., Adams, D. P., Depla, D., & Dingreville, R. (2023). *Acta Mat.*, *245.*

Phenomenological model of void trapping during film growth

As-deposited PETN cross-section

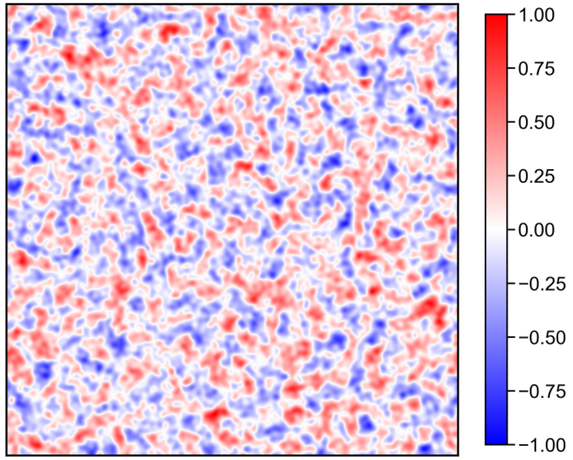
64 μm



Pixel size: 10 nm

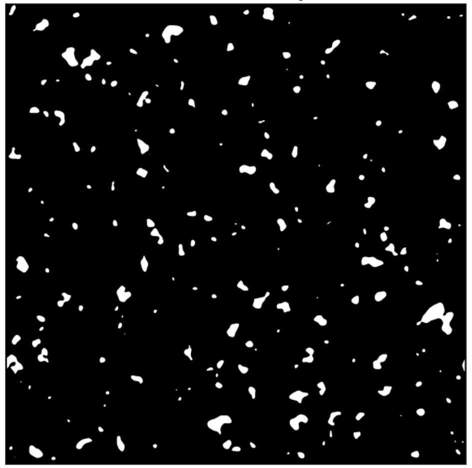
120 μm

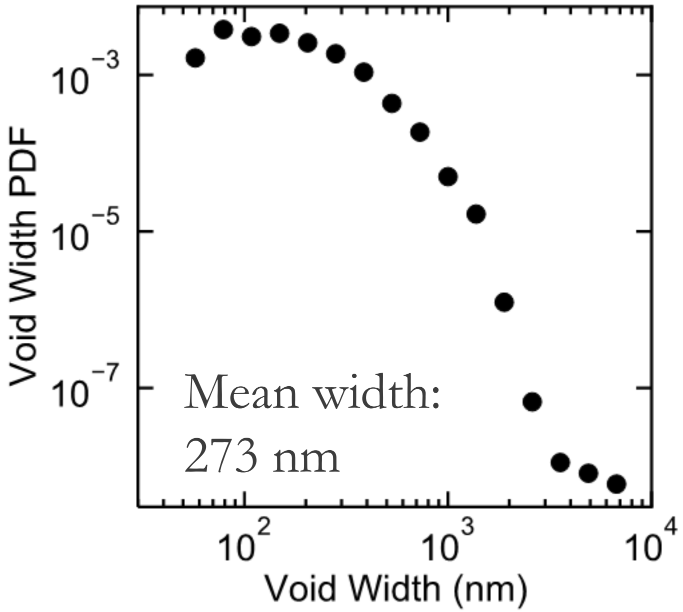
Gaussian random field

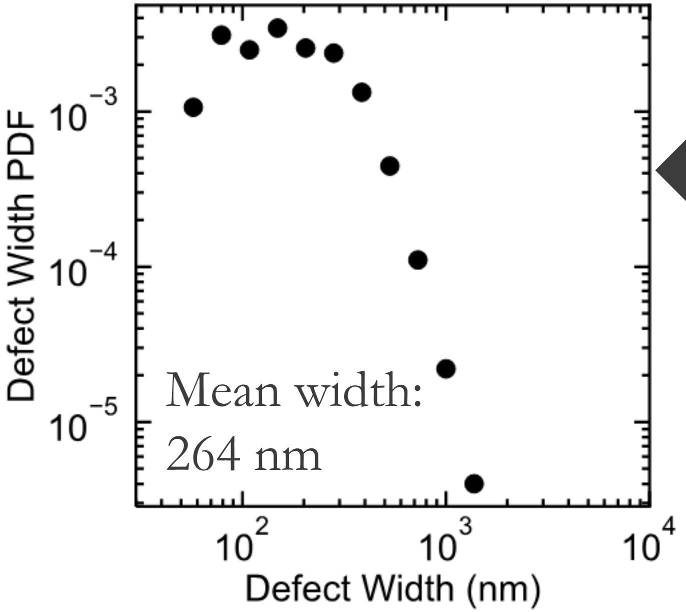


20.5 μm

Threshold by value







Defects in vapor deposition:

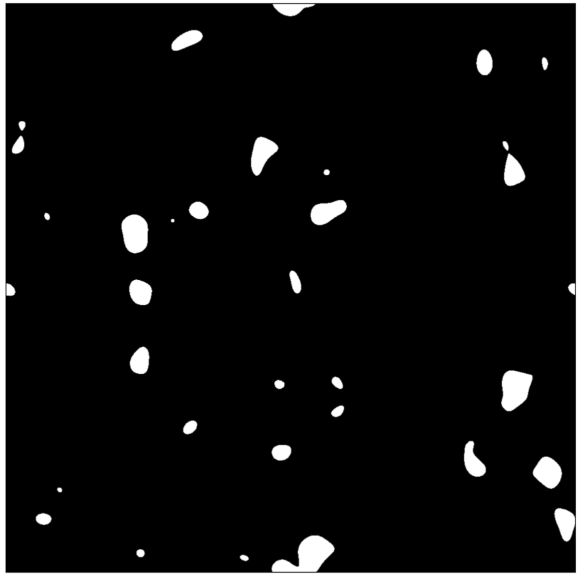
Turn off source term <u>locally</u> in defect regions as

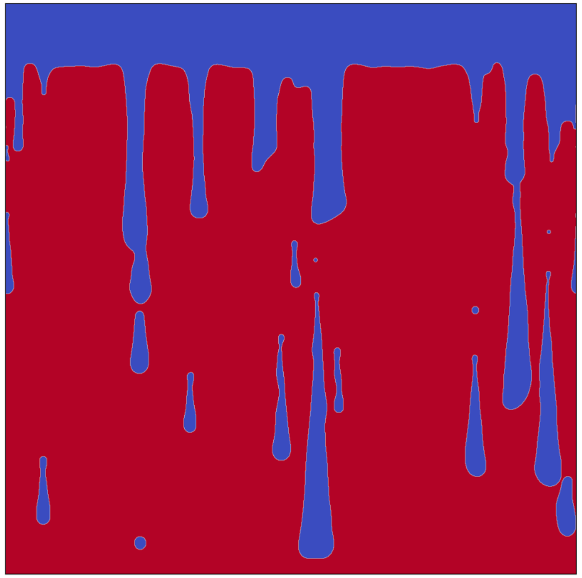
$$S(\rho, \phi, \vec{v}) = 0$$

Properties of source field drive vapor-deposited microstructure

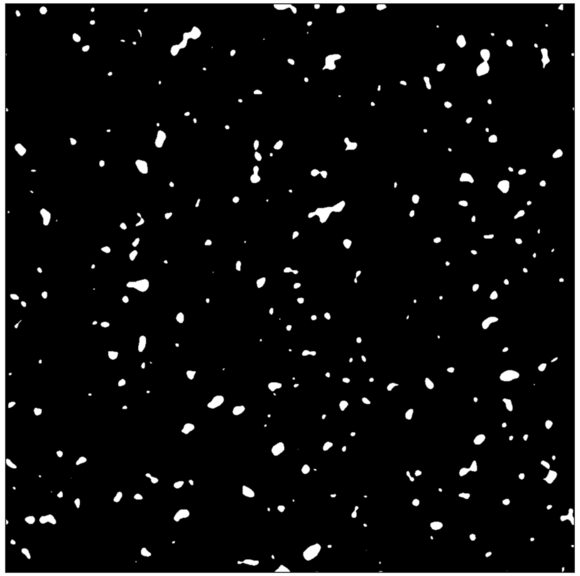
Source defects | Microstructure

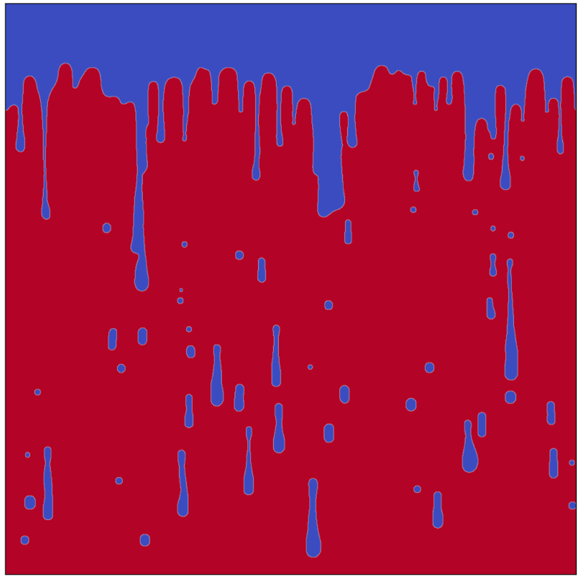
Coarse



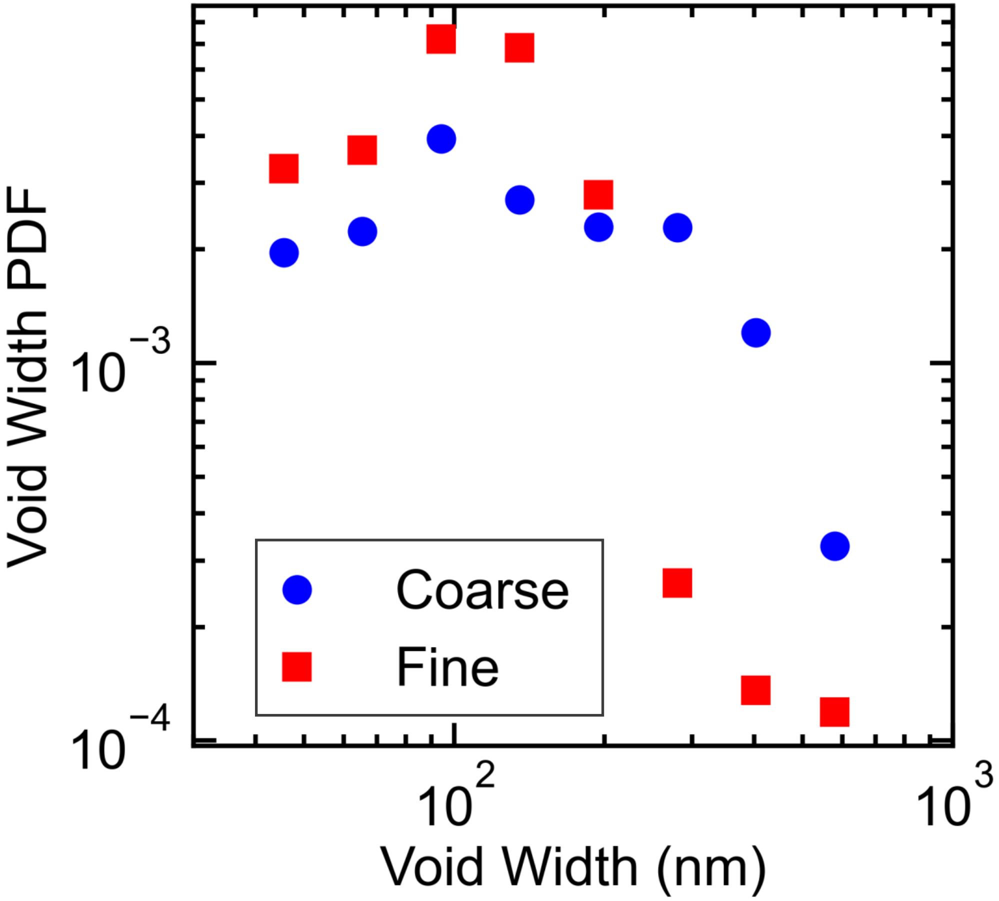


Fine





Mean void width
Experimental: 273 nm
Coarse: 245 nm
Fine: 145 nm



Key phase-field modeling features

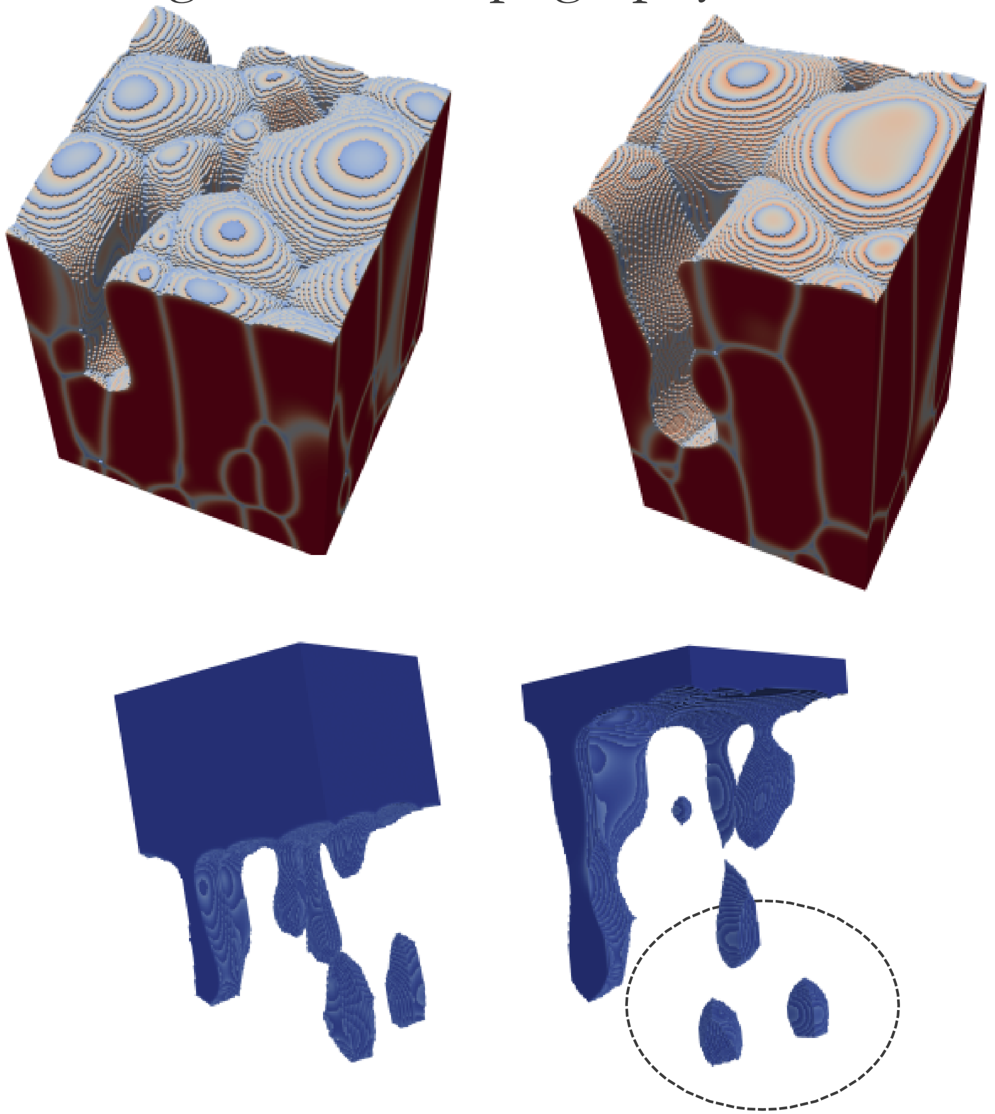
2D and 3D models incorporate concurrent vapor deposition and grain microstructure formation

- Locally inhomogeneous deposition produces **trapped pores** and **elongated voids**
- Source term defect formulation affords control over statistical properties of **porosity distribution**

Output microstructures can be used in subsequent ageing studies, and mesoscale shock initiation simulations

- Ageing following deposition shows **grain growth, surface smoothing,** and **void consolidation**

Rough surface topography formation



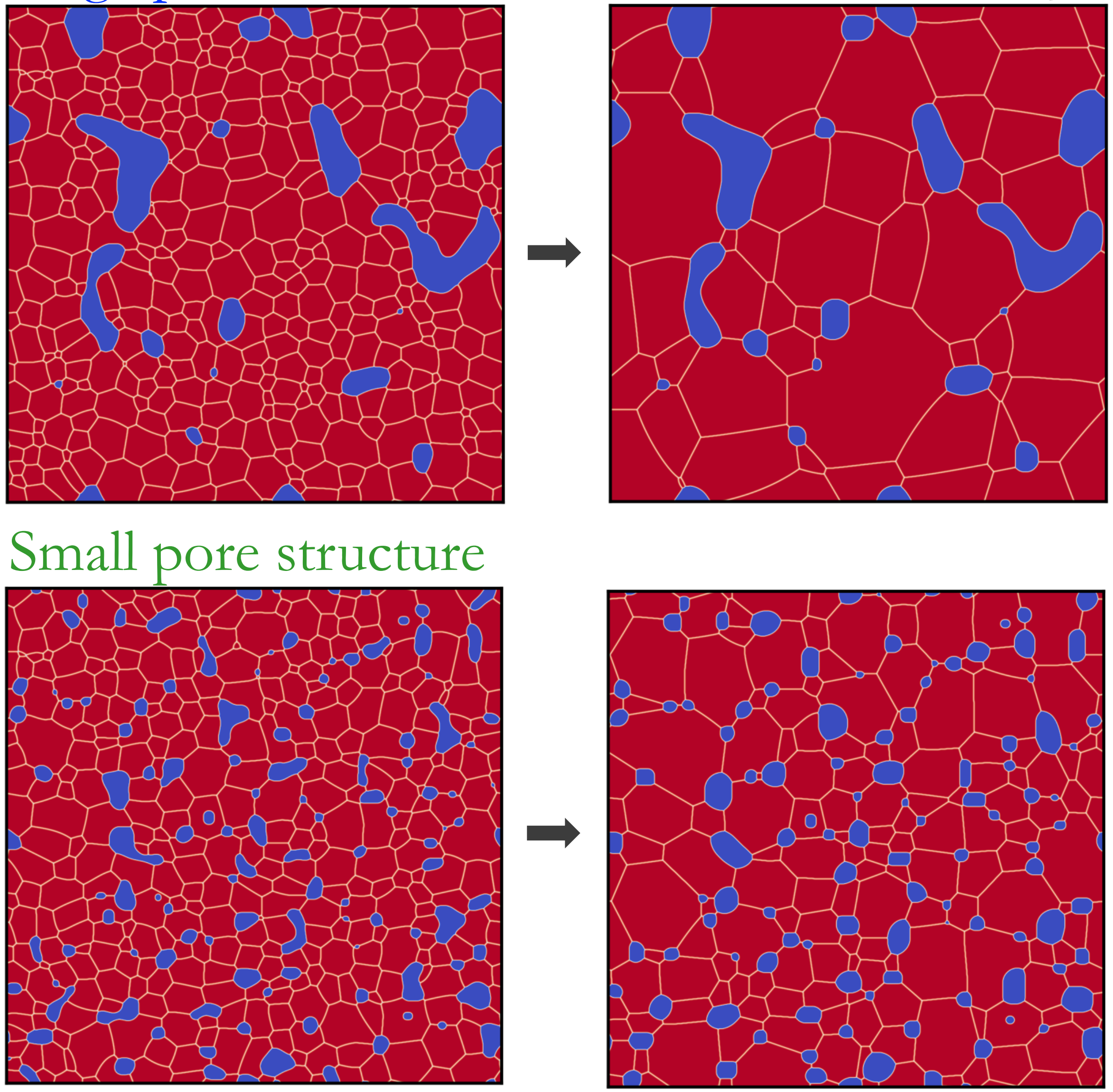
Trapped voids

Pore size dictates grain growth kinetics

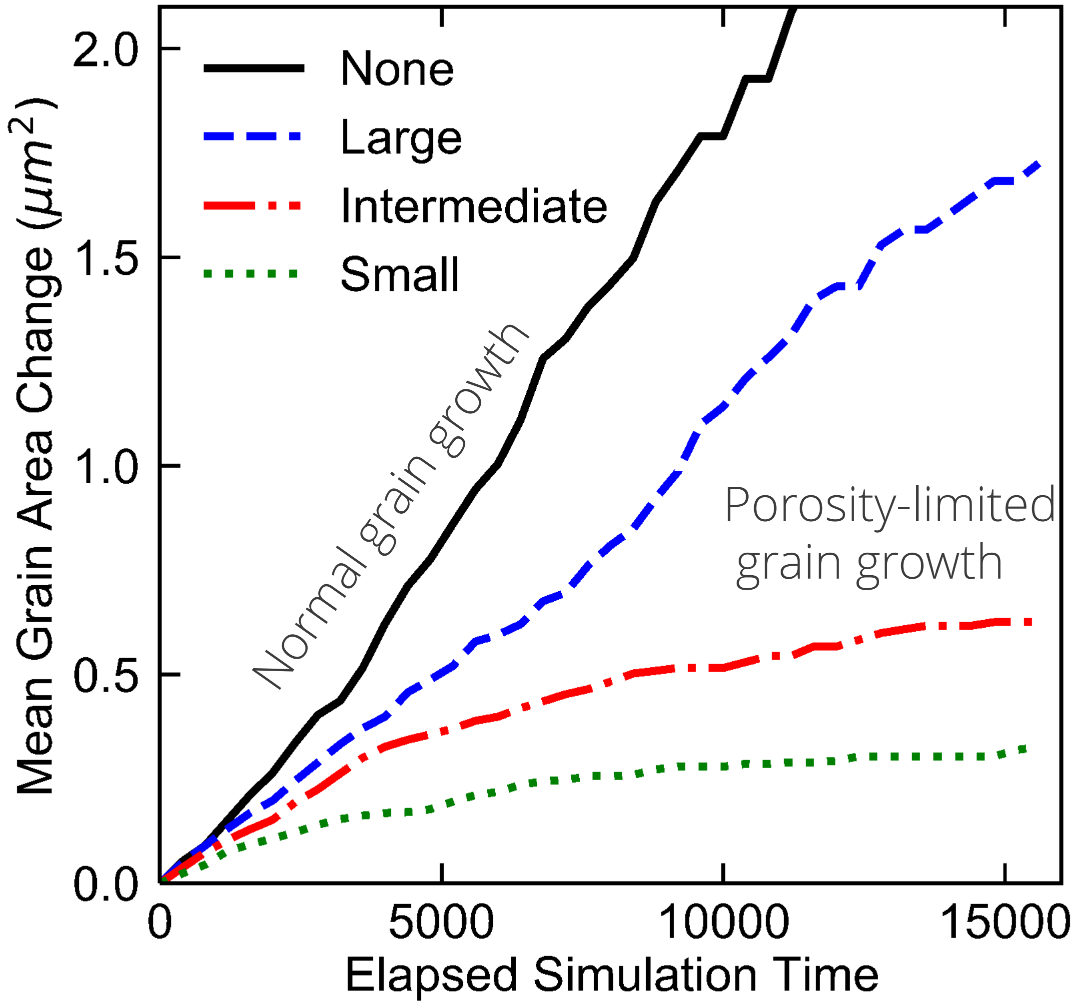
Large pore structure

10.2 μm

Small pore structure



Overall porosity ~12%



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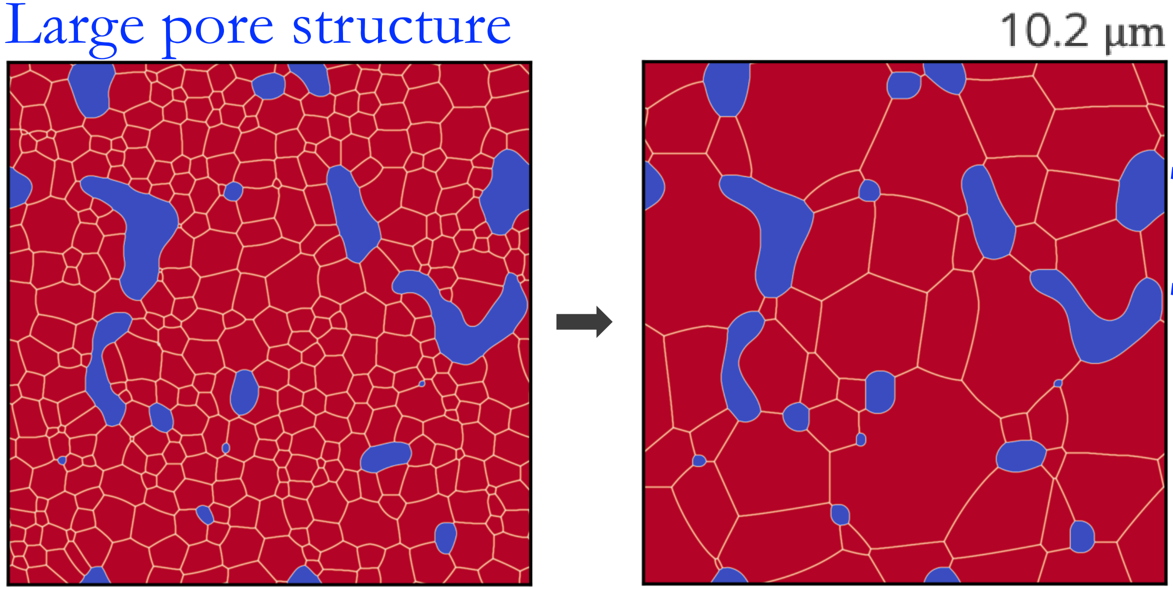
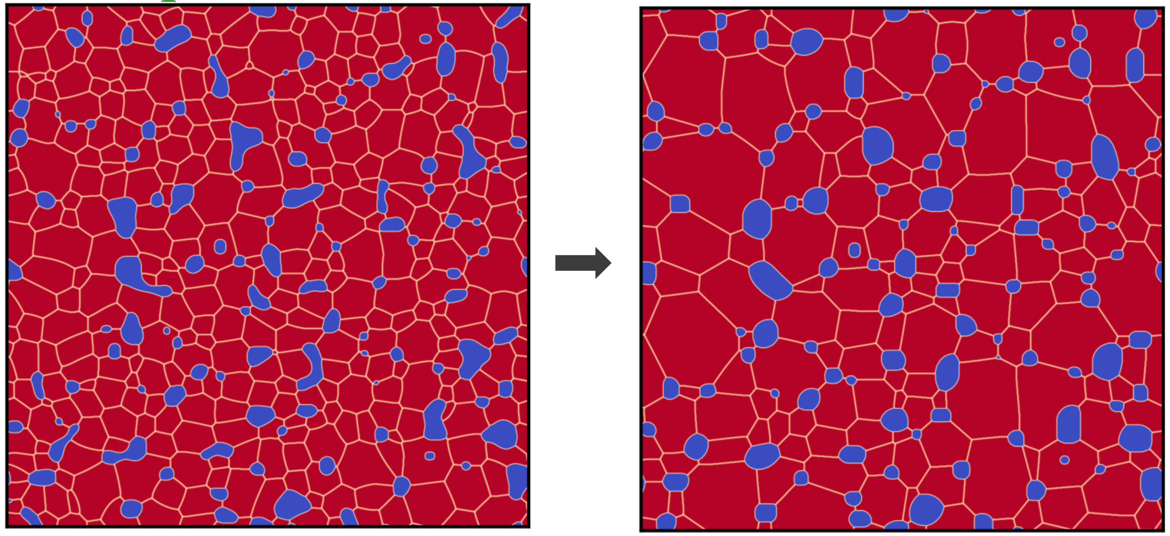


Small pore structure



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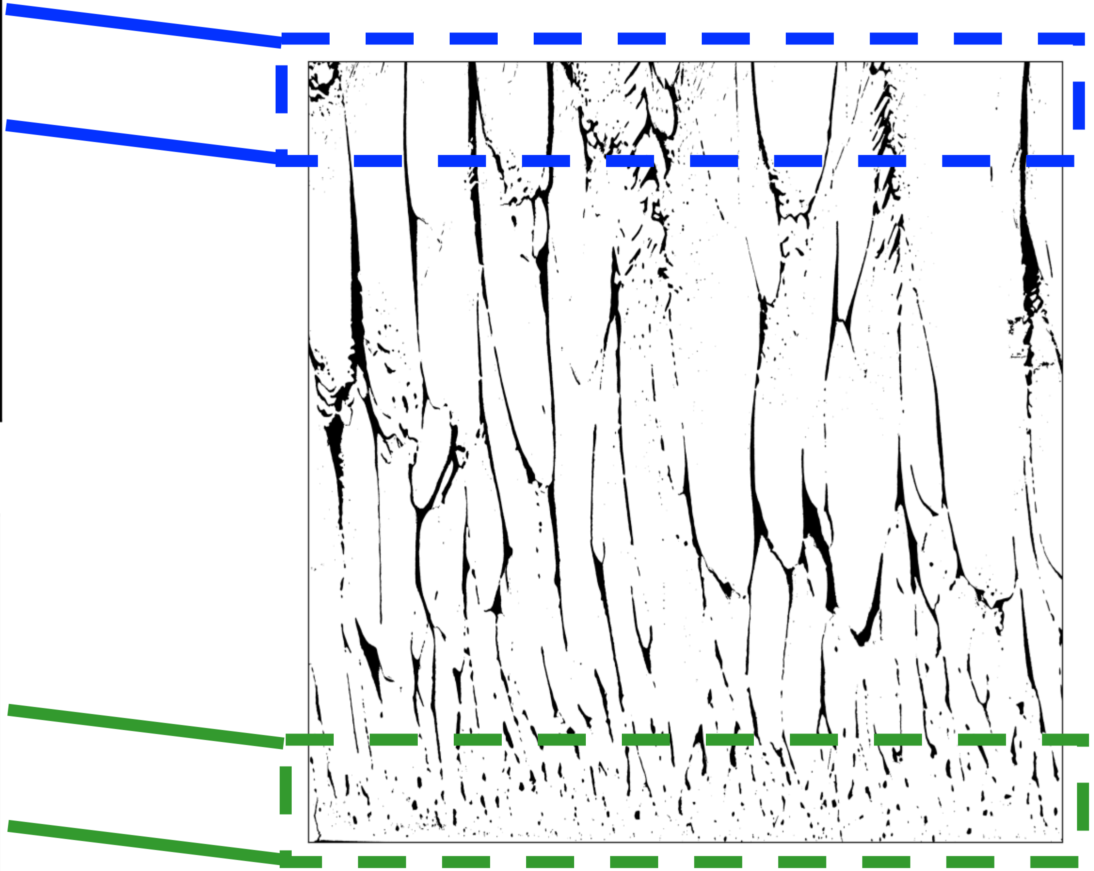

As-deposited PETN cross-section

Summary

- A coupled porous solid and grain growth phase-field model was augmented to study vapor-deposited energetic thin films with explicit vapor transport
- Defects in vapor deposition flux permitted formation of porosity distributions that qualitatively agree with experimental observations
- Simulations showed abundant, fine porosity limits grain growth more than rare, coarse porosity