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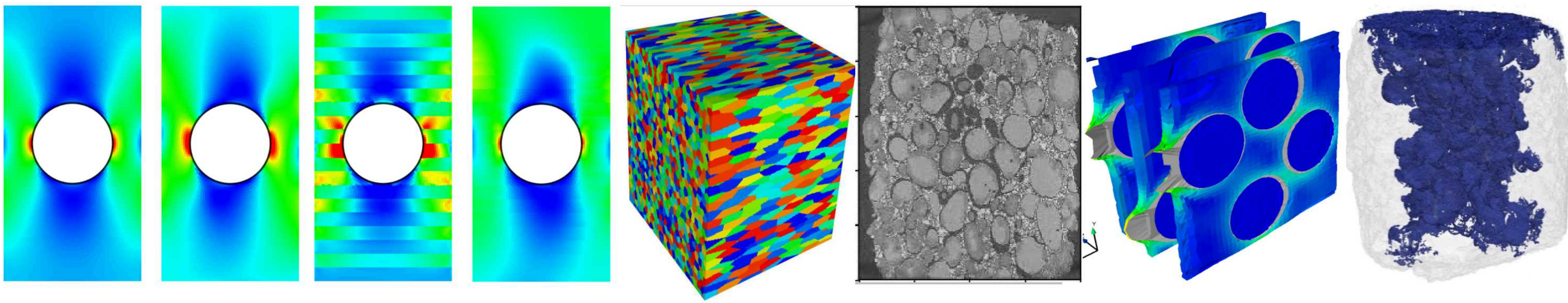

Mesoscale models to understand material variability and damage evolution

Aerospace Engineering Department, Auburn University

April 5, 2019

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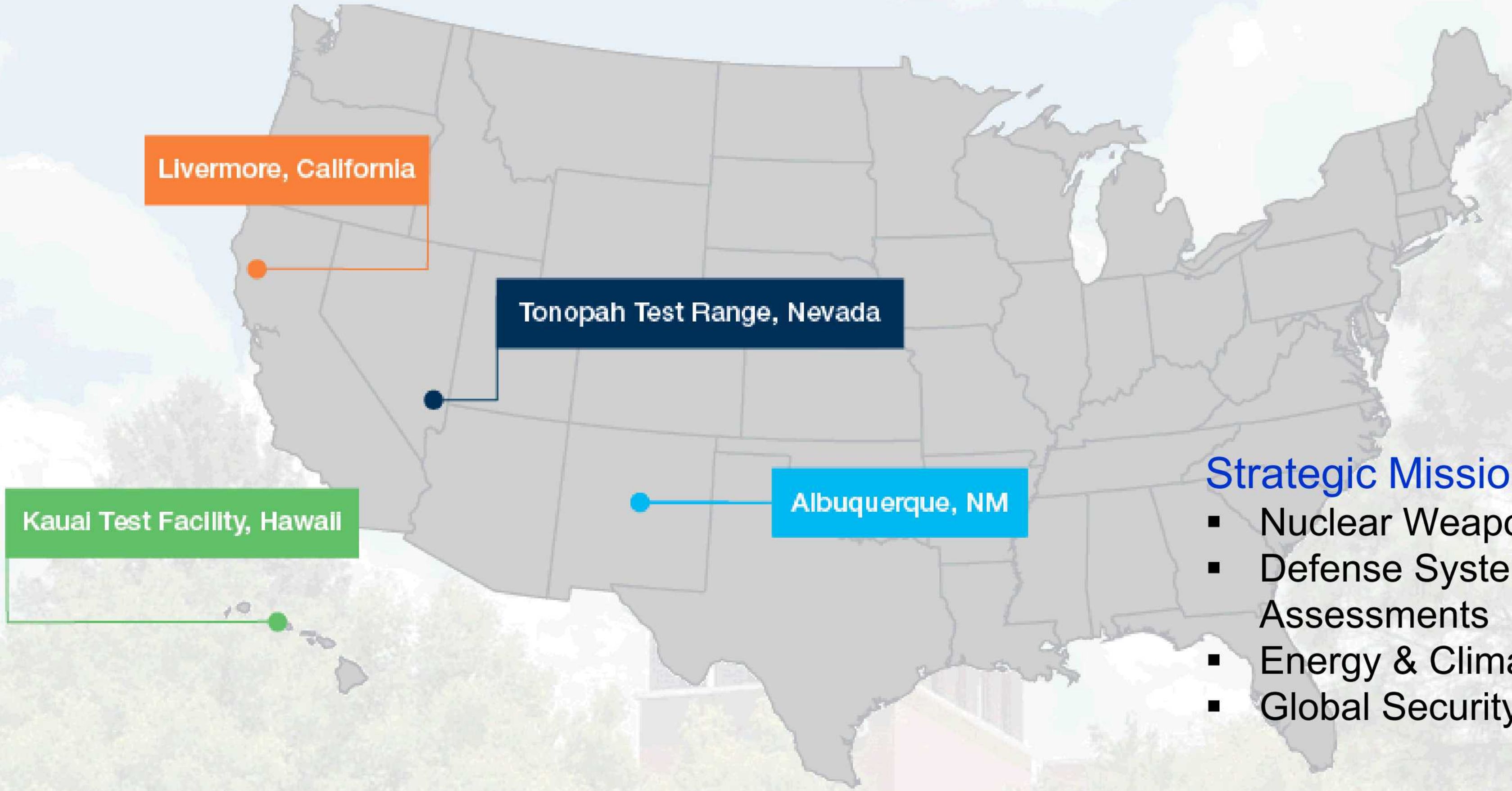
About Sandia National Laboratories



Strategic Mission Areas

- Nuclear Weapons
- Defense Systems & Assessments
- Energy & Climate
- Global Security

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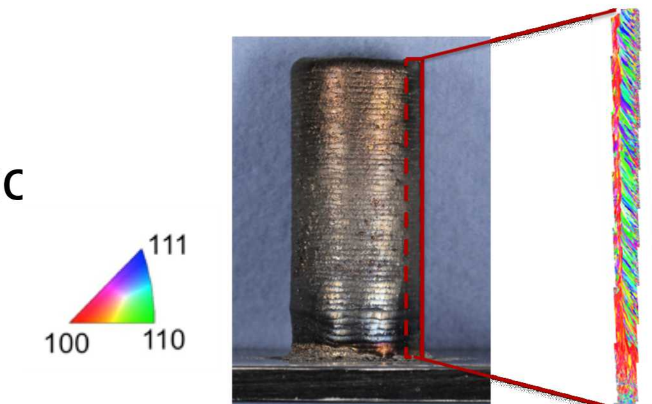
Presentation Outline

- Introduction: Why Mesoscale Models?
- Case Study 1: Thermal damage in propellants
- Case Study 2: Microstructure variability in additively manufactured metals
- Case Study 3: Damage evolution in elastc syntactic foams
- Conclusions



(K. Johnson, T. Rodgers, O. Underwood, SNL)

Collaborators

- Propellants:
  - Bill Erikson
  - Marcia Cooper
  - Stacy Guo
  - Mike Kaneshige
  - Scott Roberts
  - Dan Bolintineanu
- Additive Manufacturing:
  - Joe Bishop
  - Theron Rodgers
  - Hojun Lim
  - Mario Martinez
  - Allen Roach
- Syntactic Foams:
  - Kevin Long
  - Jay Carroll
  - Helena Jin
  - Zach Casias
  - Brad Huddleston

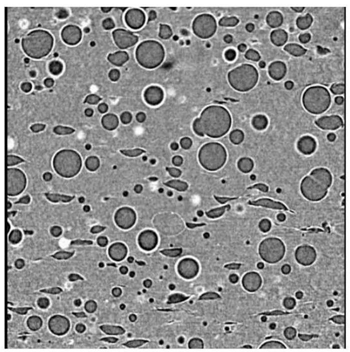
Mesoscale Phenomena in Materials

- Mesoscale— *an intermediate scale*

Mesoscale Process

Macroscale Response

Material Failure

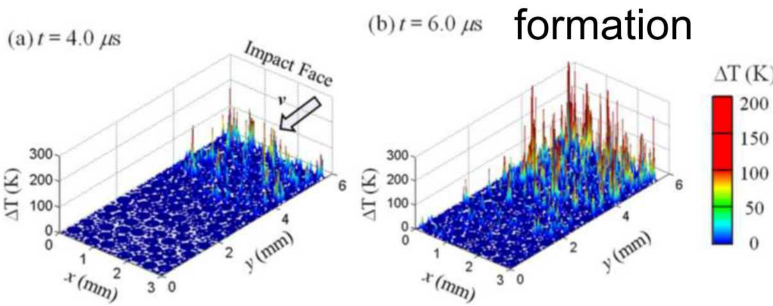


Local damage evolution

Figure 7. Shear cracks formed during plateau region on syntactic foam. Ahmadi et al., 2014

Shock Initiation of Explosives

Hot spot formation



A. Barua, S. Kim, Y. Horie, M. Zhou, J. App. Phys. 113 (2013) 064906.

https://www.quirkyscience.com/wpcontent/uploads/2012/06/Explosion-Image-by-US-Department-of-Defense.jpg

Thermal Damage in Propellants

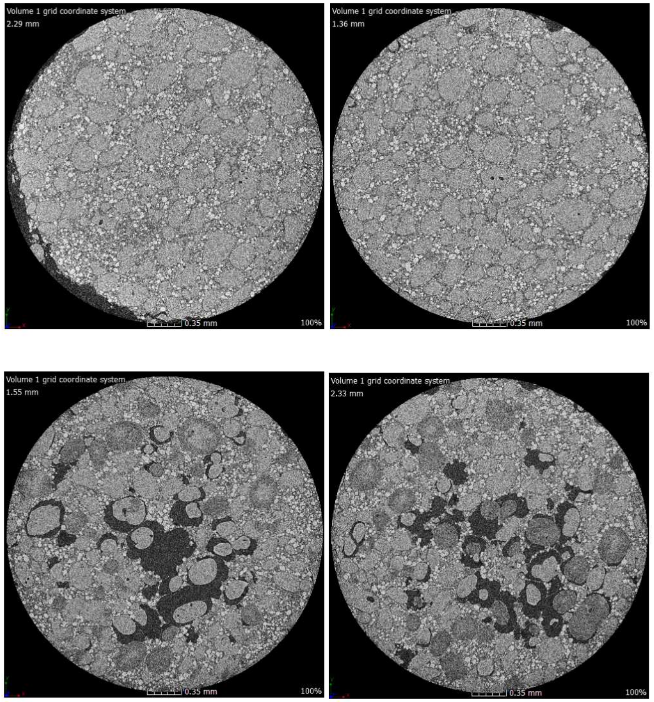
Thermal Damage in Propellants

- Why do we care?
  - Thermal Damage can result in increased reaction violence in cookoff (faster flame spread, convective combustion, DDT)
  - Hypothesis: connected porosity leads to these effects

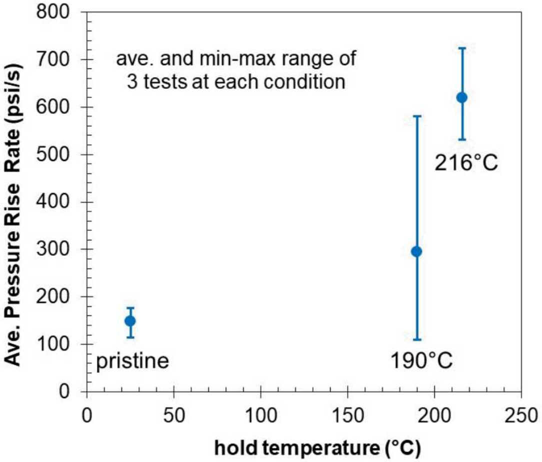
AP/HTPB propellant

Pristine

2 hrs. at 216°C



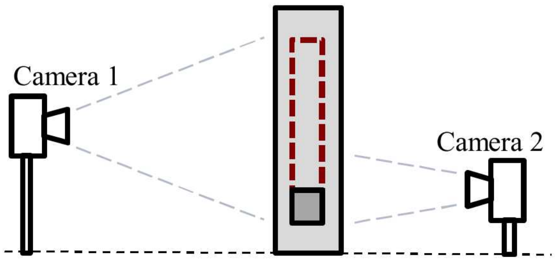
Average pressure rise rate (3 tests at each condition)



- **Implied ~4x burn rate enhancement over pristine with 216°C hold**

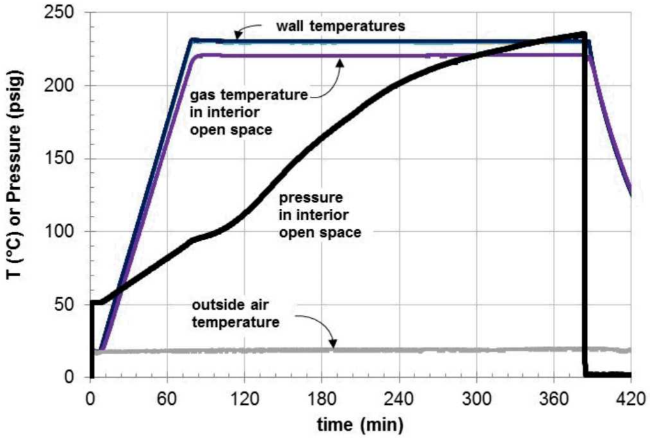
Thermal Damage Visualization (TDV) Test*

Schematic of TDV



Propellant in TDV Apparatus

Temperature and Pressure History



- Solid Propellant Material:
  - AP + Al + HTPB (IPDI cured) + aziridine bonding agent
  - Trimodal AP particle size distribution (majority is 400 μm)

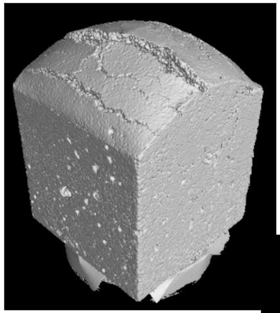
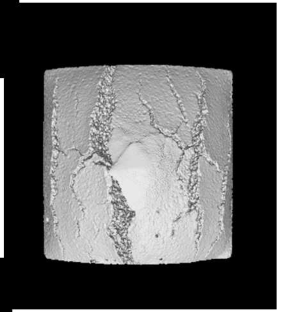
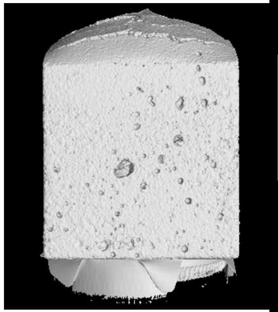
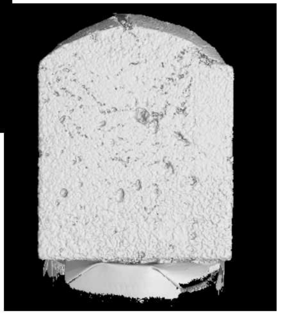
- Test Procedure:
- Test device sealed, initially 50 psi (3.4 MPa) argon.
- Heated to 230°C at 3°C/min, then hold
- Test went for ~5 hrs. with no ignition.
- Heat was cut off and pressure released.

initial state	at hold (230°C)	hold +10 min	hold +20 min	hold +30 min	hold +40 min	hold +50 min	hold +1 hr	hold +2 hr	hold +3 hr	hold +4 hr	hold +5 hr	pressure released

*Guo, S., Cooper, M. A. and Erikson, W. W., "Thermal Damage Visualization in Propellant Cookoff" JANNAF 30th PSHS Meeting, Newport News, VA, Dec. 2017.

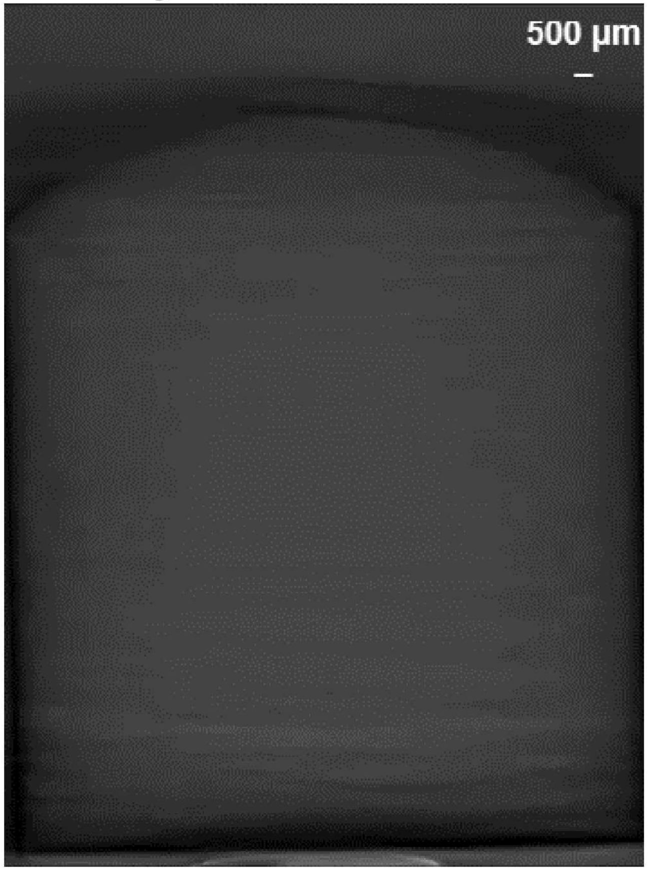
Thermal Damage Visualization CT Scan*

CT Scan of quenched sample from TDV test (pixel size ~44 µm)
Material has large AP crystals (mostly 400 µm)

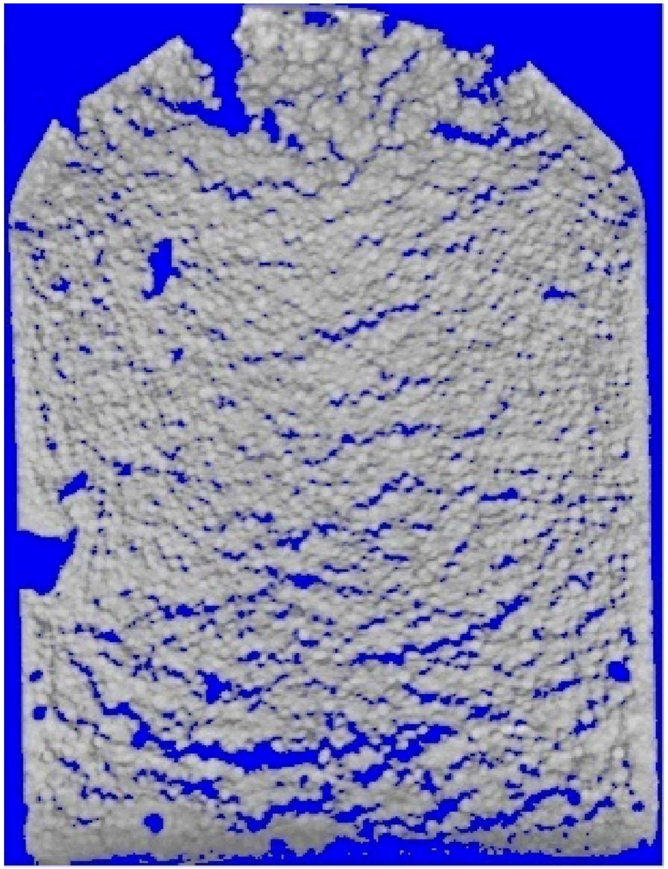





3-D Views

Grayscale Sliced View



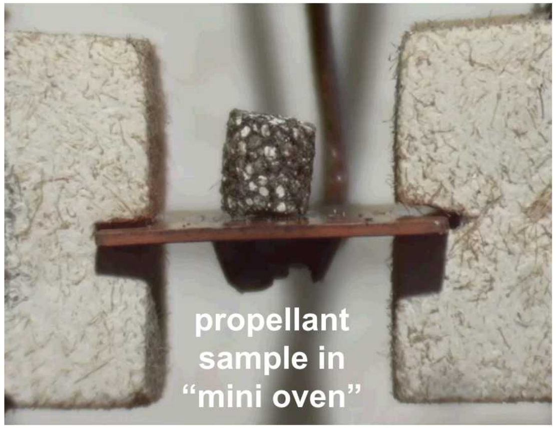
Threshold Applied (blue = void)



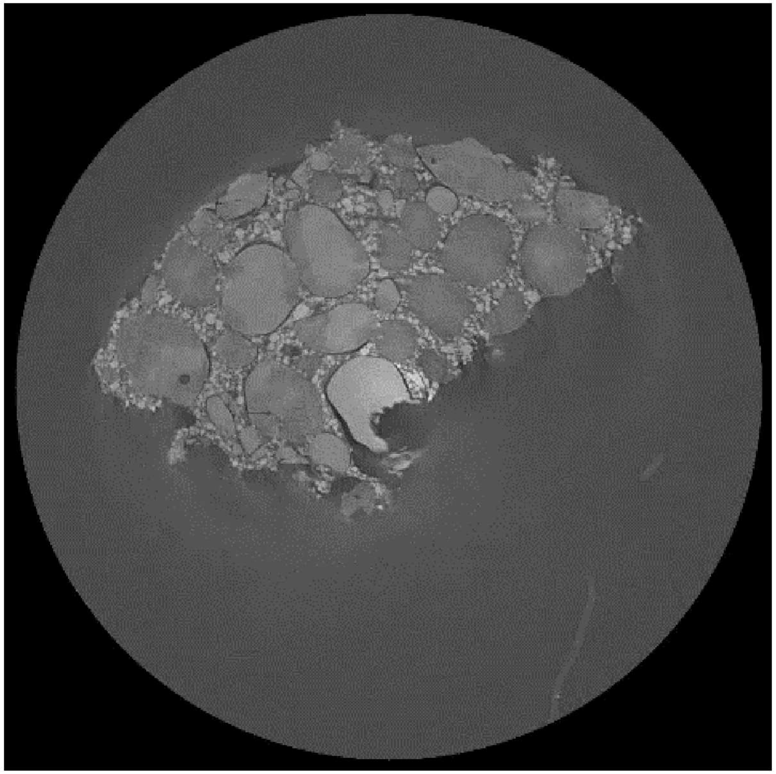
*Erikson, W. W., Cooper, M. A., Guo, S., Lechman, J. B., Noble, D. R. and Roberts, S. A., "Microstructure Analysis of Thermally Damaged AP Propellant," JANNAF 30th PSHS Meeting, Newport News, VA, Dec. 2017.

High Resolution CT Scans

- Small propellant sample (3.2 mm x 3.2 mm cylinder)
- heated unconfined in "mini-oven" at constant temperature for 2 hrs.
- CT scan performed on cooled samples.



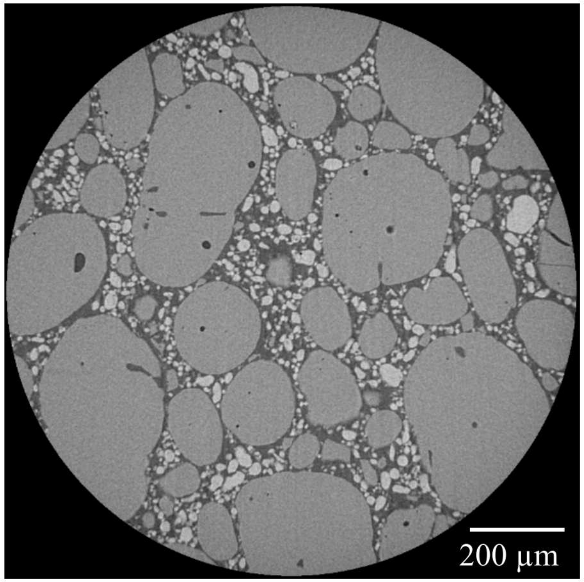
2 hr. at 215°C (3.4 μm/pixel)



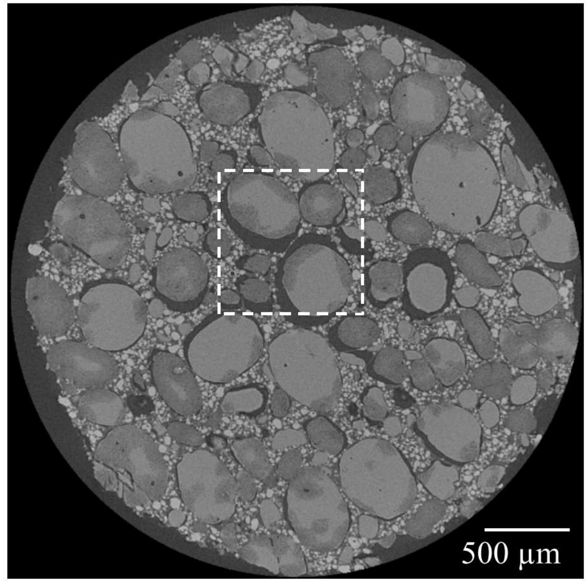
2 hr. at 240°C (3.4 μm/pixel)

Effect of Temperature

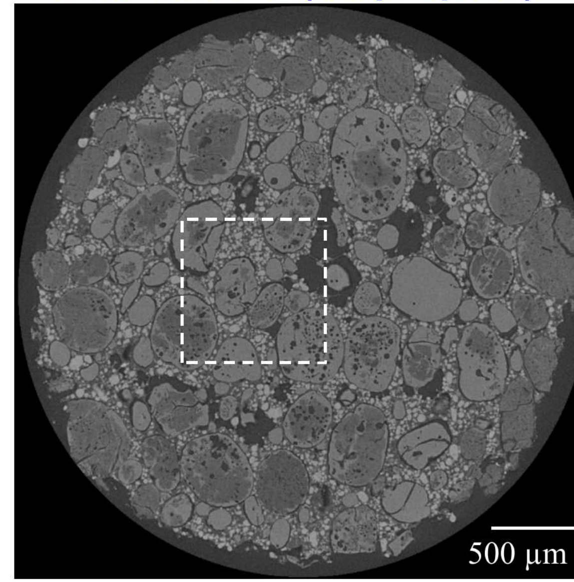
Pristine (1.24 µm/pixel)



2 hr. at 215°C (3.4 µm/pixel)

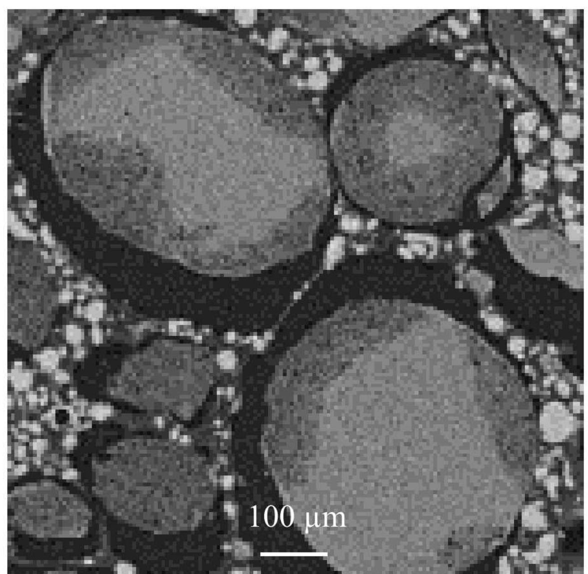


2 hr. at 240°C (3.4 µm/pixel)



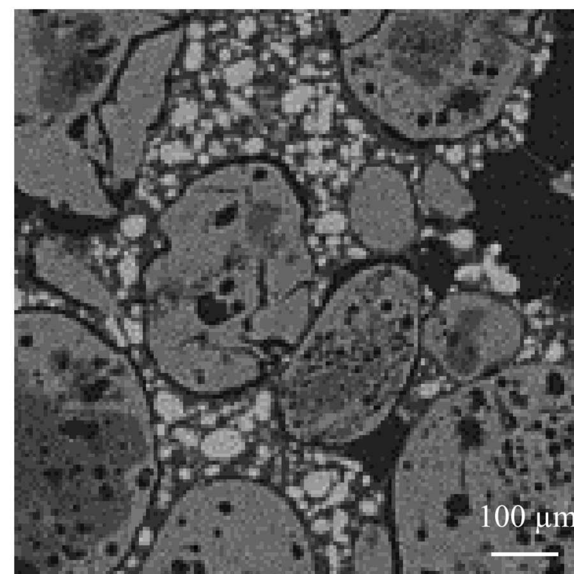
215°C Observations

- **crescent-shaped voids** around particles; more voids **toward the center** of sample
- two-tone gray of particles shows inner region is pristine; **outer is porous**



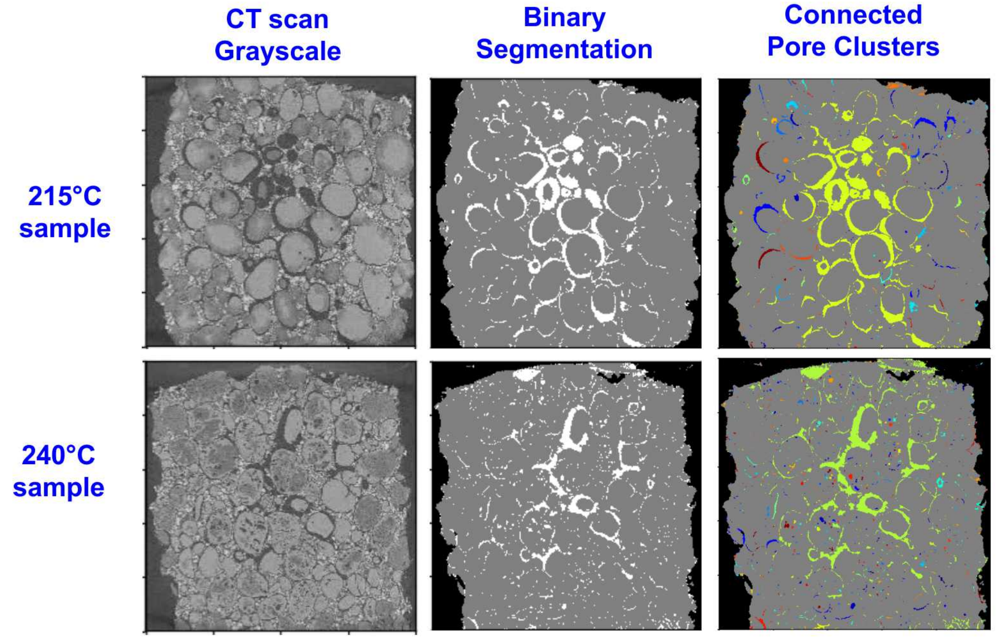
240°C Observations

- particles exhibit **cracking**
- much **more porosity within** the particles
- porosity outside particles hasn't changed much compared to 215°C

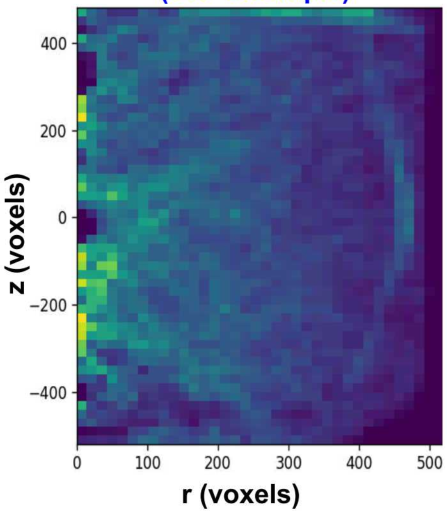


Connected Porosity in High Resolution Scans

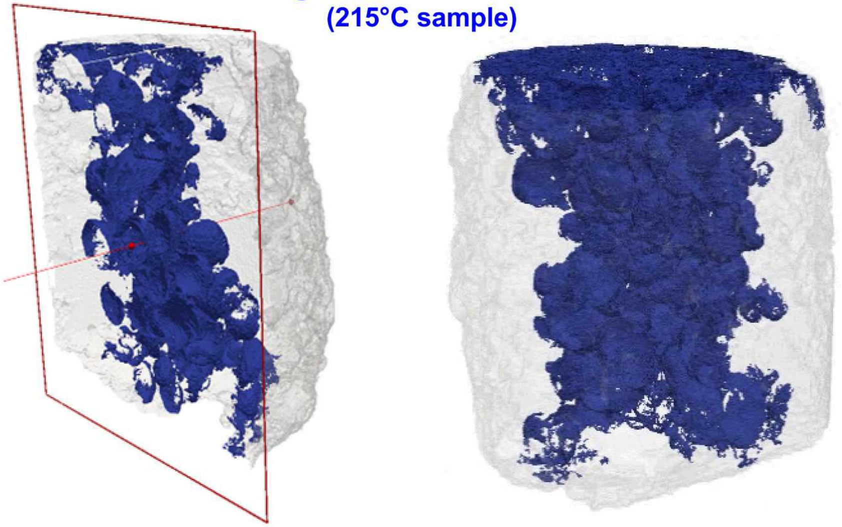
- Python-based script using open source libraries (*NumPy, scikit-image, SciPy*) was used to:
  - Remove noise, threshold, remove small features
  - Identify connected clusters (connected components labeling algorithm)
  - Determine porosity and pore surface area statistics (marching cubes algorithm)
  - Examine percolation characteristics



Porosity Map
(215°C sample)



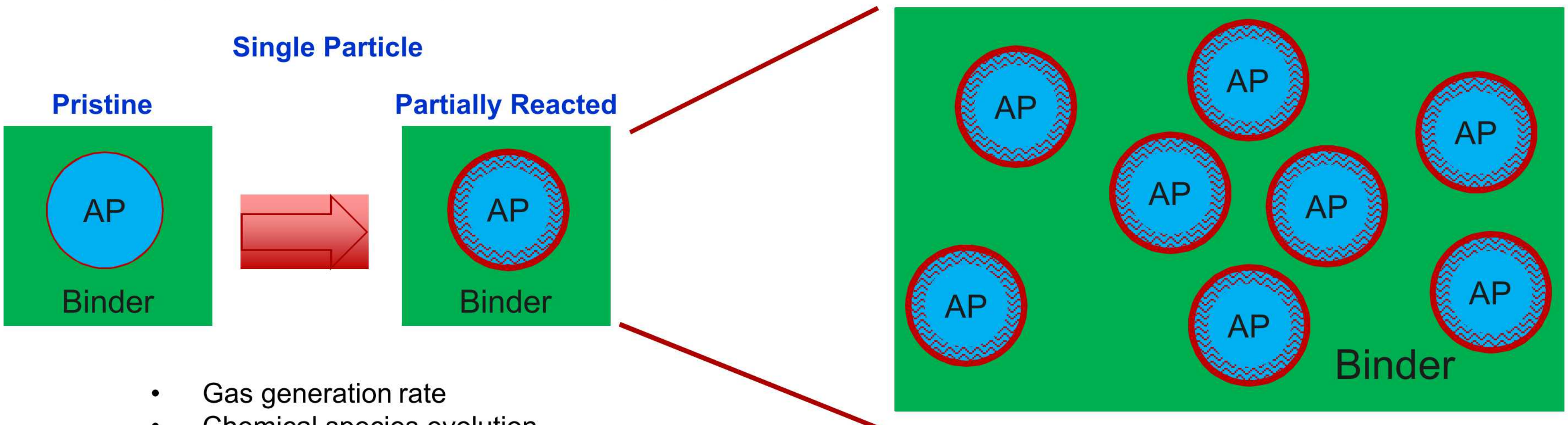
Largest Connected Cluster
(215°C sample)



Mesoscale Model of Thermal Damage

- Objectives:
  - Predict evolution of connected porosity
  - determine physics factors contributing to porosity evolution & void coalescence
  - Link pressure evolution to gas generation rates and temperature through chemistry

Multiple Particles



- Gas generation rate
- Chemical species evolution
- Particle-binder interface strength
- Decomposition product-binder chemistry

- Single particle physics +
- Local Mechanical stress states
- Particle spacing & volume fraction—how close are nearest neighbors?
- Particle & binder mechanical properties
- Global boundary conditions (confined vs. unconfined, etc)

Mesoscale Modeling Workflow

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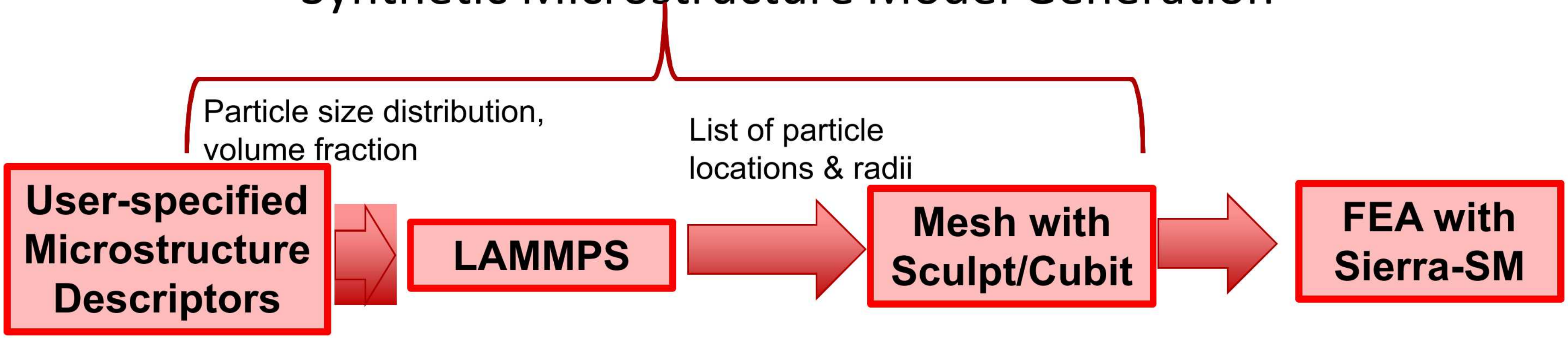
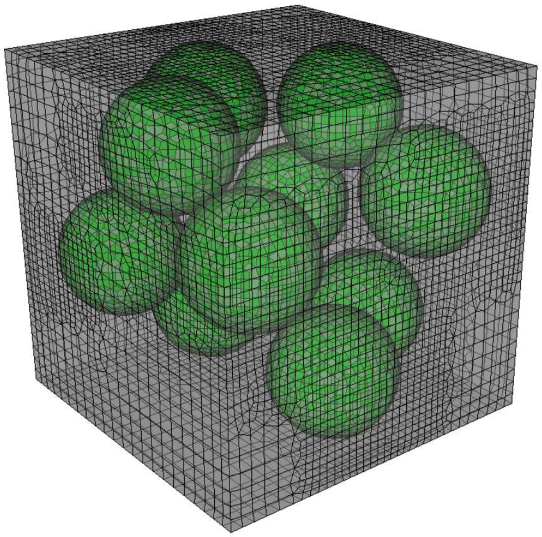
- Synthetic Microstructure Model Generation



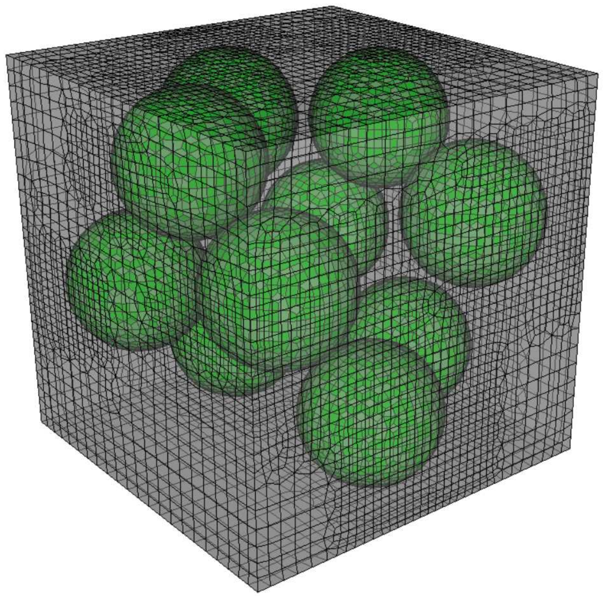
LAMMPS—Large-scale Atomic/Molecular Massively Parallel Simulator
http://lammps.sandia.gov

Sculpt—Meshing tool that generates automated all-hex mesh
S.J. Owen, **J.A. Brown**, C.D. Ernst, H. Lim, K.N. Long, “Hexahedral Mesh Generation for 3D Computational Materials Modeling,” *Procedia Engineering*, 203, (2017), pp. 167-179.



Sierra Mechanics—Finite element software, large deformations, multi-physics coupling
https://www.sandia.gov/asc/integrated_codes.html

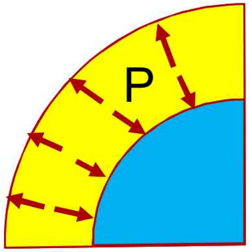
Finite Element Model



- Elastic-plastic model for AP pellets
- viscoelastic model for binder
- cohesive zone model to represent the bonded interface between particle & binder

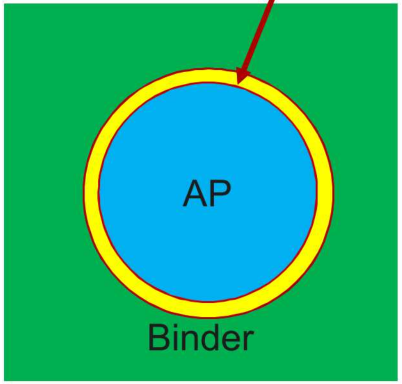
Approximately tuned to AP/HTPB properties & bond strength

$$P = \frac{nRT}{V}$$



Apply pressure boundary condition at particle-binder cohesive zone interfaces

Cohesive zone elements



Gas Generation Rates

- Ideal gas law holds: $P = \frac{nRT}{V}$
- At low temperatures, AP decomposition follows a **sigmoidal pattern** (induction, acceleration, deceleration), with a **max. decomposition level** (typically 30%).
- First-cut representation of the gas generation (moles per time) we assume:
  - 1 mol AP → 4 moles gas (N_2, H_2O, …)
  - Experimental data for decomposition ($d\alpha/dt$) taken at one temperature was related to other temperatures by assuming: $$\frac{d\alpha}{dt} = f(\alpha)k(T)$$

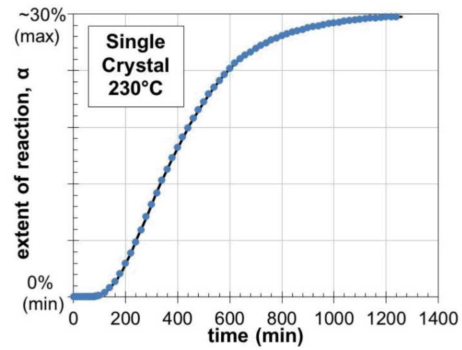
$$k(T) = Ae^{\frac{-E_a}{RT}}$$

α is extent of reaction
f(α) is a reaction model (sigmoidal behavior)
(E_a chosen at 80 kJ/mol)

$$E_a = 80kJ/mol$$

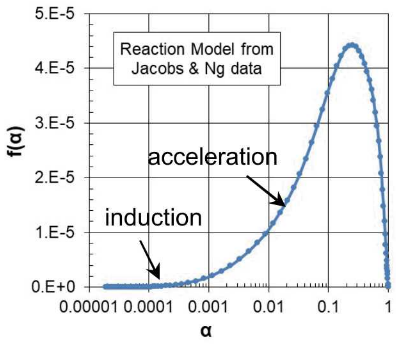
- Moles of gas evolved per particle, n(t) is directly proportional to α(t). Calculated for 190, 215 and 240°C.

AP Decomposition Data

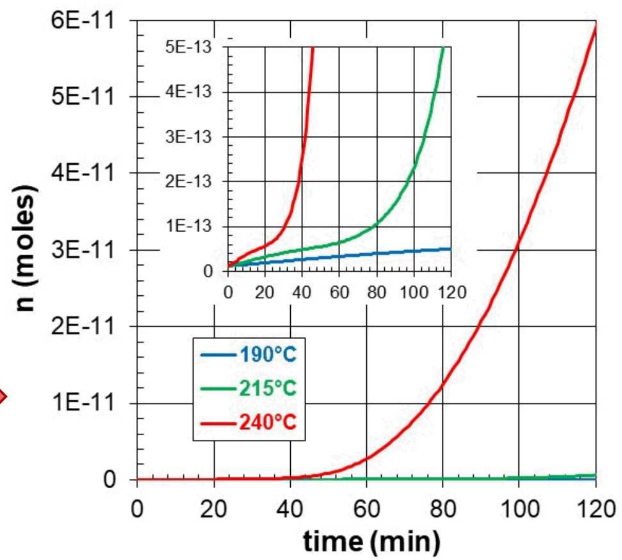


Jacobs & Ng. *Proc. of 7th Int'l. Symp. on the Reactivity of Solids.* Bristol, England: Chapman and Hall. 398-410 (1972).

AP Rxn. Model

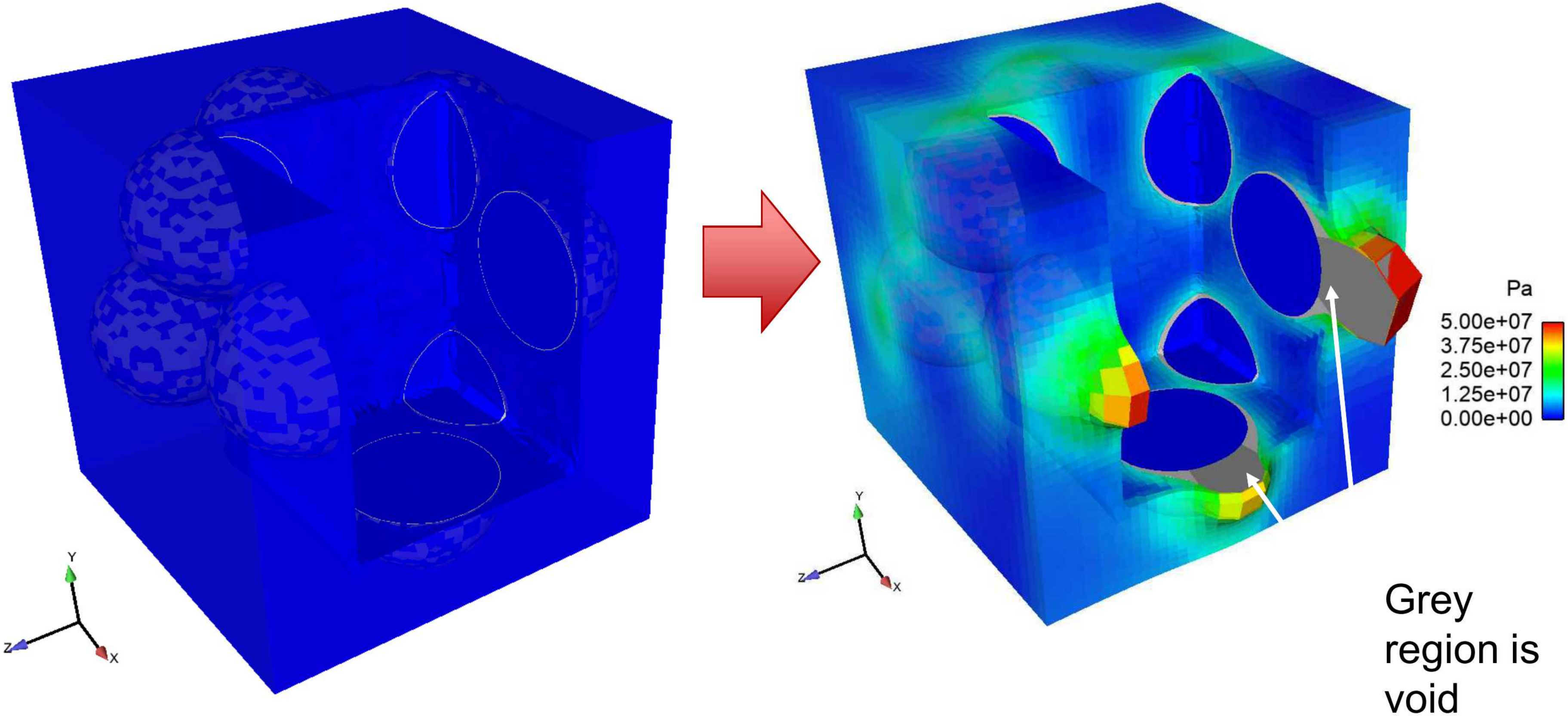


Gas Evolved for 400 µm AP particle



Porosity Evolution

Pristine | 85 min at 240C

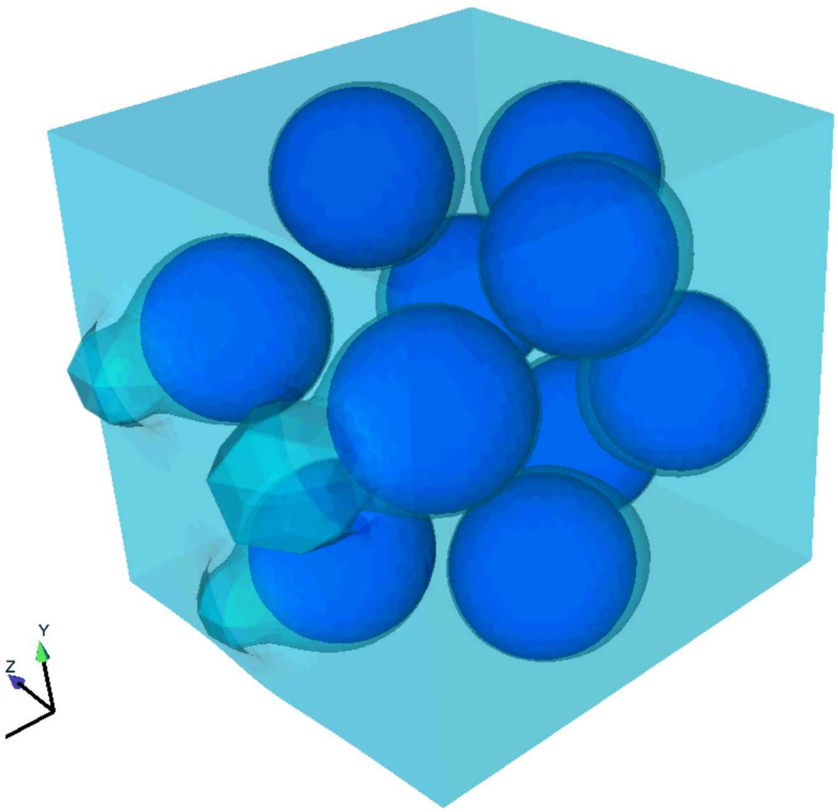


- High stress regions form in-between particles as gas pressure increases
- A free surface allows large deformation of binder and would likely result in venting

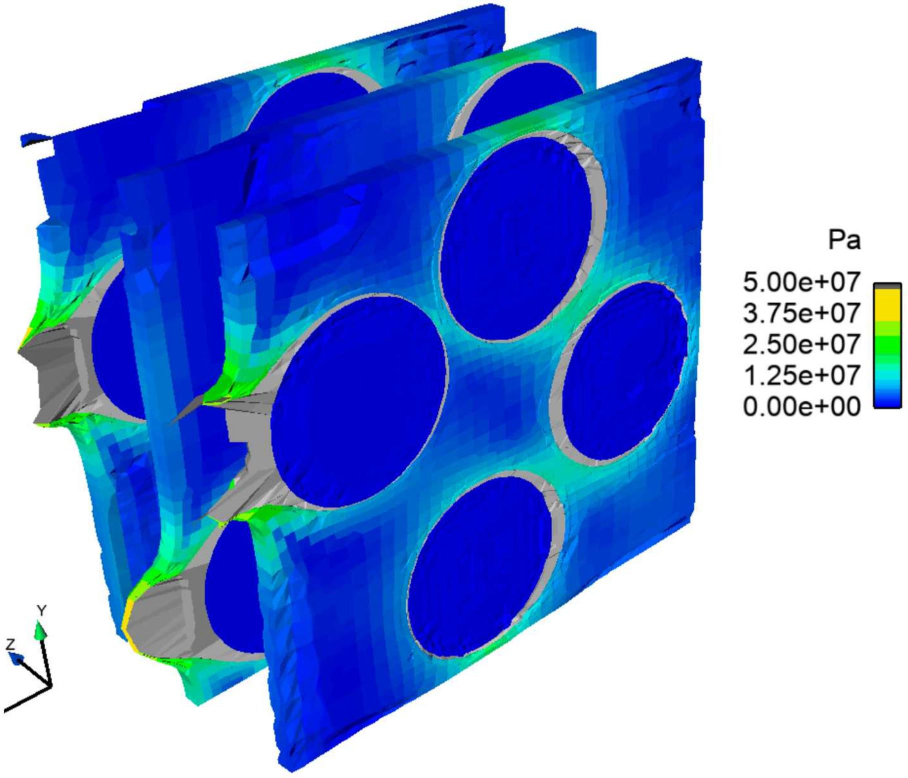
Porosity Evolution

85 min at 240C

3D view (transparent matrix)



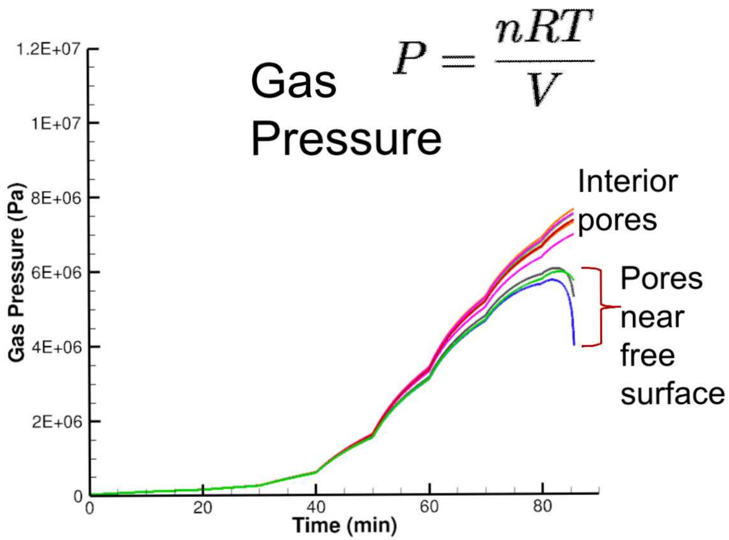
2D slices along Z axis

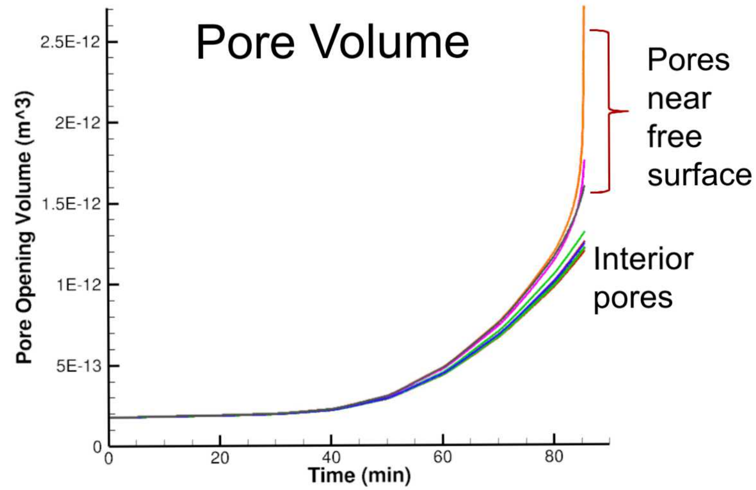


Pressure and Pore-Volume Histories

With Chemistry

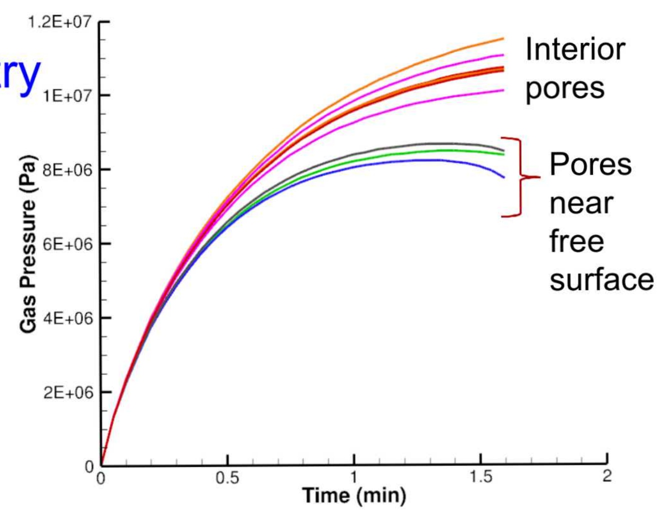
$$n = f(\alpha, t, T)$$

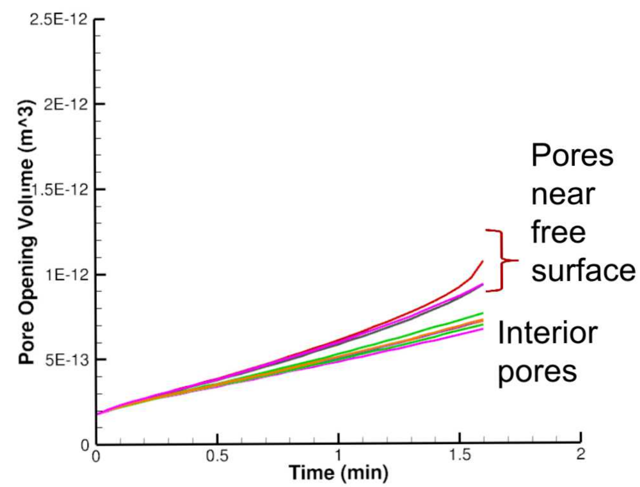




Without Chemistry

$$n = constant$$





Comparison of Model and Experiment

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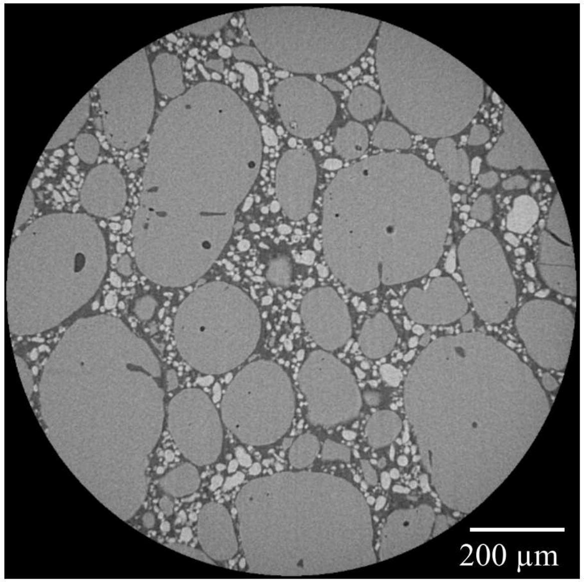
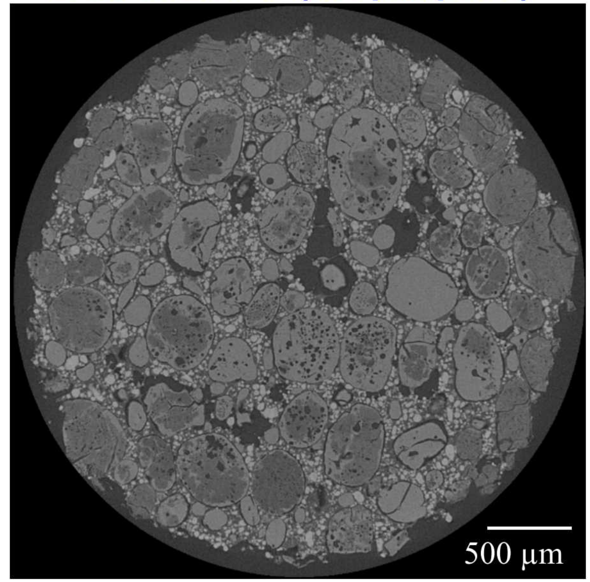
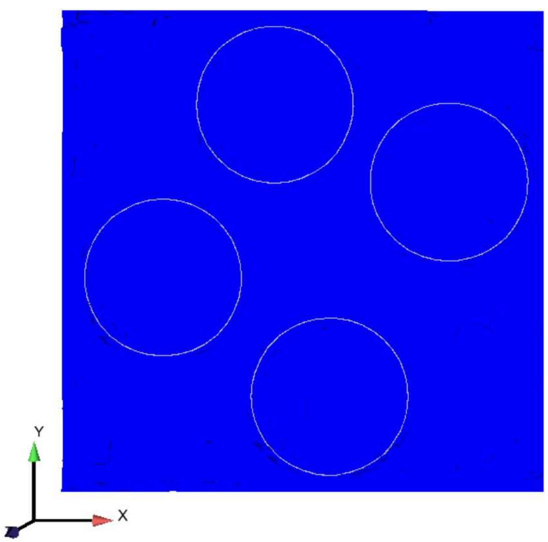
Pristine (1.24 µm/pixel)



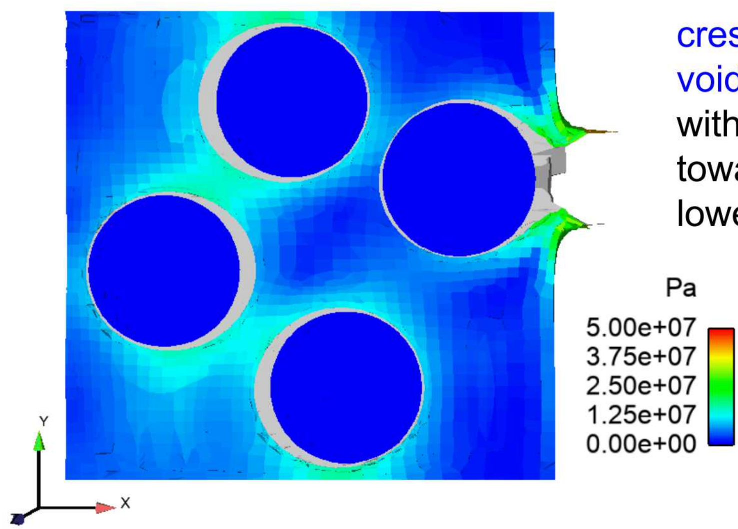
2 hr. at 240°C (3.4 µm/pixel)



- Observations from CT scan images show crescent-shaped voids surrounding the particles; presumably from decomposition gases trapped in the gas-tight binder



Model cross-section

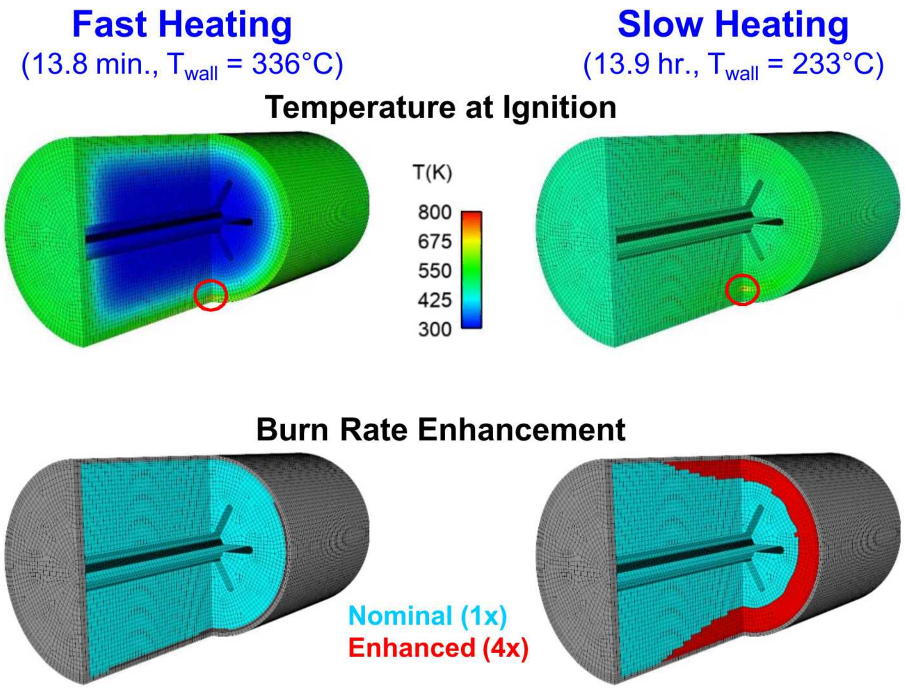


crescent-shaped voids develop with preference toward regions of lower stress

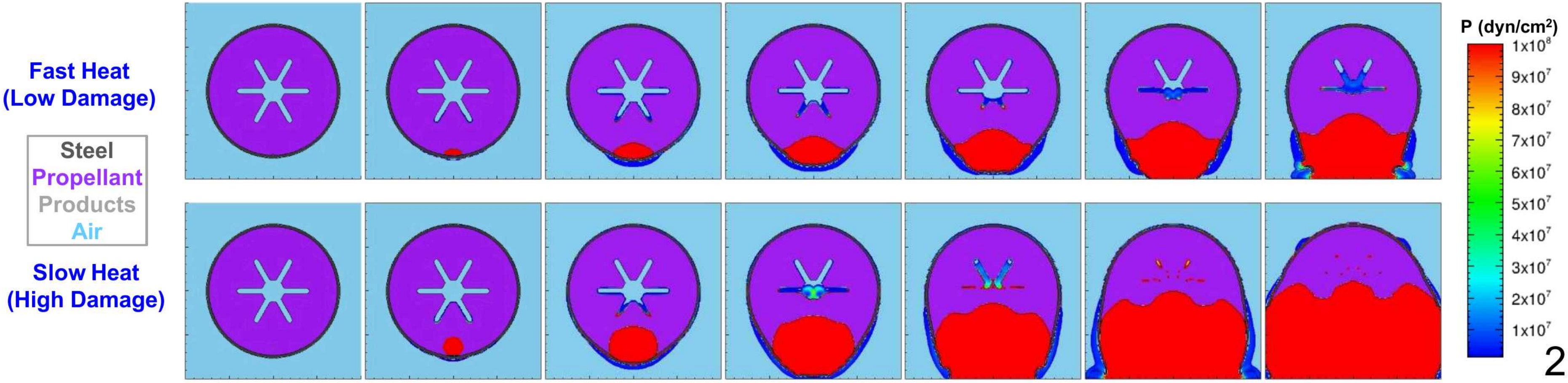
von Mises Stress (Pa)

Informing Macroscale Cookoff Models

- Two Test cases with simplified geometry (pseudo rocket motor)
  - Slow Heating (15°C/hr. rate),
  - Fast Heating (800 K radiant source)
- Locations with extent of rxn. > 0.75% were deemed “damaged” (mesoscale sims) and given a 4x burn enhancement value (from combustion bomb measurements).



2D Slice of Pressure & Materials (20 μs image spacing)



Summary:

- High-resolution CT scans show crescent-shaped voids form around large AP particles
  - Significant amount of connected (percolating) porosity
- Model predicts crescent-shaped voids develop with preference toward regions of lower stress
  - governed by global boundary conditions and local nearest-neighbor distances

Future Work:

- Add failure criteria for binder material—growth of connected porosity
- Add failure criteria for AP particles—particle cracking
- Extend approach to include larger volumes, experimentally determined particle size distributions

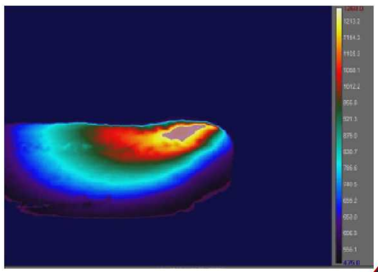
22

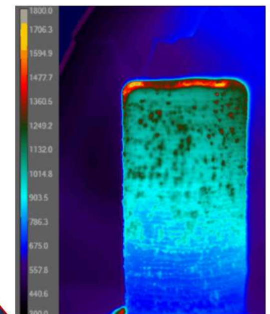
Accounting for Microstructure Variability in Additively Manufactured Metals

J.A. Brown, J.E. Bishop, *Modelling Simul. Mater. Sci. Eng.* 27 (2019) 025003 (22pp).

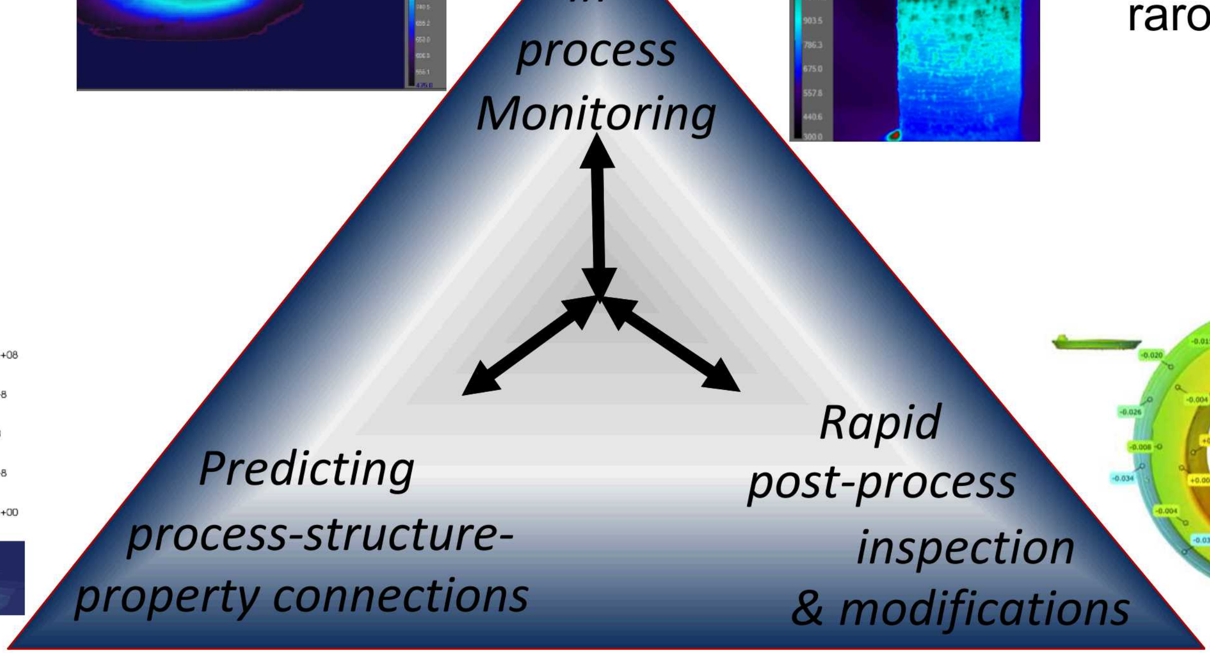
AM for Design Paradigm Change

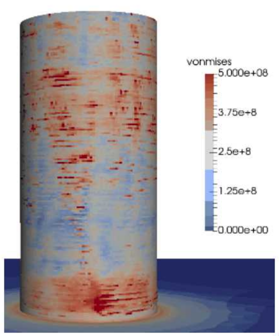
- Sandia is developing an assurance capability that is rapid, flexible, and practical that exploits disruptive capabilities of Additive Manufacturing
- Develop deep materials & process understanding by integrating validated, predictive capability with real-time and ex-situ diagnostics to realize Uncertainty Quantification driven qualification of design and process

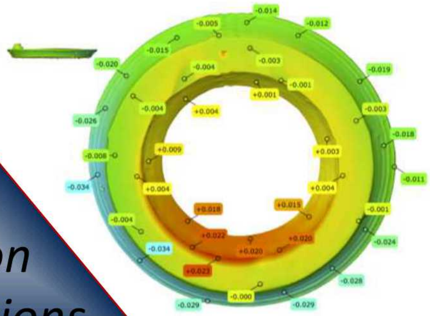




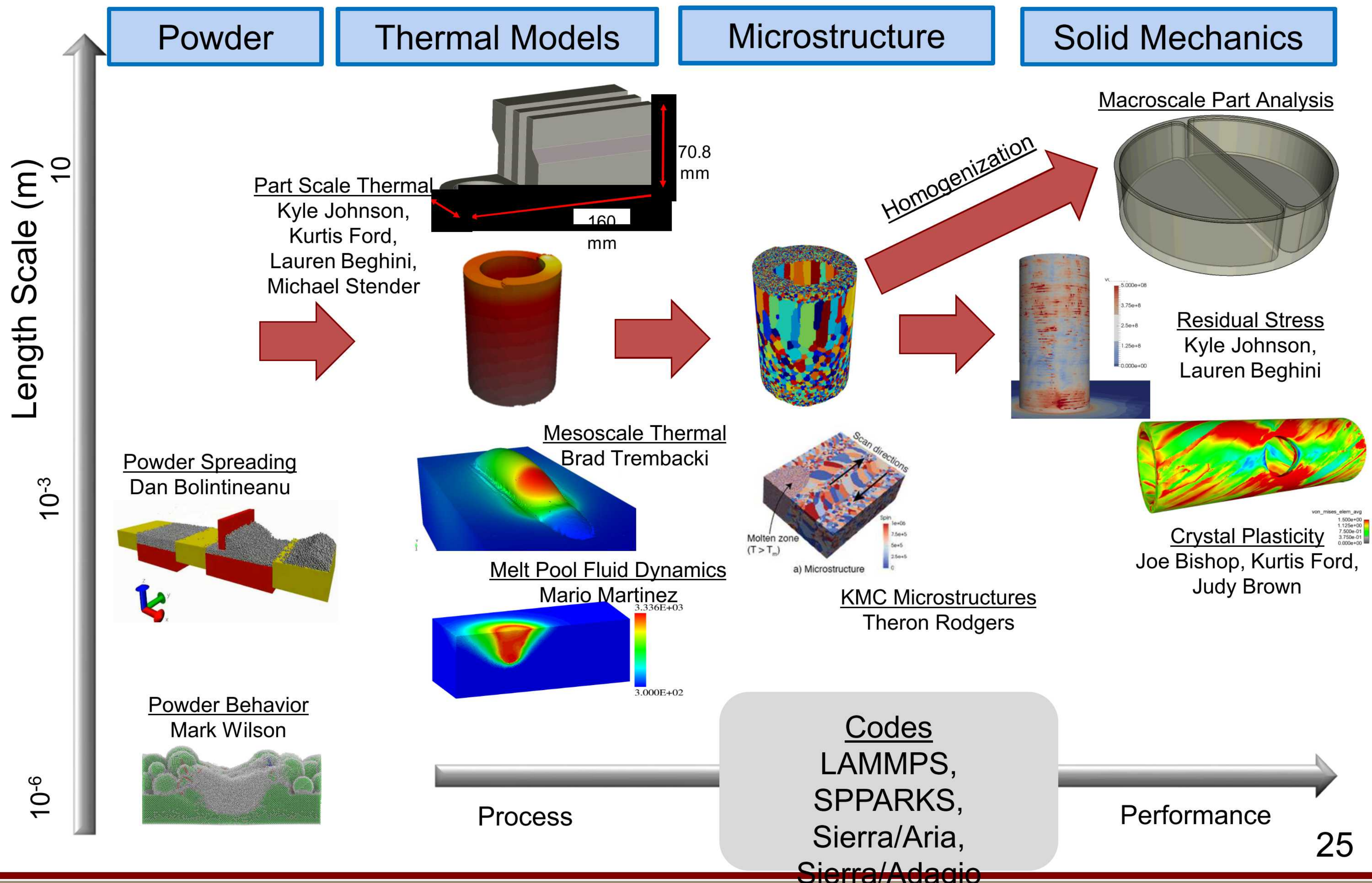
Born Qualified Grand Challenge LDRD
POC: Allen Roach
raroach@sandia.gov







AM Modeling Efforts at Sandia

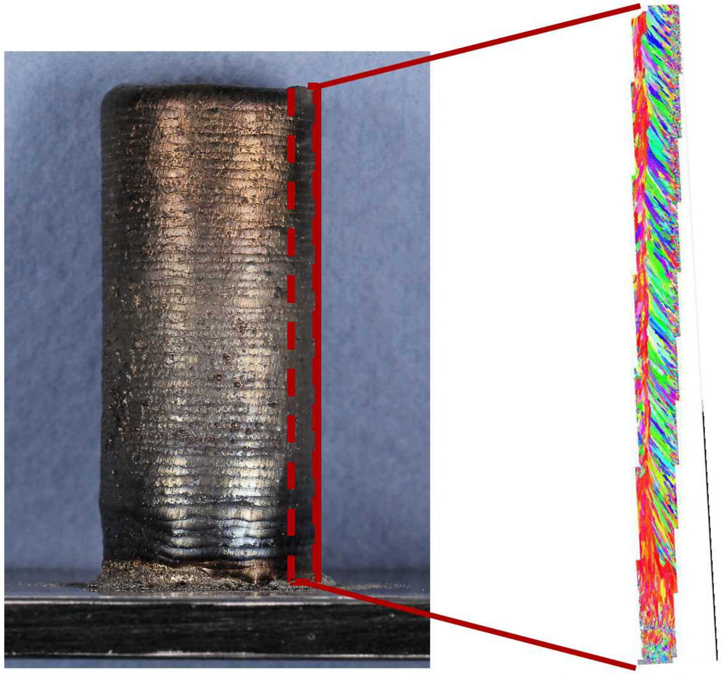


Unique Microstructure in AM Structures

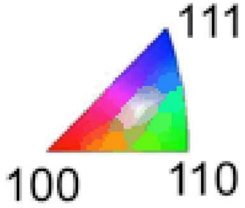
- Highly process-dependent: AM process, local thermal history, melt pool shape, scan pattern & velocity

- How should we choose material models for macroscale AM structures?
  - Is there part-scale texture/anisotropy?
  - Regions of local texture?

- Quantify errors introduced by simplified material models used for welds and AM structures
  - Model-form error estimation
  - Unknown/uncertain material properties
  - Effects of microstructural variability



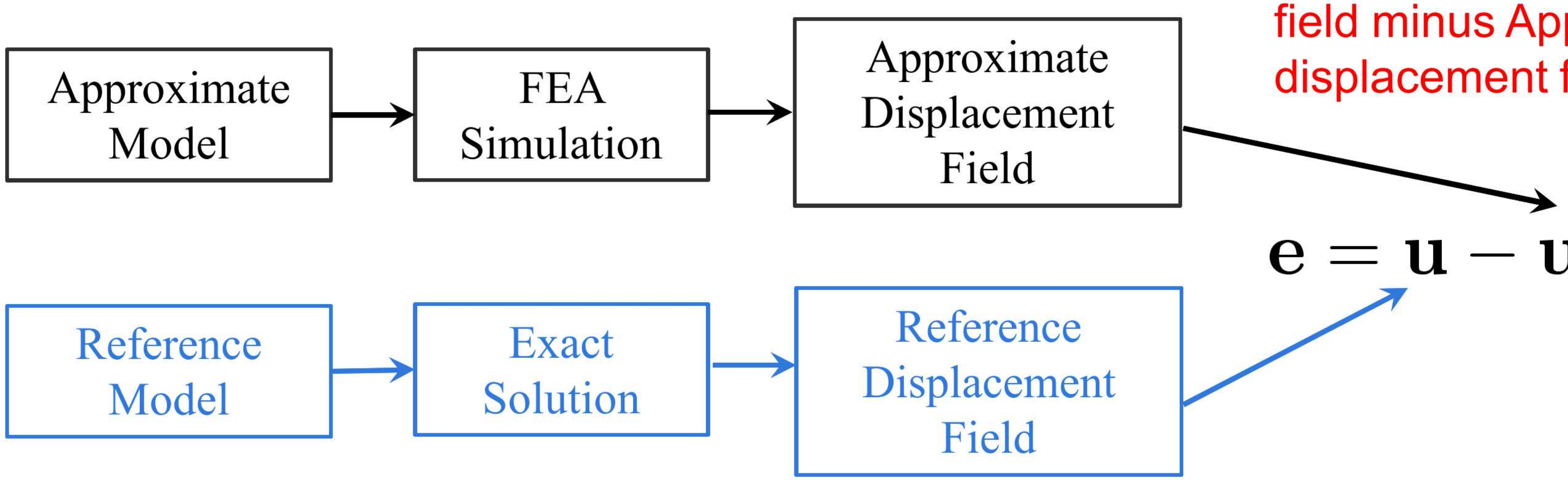
(K. Johnson, T. Rodgers, O. Underwood, SNL)



A Posteriori Modeling Error

- What is error introduced by using an approximate material model?

Exact Error:
Reference displacement field minus Approximate displacement field



$$\mathbf{e} = \mathbf{u} - \mathbf{u}^{0,h}$$

$$||\mathbf{e}||_E = ||\mathbf{u} - \mathbf{u}^{0,h}||_E \leq \underbrace{||\mathbf{u} - \mathbf{u}^{0}||_E}_{\text{Model-form error}} + \underbrace{||\mathbf{u}^{0} - \mathbf{u}^{0,h}||_E}_{\text{Discretization error of approximate model}}$$

Model-form error

Discretization error of approximate model

Error Estimation: Material Model Error

(Zohdi, Oden, Rodin, 1996, “Hierarchical modeling of heterogeneous bodies”, CMAME)

Energy Norm of Displacement Error

Approximate solution

Error Indicator

$$||\mathbf{u}-\mathbf{u}^0||_E^2 \leq \int_\Omega (\boldsymbol{\varepsilon}^0-\bar{\boldsymbol{\varepsilon}}) : (\bar{\boldsymbol{\sigma}}-\boldsymbol{\sigma}^0)\, d\Omega \approx \sum_{i=1}^{N} V_e\, \eta_i^2$$

displacement field using true material model: **generally unknown**

approximate displacement field from simplified or approximate material model

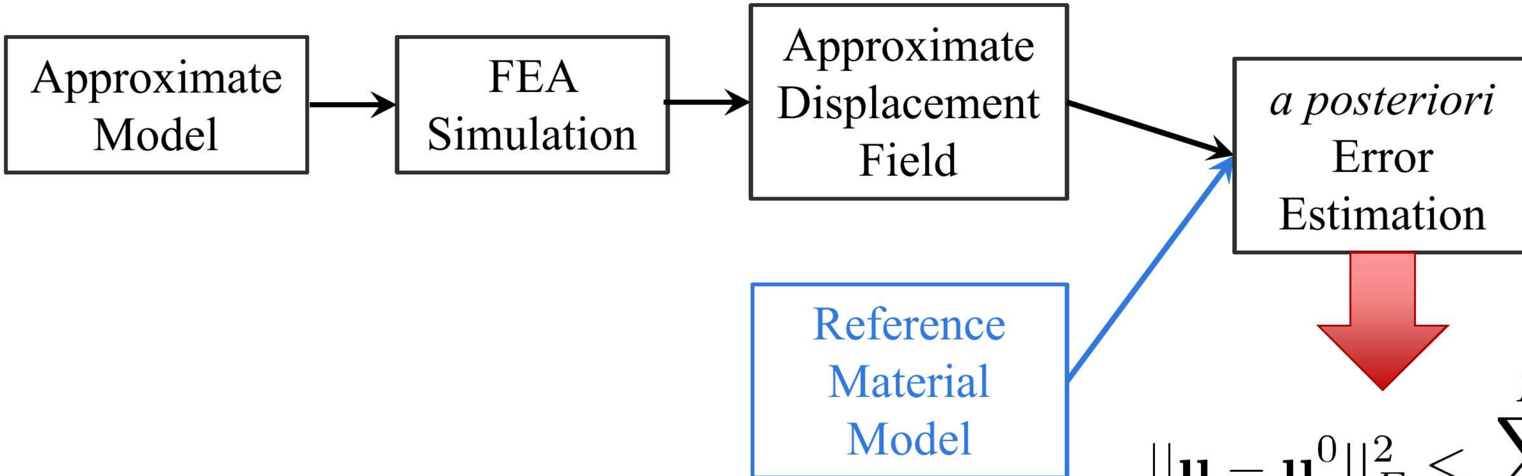
strain field resulting from approx. stress field but true material model

stress field resulting from approx. strain field but true material model

$$\eta_i^2 \approx \left(\boldsymbol{\epsilon}^0-\bar{\boldsymbol{\epsilon}}\right) : \left(\bar{\boldsymbol{\sigma}}-\boldsymbol{\sigma}^0\right) = \left(\mathbb{I}-\mathbb{C}^{-1}\,\mathbb{C}^0\right)\boldsymbol{\epsilon}^0 : \left(\mathbb{C}-\mathbb{C}^0\right)\boldsymbol{\epsilon}^0$$

- Key Point: Can bound error using only known quantities: approximate stress & strain fields and reference material properties

Error Estimation: Material Model Error



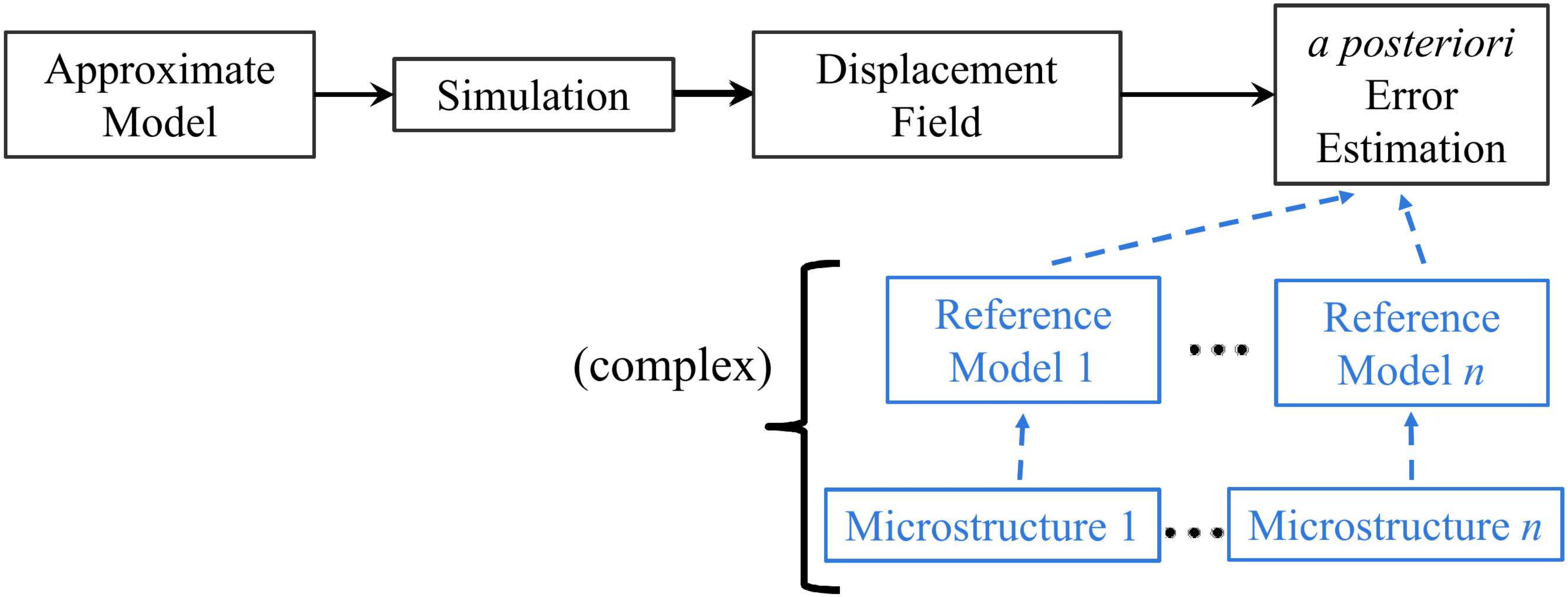
$$||\mathbf{u} - \mathbf{u}^0||_E^2 \leq \sum_{i=1}^{N} V_e \, \eta_i^2$$

$$\eta_i^2 \approx \left(\boldsymbol{\epsilon}^0 - \bar{\boldsymbol{\epsilon}}\right) : \left(\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0\right) = \left(\mathbb{I} - \mathbb{C}^{-1}\,\mathbb{C}^0\right)\boldsymbol{\epsilon}^0 : \left(\mathbb{C} - \mathbb{C}^0\right)\boldsymbol{\epsilon}^0$$

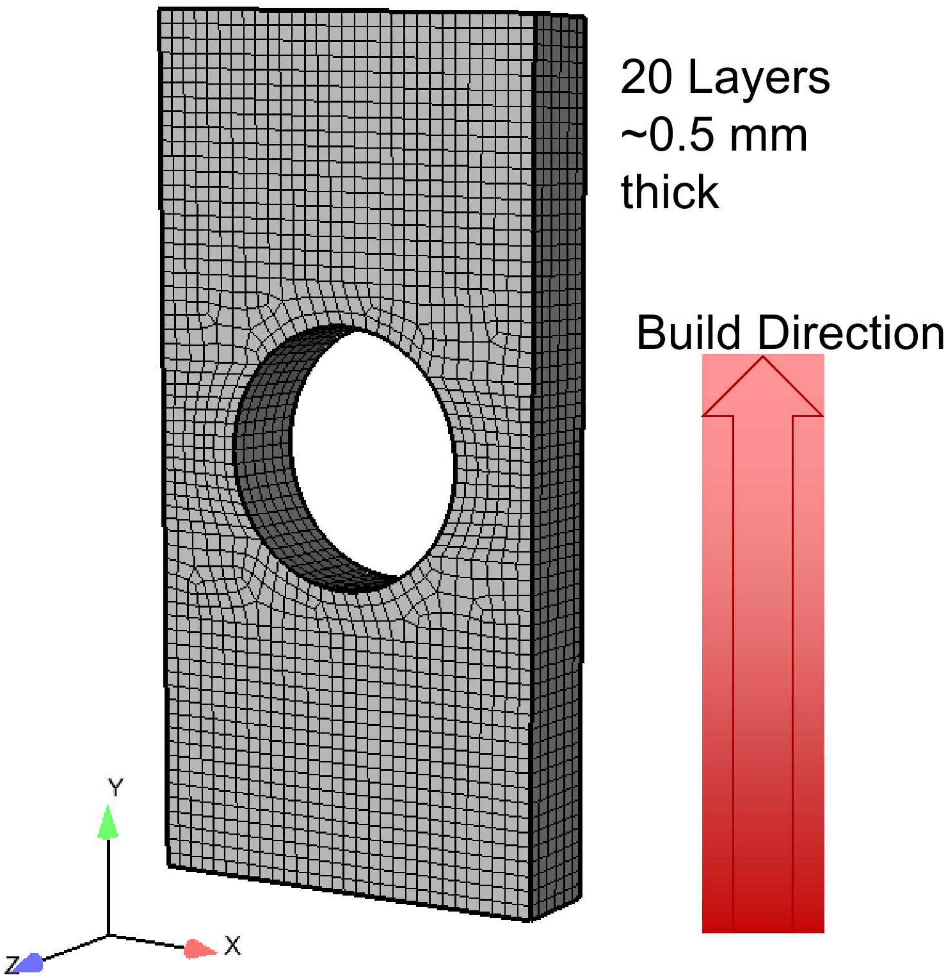
- Key Point: Don’t need to run reference model simulation, just need to know reference material model.

Error estimation as UQ

- What if the true material properties are unknown or properties vary throughout the structure?



Example AM Structure

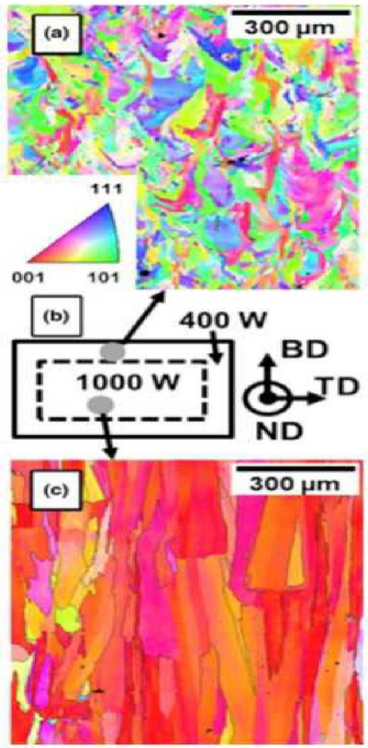


- Finite Element Model, ~74,000 Hex8 elements
- Uniaxial tension traction BC
- Unit load to study small-strain elastic response
- Plate Material: 304L Stainless Steel
  - Approximate Model:
    - Isotropic, E = 200 GPa, ν = 0.3

"Best Engineering Guess" at material properties and model form

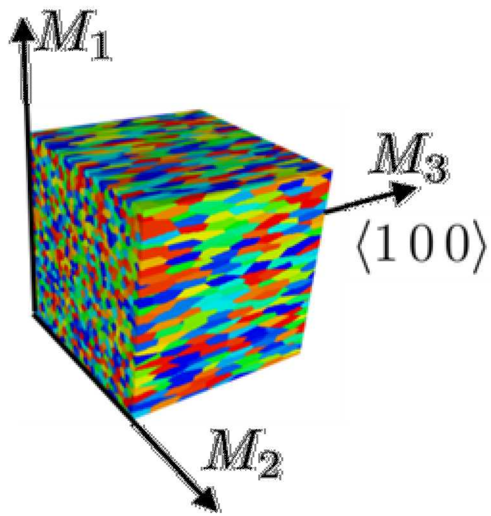
Reference Material Model

- Based on the strong <100> fiber textures seen in many AM structures

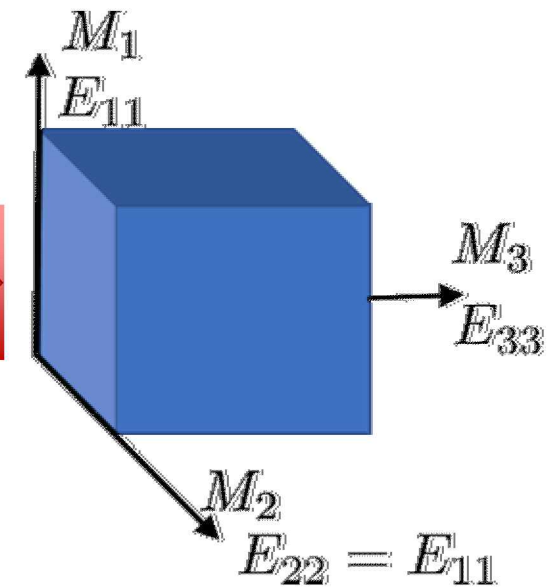


T. Niendorf, et. al., MMT-B (2013) 44B: 794-796

Representative Volume Element

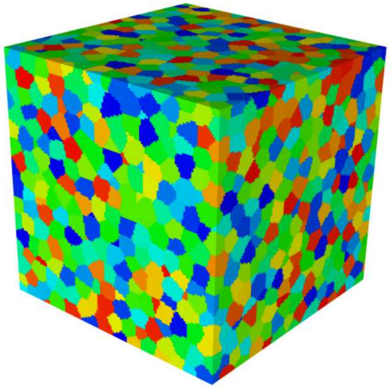


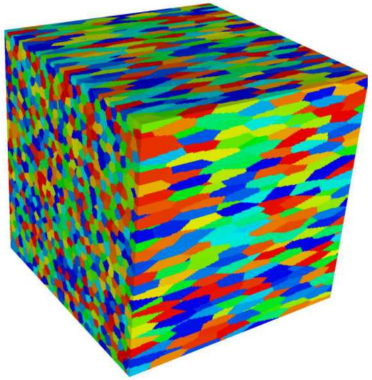
Transversely Isotropic Homogenized Properties



Material: 304L Stainless Steel

Homogenized Reference Properties





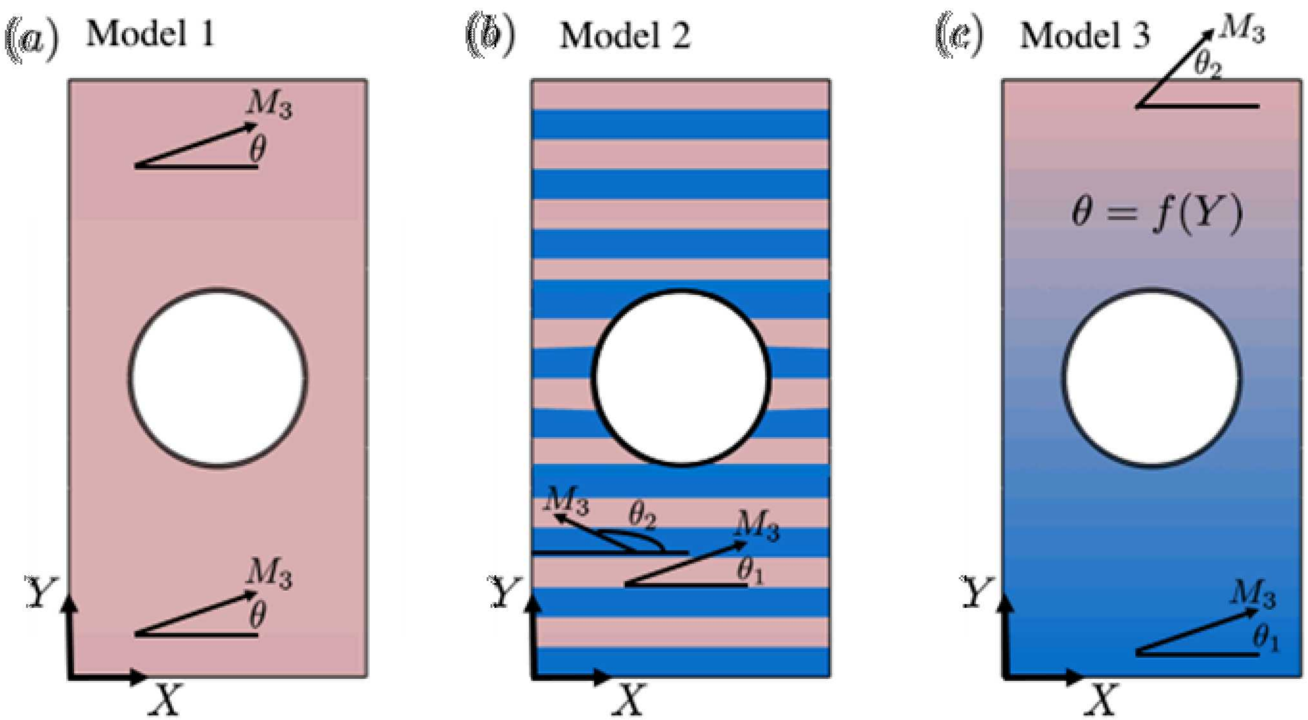
	E_{11}	E_{22}	E_{33}	ν_{12}	ν_{23}	ν_{13}	G_{12}	G_{23}	G_{13}
Random Orientations	198			0.294			76.5		
Pure Fiber Texture	143	143	90.9	0.114	0.615	0.615	58	126	126

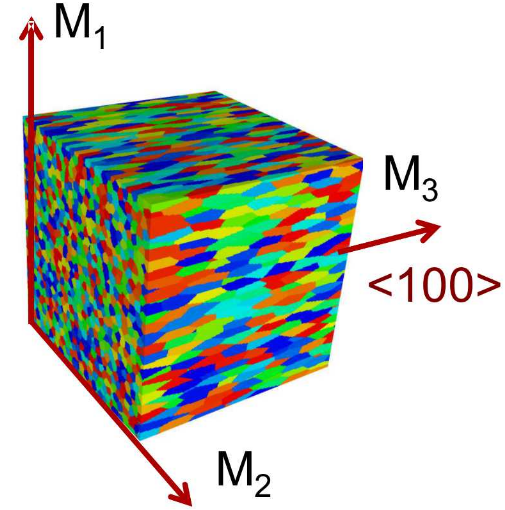
E, G values given in GPa

Relate Fiber Texture to Structure Geometry for Reference Models

- Material coordinate system (M_1, M_2, M_3)
- Structure coordinate system: (X,Y,Z)

Uniform Orientation | Alternating Orientation by Layer | Orientation Gradient Along Height

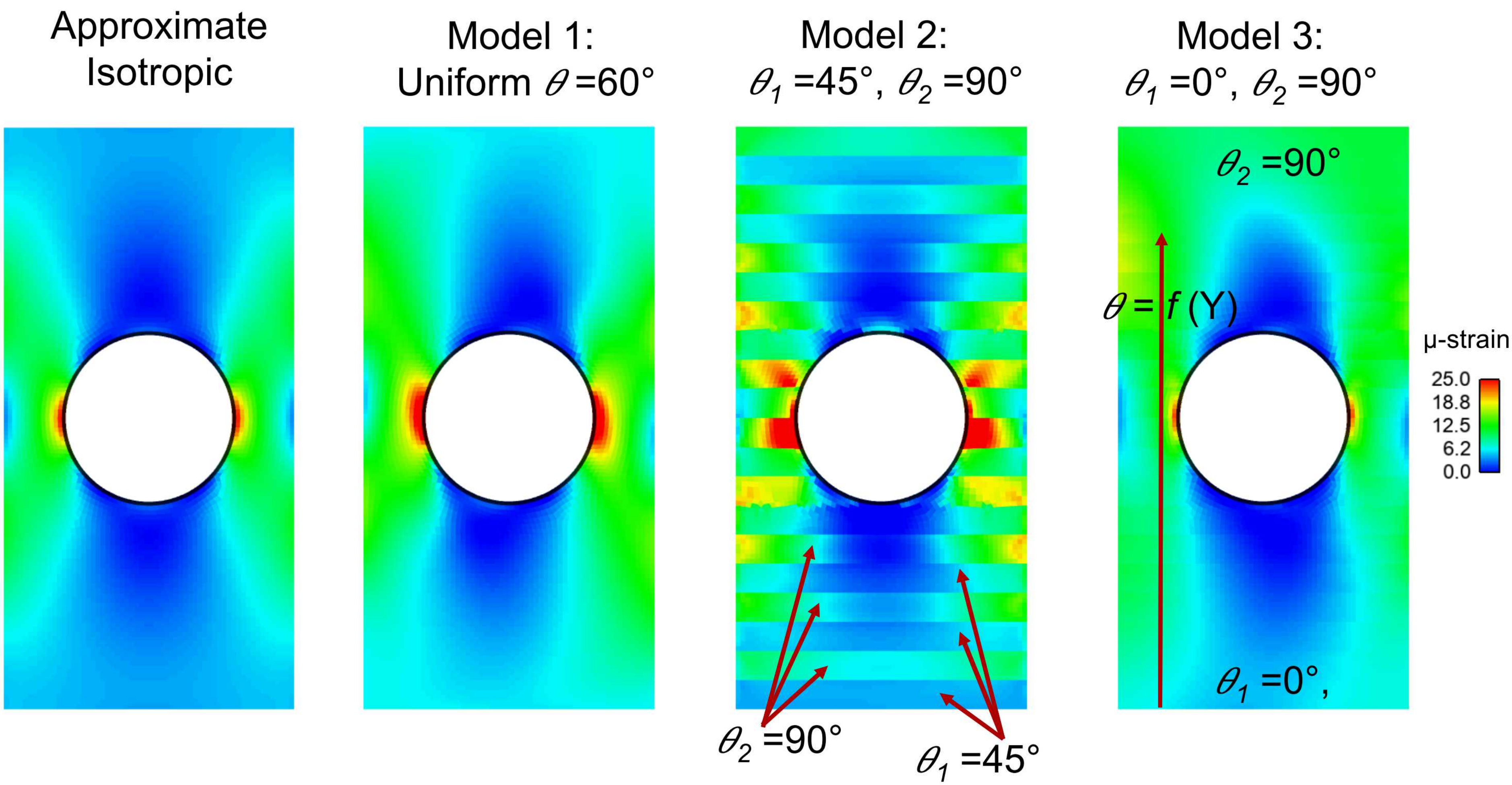




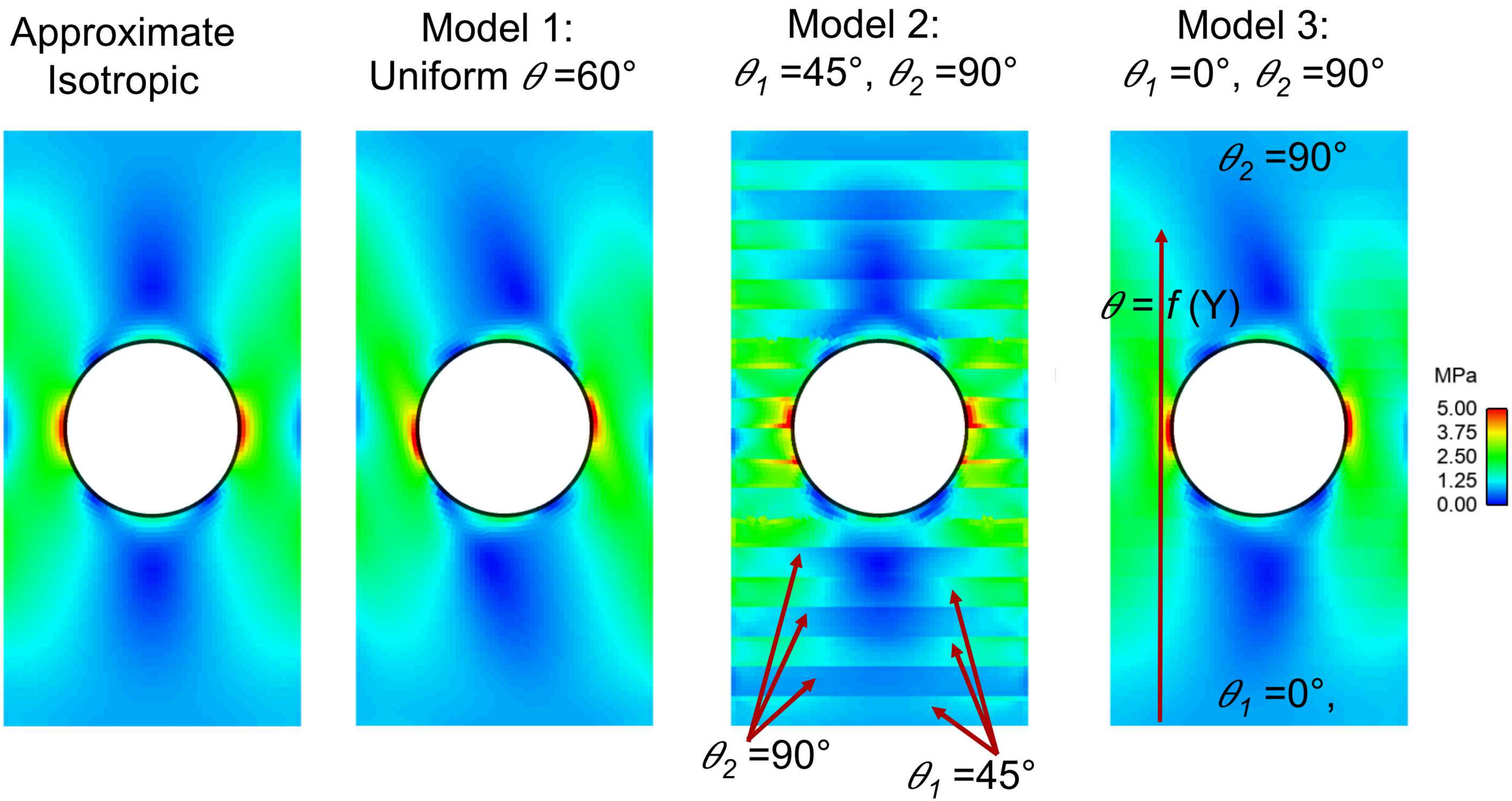
Pure Fiber Texture Homogenized Properties

$$E_{11} = 143 \text{ GPa}$$
$$E_{22} = 143 \text{ GPa}$$
$$E_{33} = 90.9 \text{ GPa}$$
$$\nu_{12} = 0.114$$
$$\nu_{23} = 0.615$$
$$\nu_{13} = 0.615$$
$$G_{12} = 58 \text{ GPa}$$
$$G_{23} = 126 \text{ GPa}$$
$$G_{13} = 126 \text{ GPa}$$

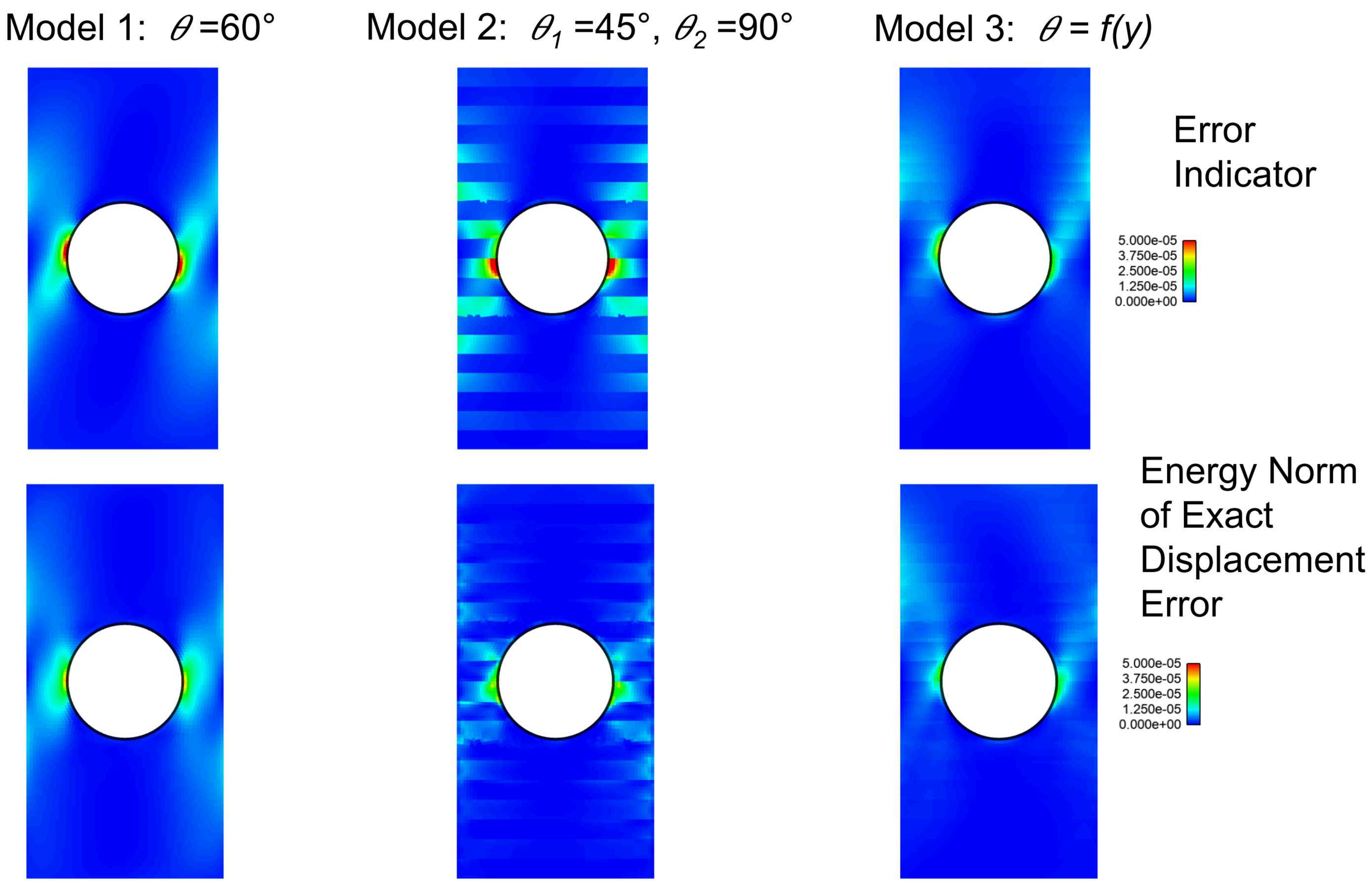
Strain Responses



Von Mises Stress Response



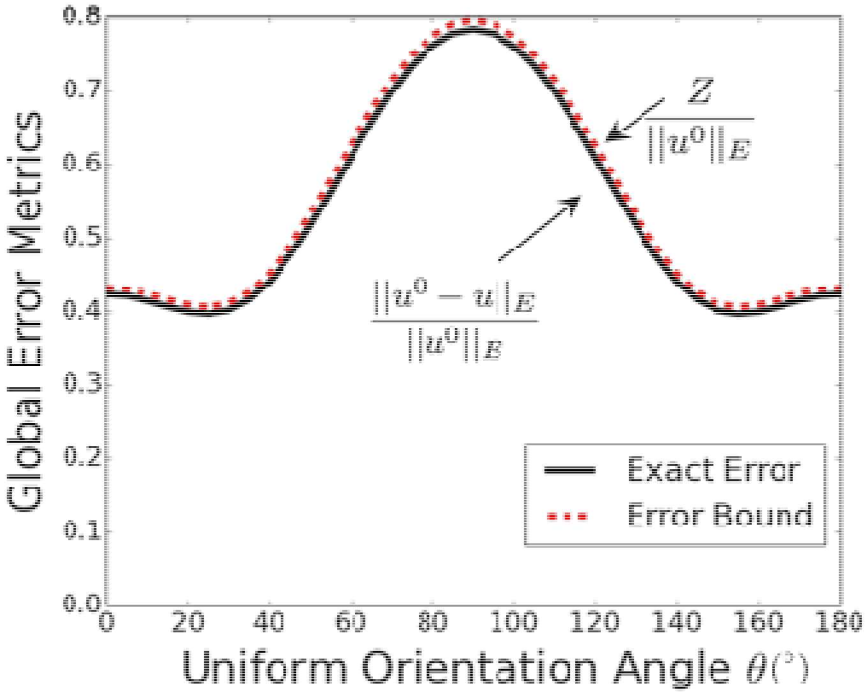
Error Indicator Verification

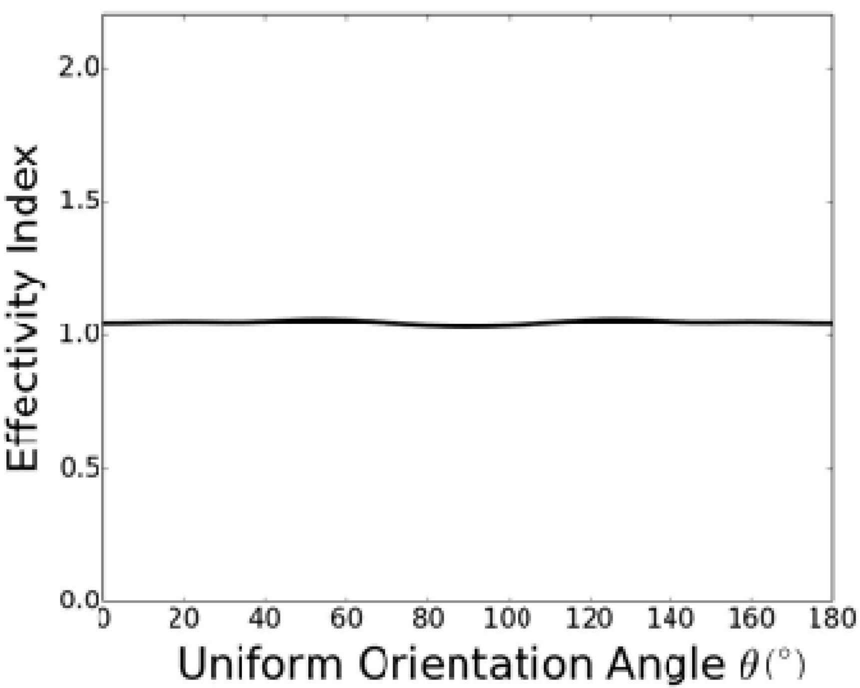


Error Estimation as UQ

- Sweep over multiple reference model possibilities to obtain range of error bounds

Model 1:
Uniform Material Orientation θ

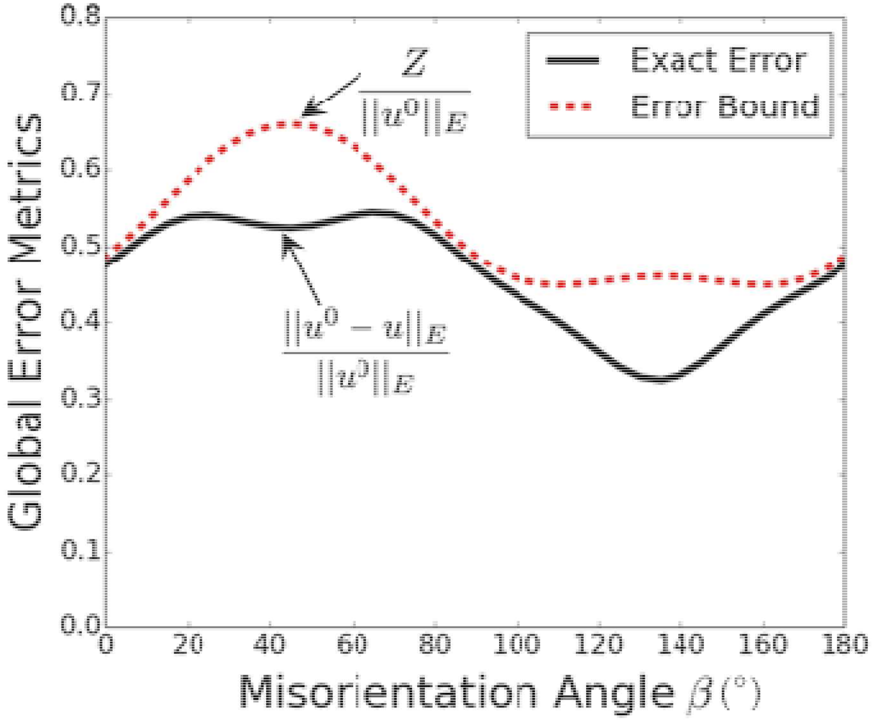


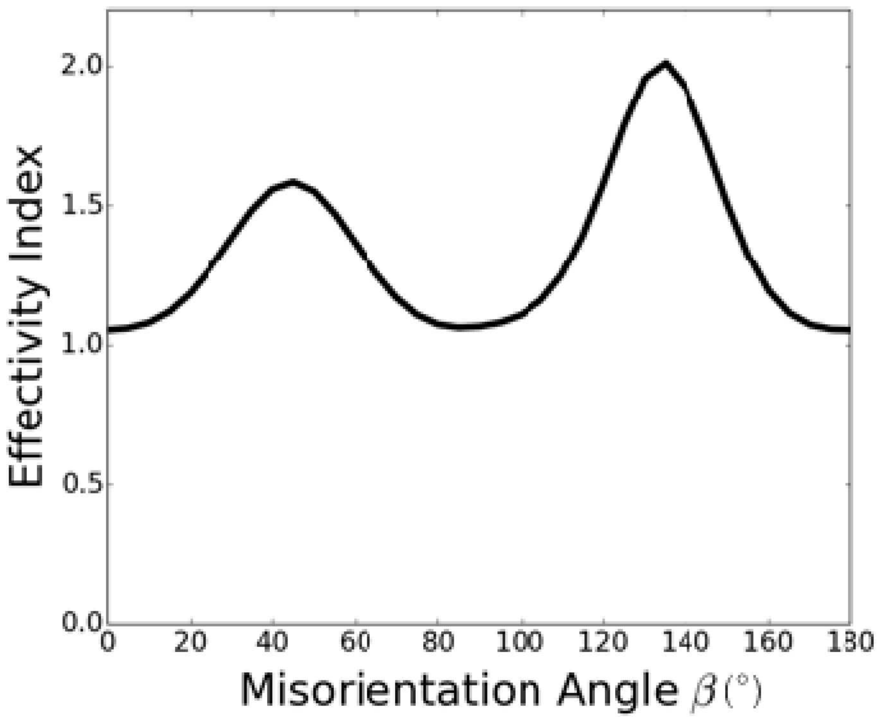


Error Estimation as UQ

- Sweep over multiple reference model possibilities to obtain range of error bounds

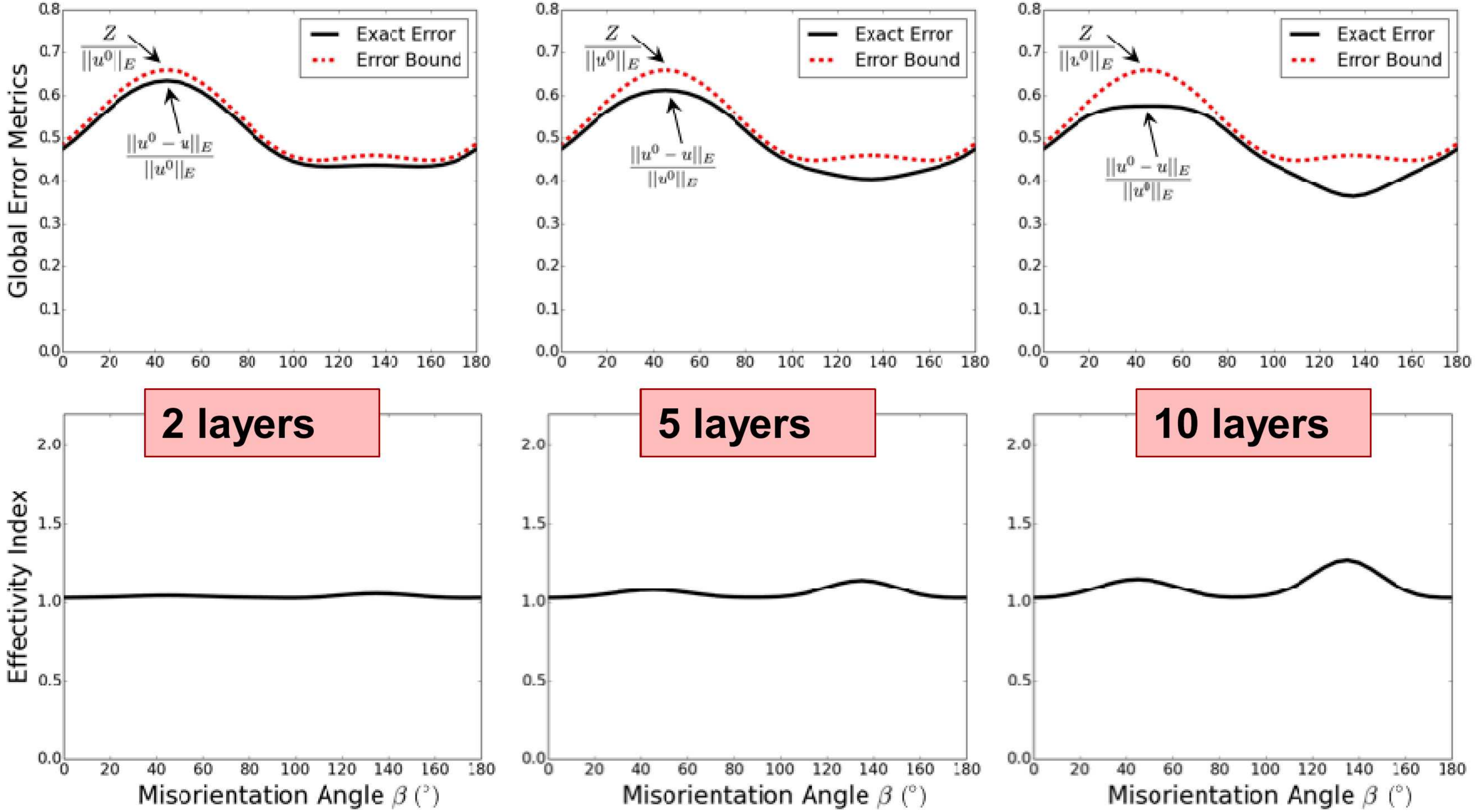
Model 2:
Alternating Material Orientation per Layer θ_1, θ_2





The Need for Multi-Scale

- Interfaces with distinctly different material properties introduce pollution errors the bound does not account for



Summary:

- Error Indicators calculated *a posteriori* can provide bounds and spatial locations of deviations from an approximate model
- Presence of macro or micro texture can affect quantities of interest in AM structures

Future Work:

- Multi-scale error estimation, extend reference models to grain scale (crystal elasticity, crystal plasticity)
- Use P-S-P model framework to develop process-linked reference microstructures
- Extend approach to study plastic deformation regime and other quantities of interest (failure, porosity, etc.)

Damage Evolution in Elastomeric Syntactic Foams

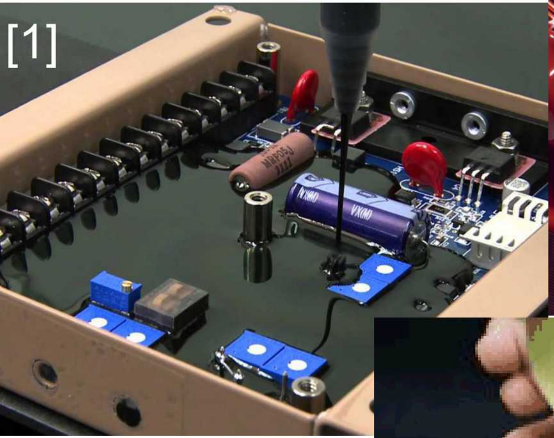
J.A. Brown, J.D. Carroll, B. Huddleston, Z. Casias, K.N. Long, J. Mater. Sci. (2018) 53: 10479-10498.

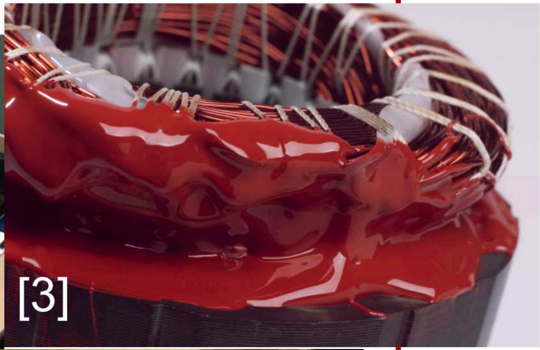
B.P. Croom, H. Jin, B. Mills, J. Carroll, K. Long, J. Brown, X. Li, Composites Sci. Tech. 169 (2019) 195-202.

Syntactic Foams for Potting and Encapsulation

Potting and Encapsulation

- Vibration dampening
- Electrical & environmental insulation

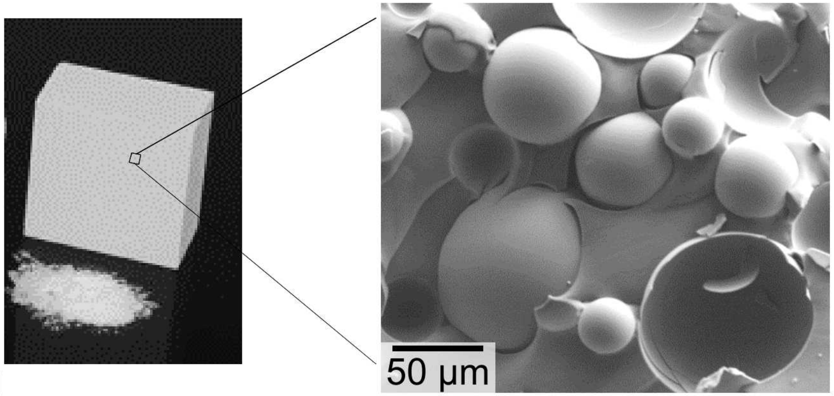




Sylgard/GMB Syntactic Foam

Sylgard® 184 (PDMS) matrix with embedded Glass Microballoons (GMBs) (3M® A16/500)

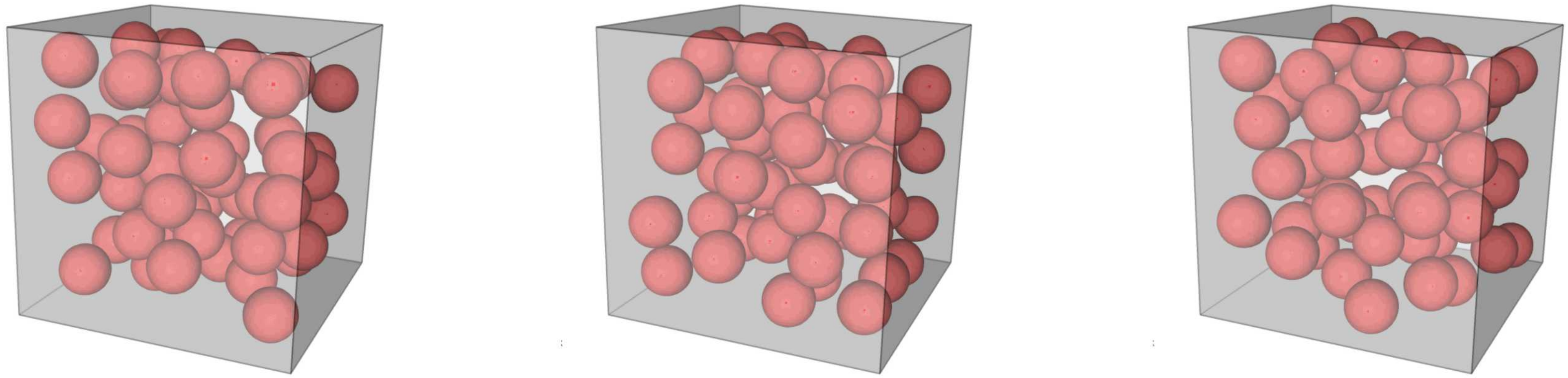
- Crushable foam
- Increased stiffness
- Low Density
- Reduced thermal expansion



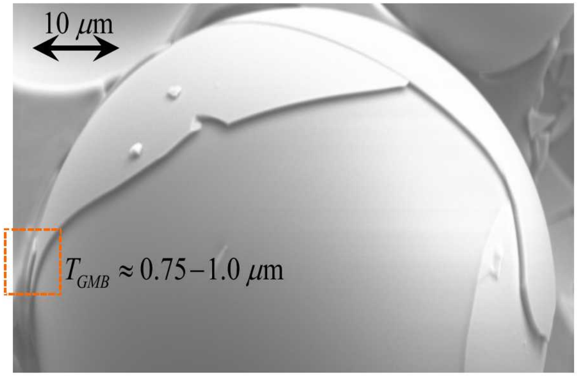
[1] http://www.ecopoxy.com/epoxy-casting-system-for-electronics-encapsulation/
[2] https://www.masterbond.com/tds/ep17ht-100
[3] http://www.directindustry.com/prod/star-technology/product-114815-1369531.html

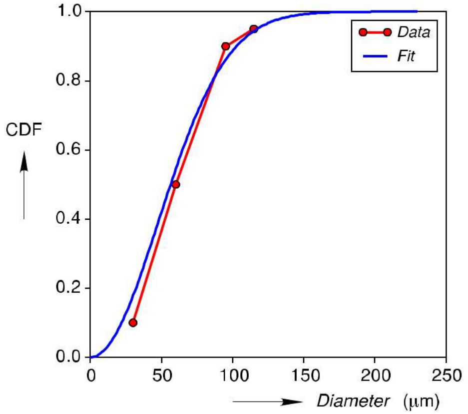
Synthetic Microstructure Generation

- Generate Stochastic Volume Element (SVE) models of Sylgard/GMB microstructure



Estimate Characteristic GMB Thickness: 1 µm

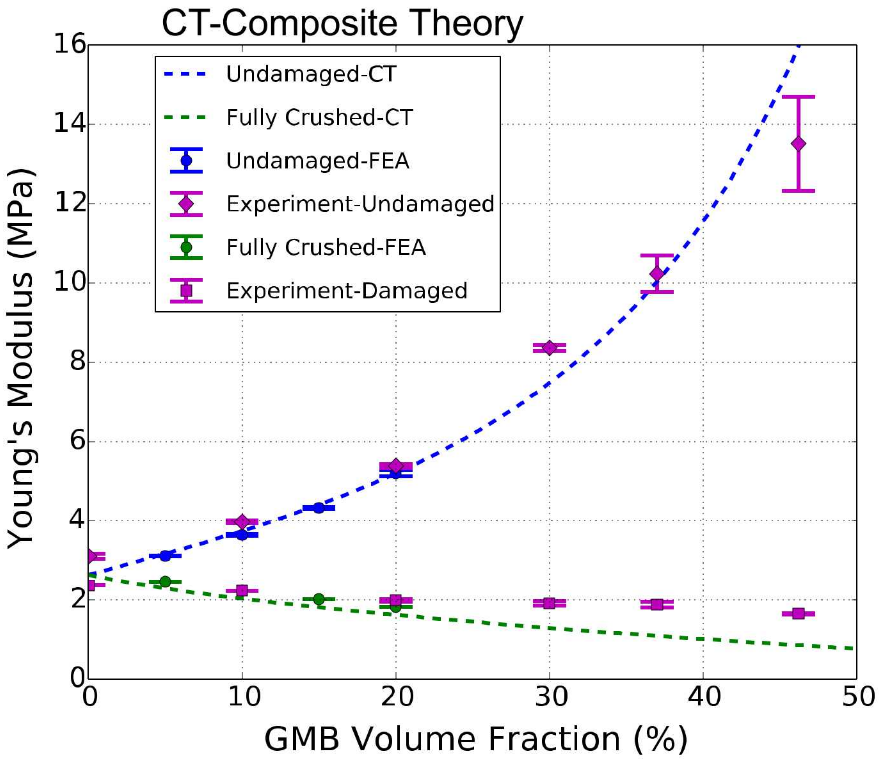


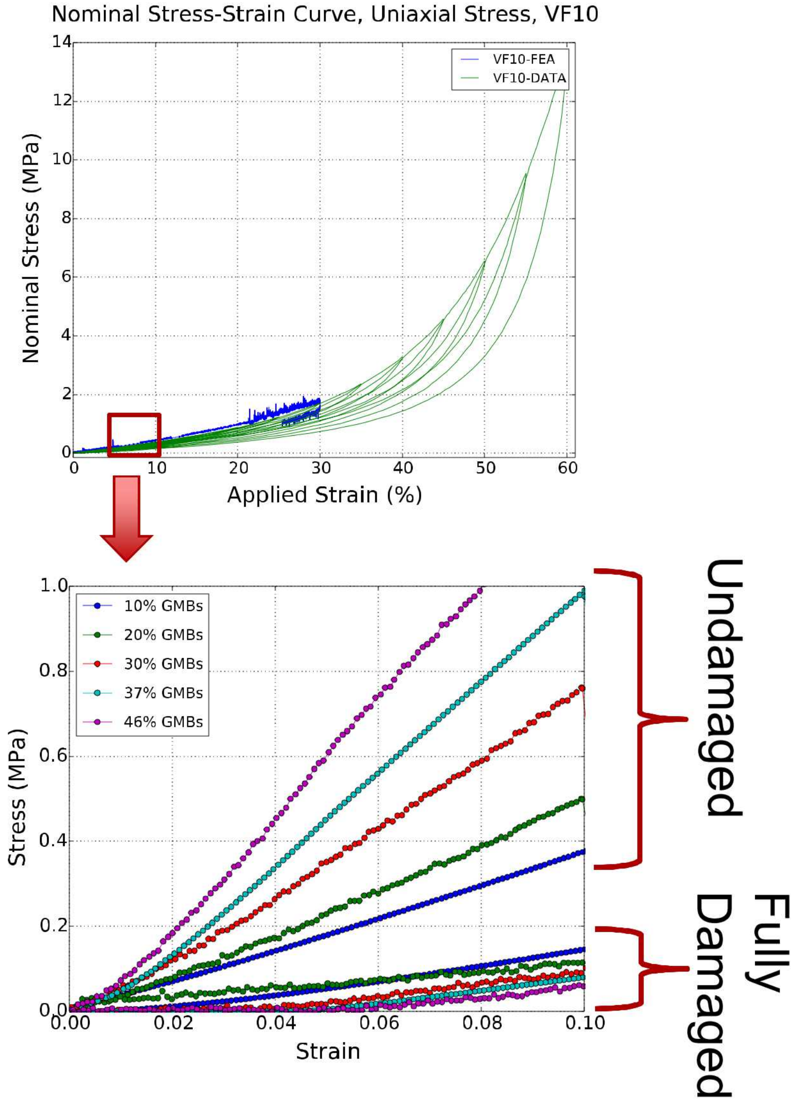


Manufacturer's (3M®) Cumulative Distribution Data for A16/500 GMB

Average GMB Diameter: 60 µm

Effect of Volume Fraction on Young's Modulus



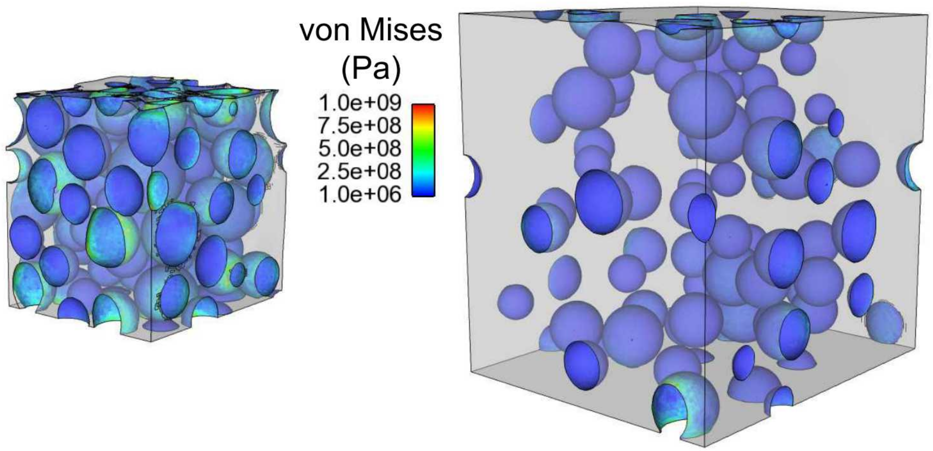


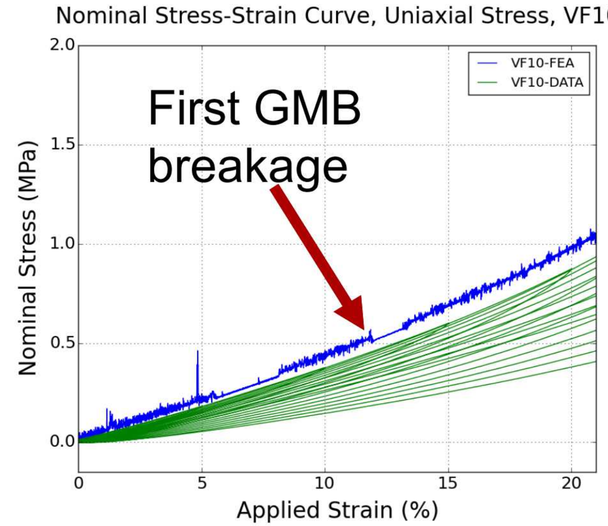
Increasing GMB Volume Fraction also increases the initial composite Young's Modulus
--Well predicted by FEA and composite theory

Effect of GMB Volume Fraction on Damage

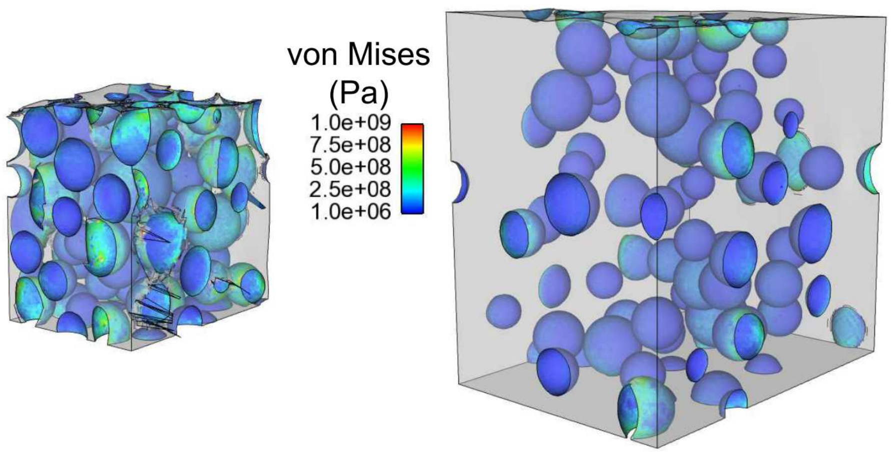
46% GMBs | 10% GMBs

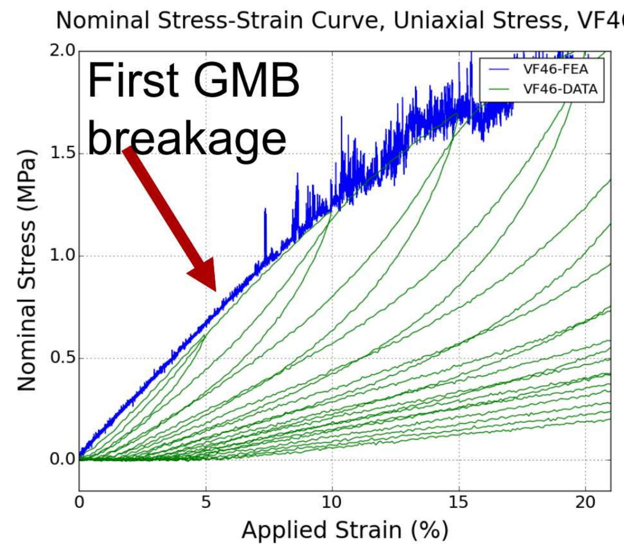
10% strain



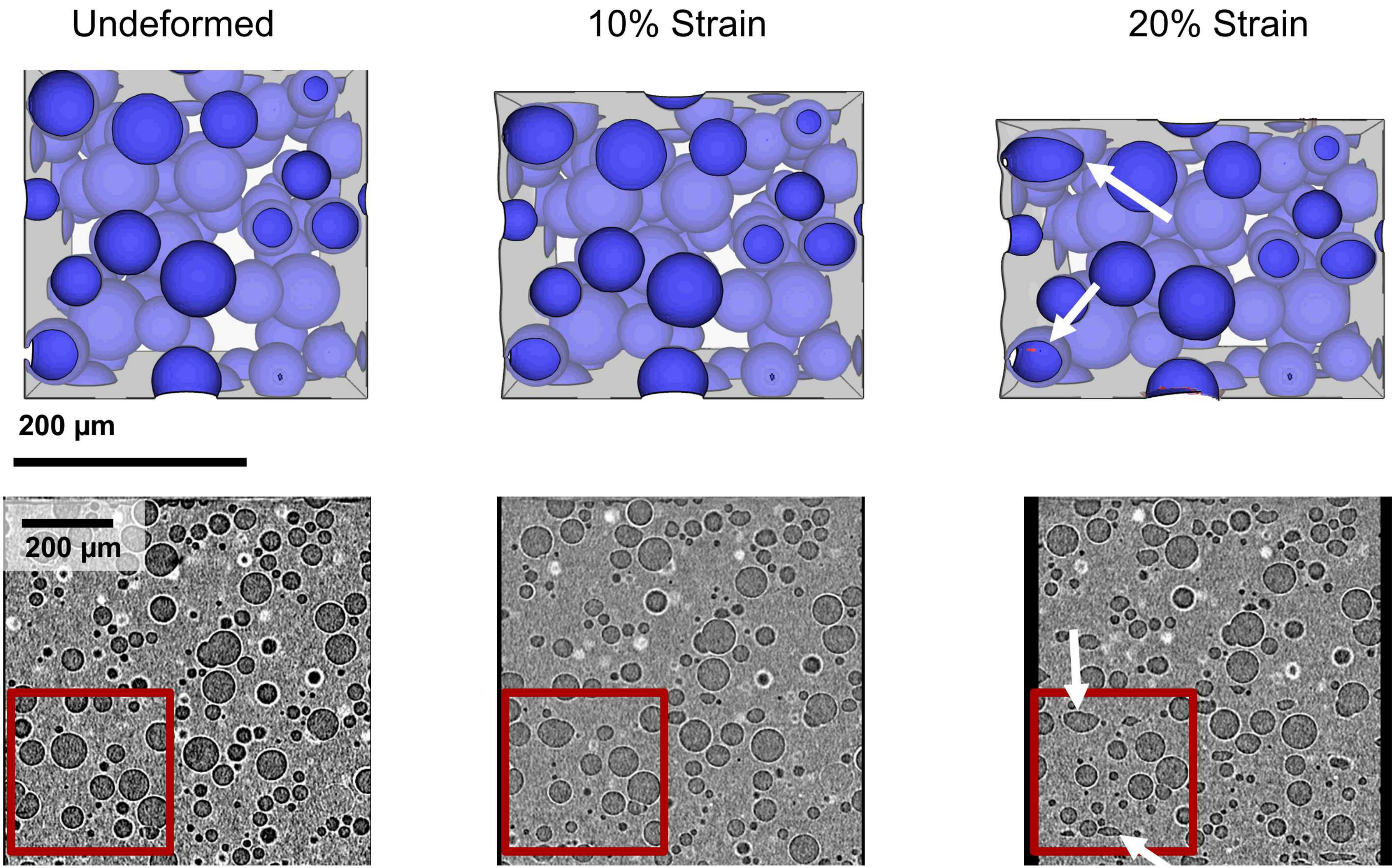


20% strain





Comparison with X-Ray CT, 25% GMBs



Summary:

- GMB breakage is the primary damage mechanism
  - However, some GMBs remain intact!
- As GMB volume fraction increases:
  - Initial undamaged Young's modulus increases
  - material incurs damage at smaller strains

Future Work:

- Refine failure criteria used for GMBs
- Macroscale constitutive model development
- Exemplar problem for numerical tool development

Conclusions

- Mesoscale models coupled with experiments help provide understanding of underlying physical mechanisms
  - Ultimate goal is transfer of these insights to part-scale models

- Case Study 1:
  - Tie AP decomposition chemistry to local stress states and porosity formation to predict thermal damage in AP/HTPB propellant materials

- Case Study 2:
  - Use *a posteriori* calculations to asses model form error bounds in performance predictions for additively manufactured metals with uncertain microstructure

- Case Study 3:
  - Mesoscale model enables study of damage evolution processes in foams with varying design parameters (e.g. filler volume fraction, filler design, matrix material)

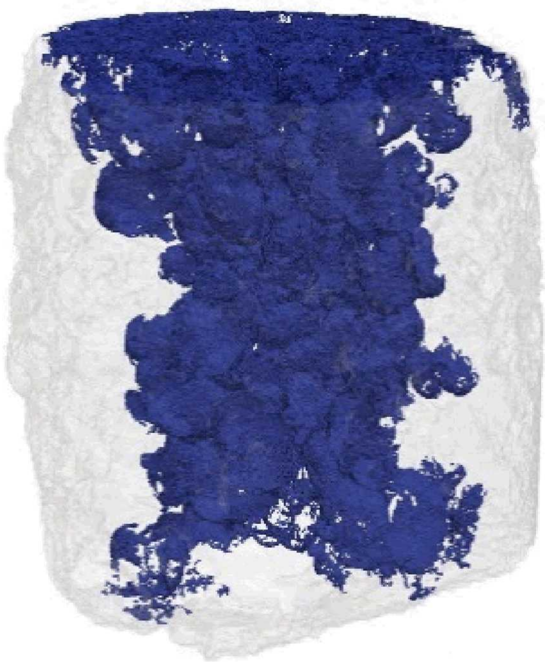
49

Acknowledgements:

- Sophia Lefantzi for management support
- Mike Oliver, Burke Kernan, and Andres Chaves for experimental support
- Funding provided by JMP TCG-III, JIMTP MATG-I, Born Qualified LDRD, and ASC PEM

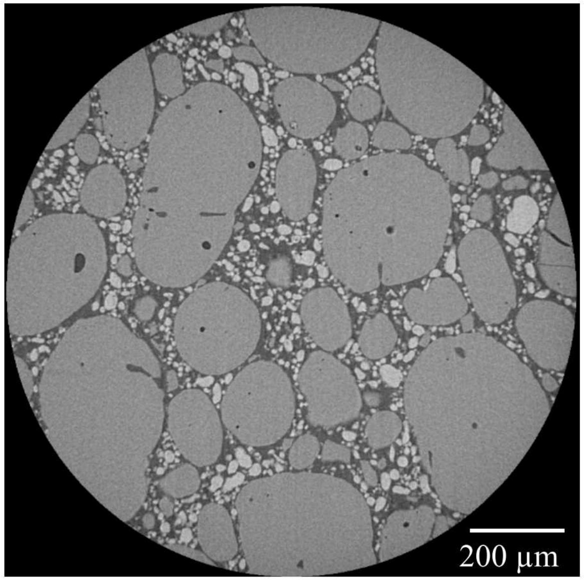
Thermal Damage in Propellants

- Why do we care?
  - Thermal Damage can result in increased reaction violence in cookoff (faster flame spread, convective combustion, DDT)
  - Hypothesis: connected porosity leads to these effects
- Material / Experiments
  - Thermal Damage Visualization test (TDV)
    - Both large and small samples
  - Pre & Post test X-ray CT Scans as a tool to characterize porosity
- Methods for analysis:
  - Image processing/threshold effects
  - Mesoscale multiphysics model for porosity evolution
- Conclusions

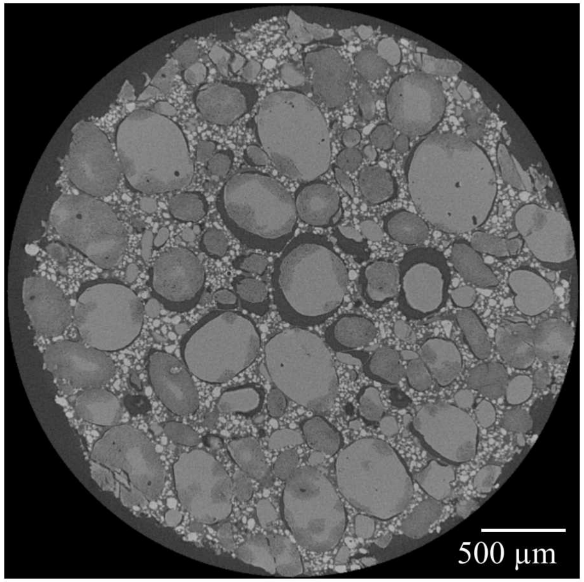


Comparison of Simulation and Experiment

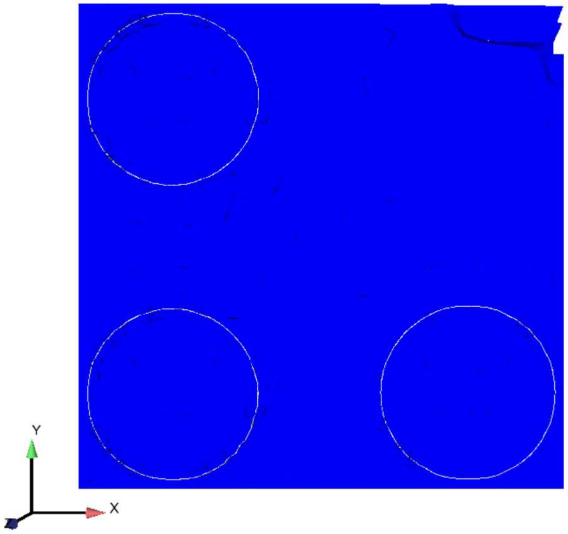
Pristine (1.24 µm/pixel)



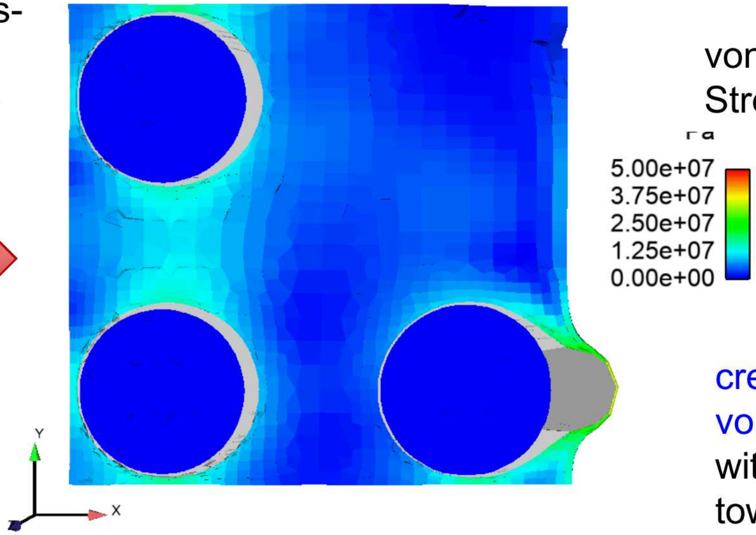
2 hr. at 215°C (3.4 µm/pixel)



- Observations from CT scan images show crescent-shaped voids surrounding the particles; presumably from decomposition gases trapped in the gas-tight binder



Model cross-section at center of Z-dimension

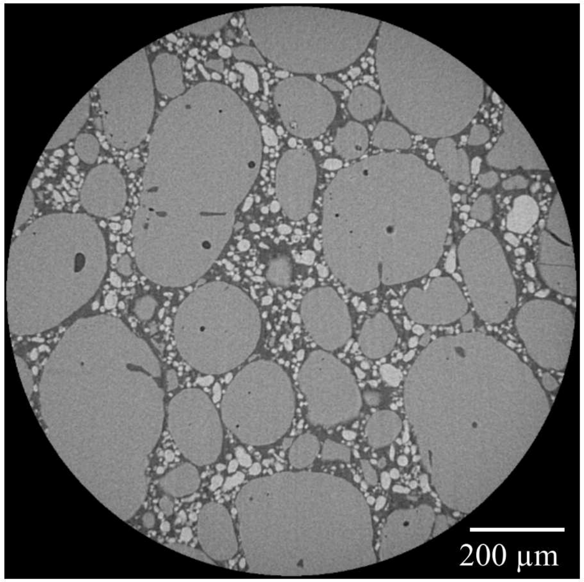


von Mises Stress (Pa)

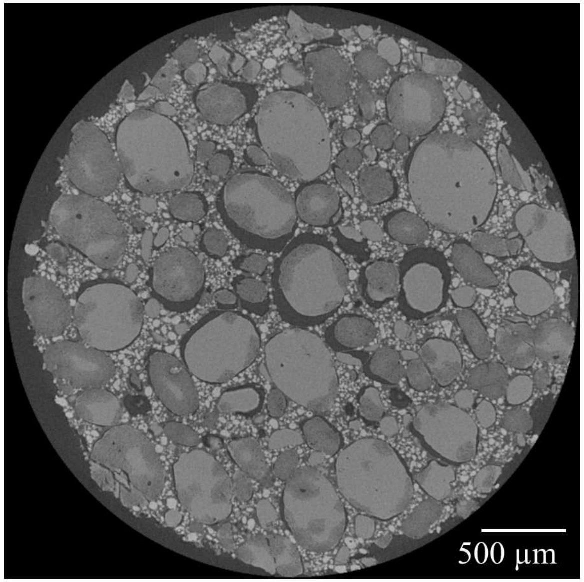
crescent-shaped voids develop with preference toward regions of lower stress

Comparison of Simulation and Experiment

Pristine (1.24 µm/pixel)



2 hr. at 215°C (3.4 µm/pixel)



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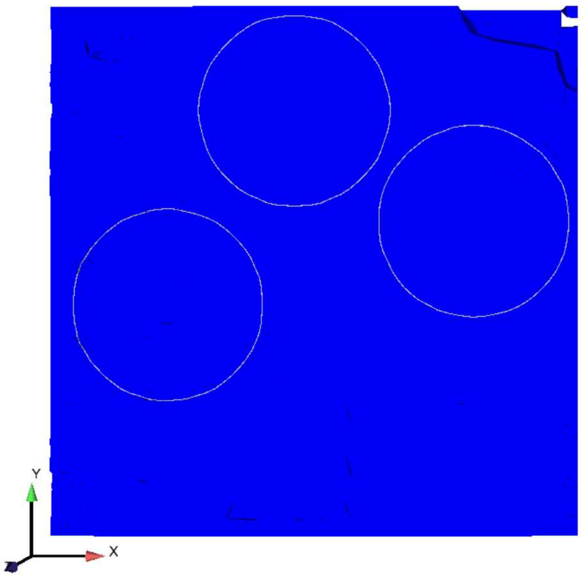
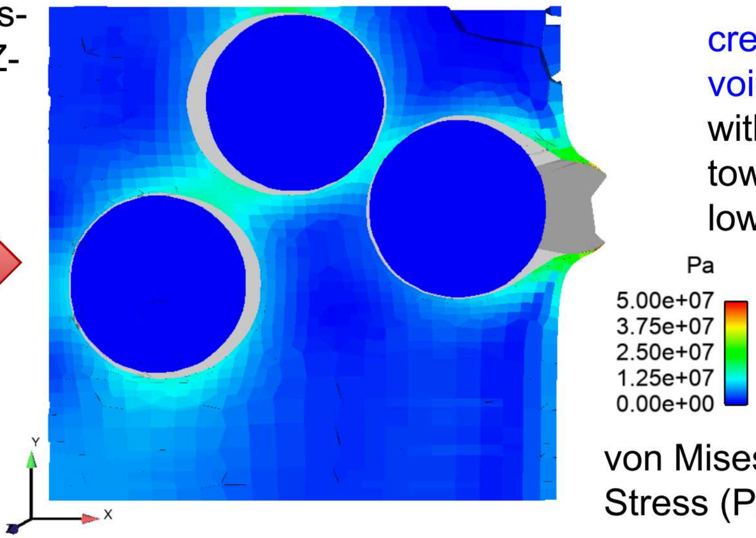


Model cross-section at Z-front



crescent-shaped voids develop with preference toward regions of lower stress

von Mises Stress (Pa)

Sources of Uncertainty in AM parts

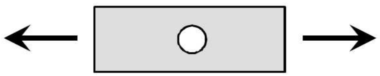
- Defects:
  - Porosity
  - Inclusions/contaminants/oxide particles
  - Compositional differences
- Thermal History
- Residual Stress
- Variability within a part
- Variability between parts/builds
- Powder feedstock

- Microstructure
  - Local/Global texture
  - Dislocation density
  - Solute segregation at grain boundaries (alloys)
  - Different phases
  - Cellular sub-grain structure

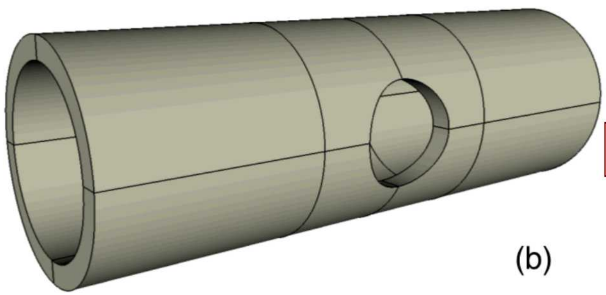
- Identify "critical" defects
- Predict performance probabilistically
- Science-based modeling approach

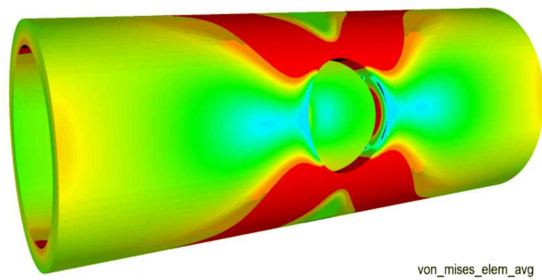
What if the Exact Microstructure/Properties are Unknown?

Sandia National Laboratories



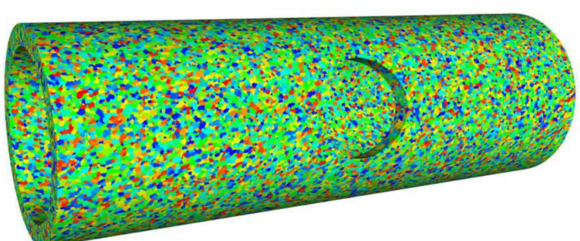
FEA with simple material model



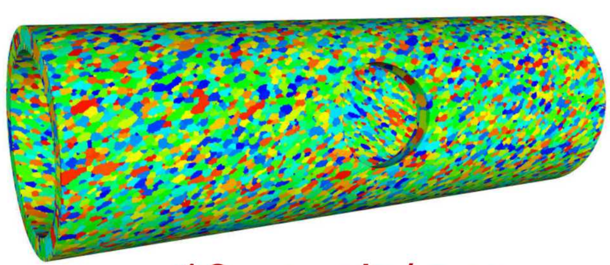


Engineering Quantities of Interest

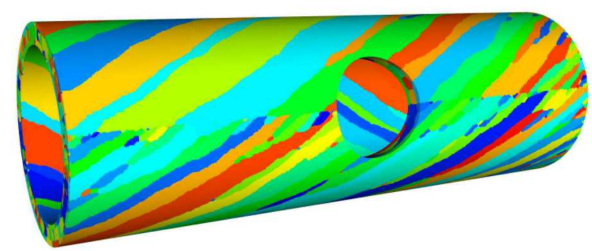
Model Form Error Estimation as UQ method for variable microstructures (postprocessing)



20 voxels/mcs



10 voxels/mcs



5 voxels/mcs

How to Obtain Representative Reference Properties?

Computational Homogenization

Material: 304L Stainless Steel

Material Model: FCC Crystal Plasticity:
(K. Matous, A. Maniatty, 2004, *IJNME*)

Single crystal elastic constants (austenite):

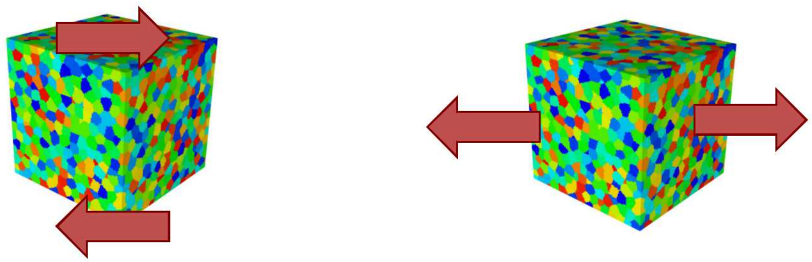
$$C_{11} = 204.6 \;\; \text{GPa}$$
$$C_{12} = 137.7 \;\; \text{GPa}$$
$$C_{44} = 126.2 \;\; \text{GPa}$$

anisotropy ratio

$$A = \frac{2C_{44}}{C_{11} - C_{12}} = 3.77$$

Uniaxial and Shear Boundary Value Problems on Stochastic Volume Element

Shear Uniaxial



Volume averages of local quantities

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{\Omega_v} \int_{\Omega_v} \boldsymbol{\sigma}(x) d\Omega$$
$$\langle \boldsymbol{\varepsilon} \rangle = \frac{1}{\Omega_v} \int_{\Omega_v} \boldsymbol{\varepsilon}(x) d\Omega.$$

Populate Stiffness Tensor via Hooke's Law

$$\langle \boldsymbol{\sigma} \rangle = \mathbb{C} \langle \boldsymbol{\varepsilon} \rangle.$$

Literature-Based Library of Possible Microstructures

- Uniform angle throughout microstructure (pure fiber texture)

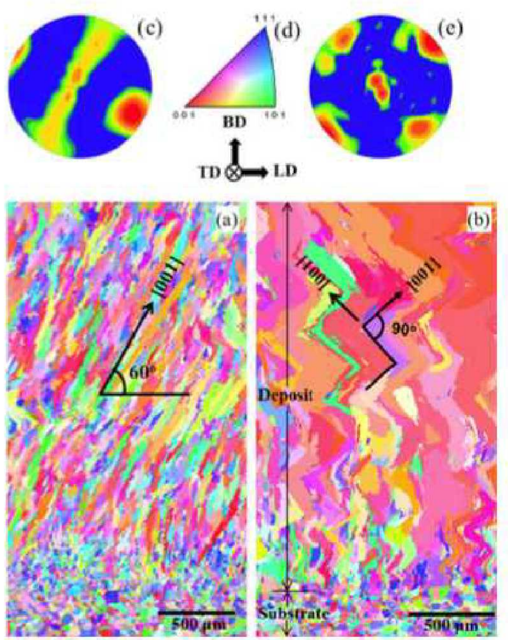
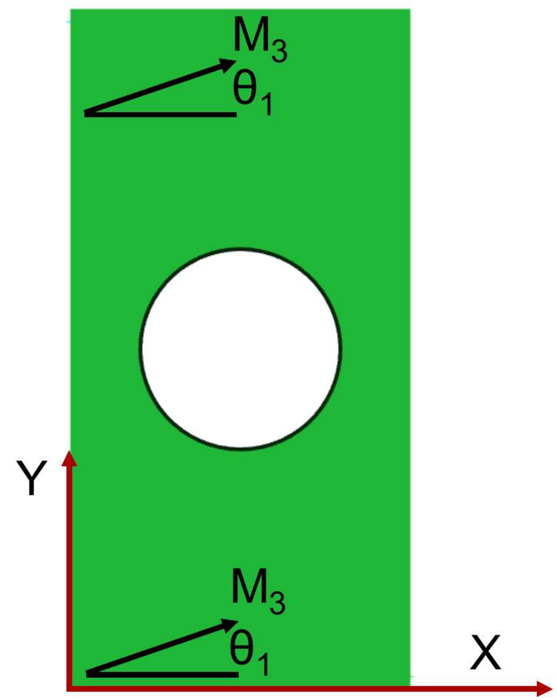
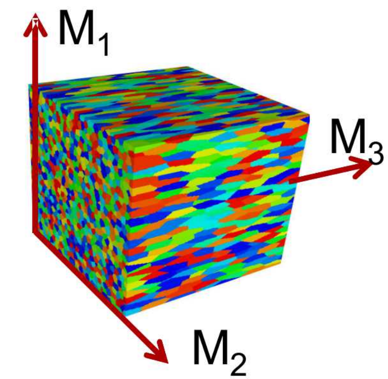


Figure 4. EBSD maps of the as-deposited IN718. (a) Inverse pole figure (IPF) colored OIM map of deposit A, (b) OIM of deposit B, (c) (100) pole figure of deposit A, (d) IPF and (e) (100) pole figure of deposit B.

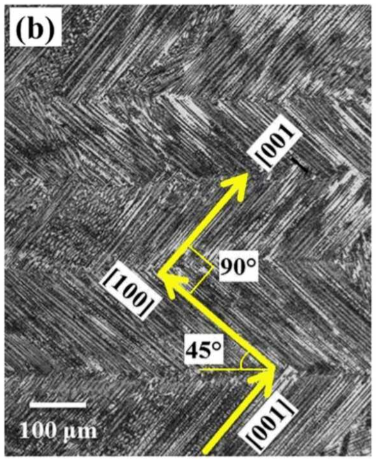
G.P. Dinda, A.K. Dasgupta, J. Mazumder, Scripta Materialia (2012) 67: 503-506

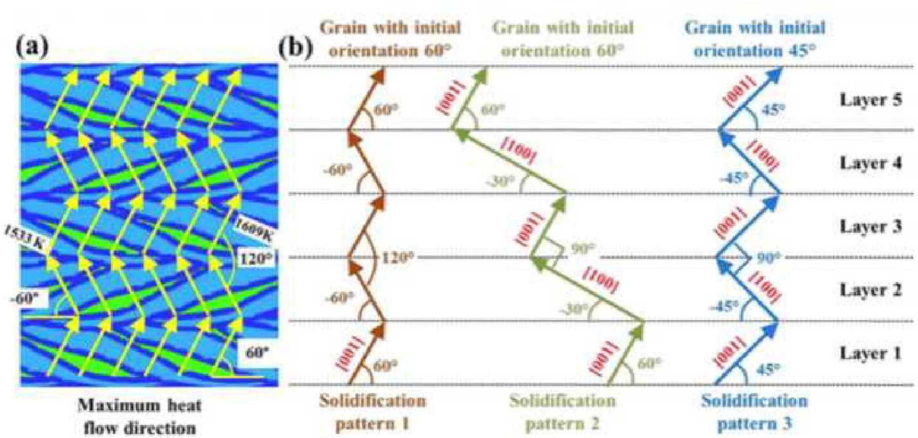




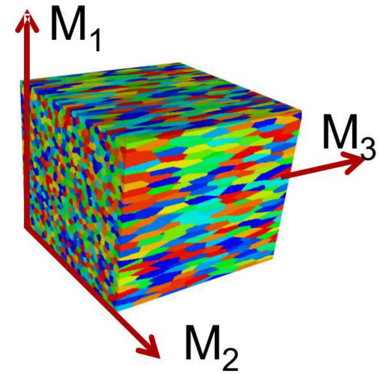
Literature-Based Library of Possible Microstructures

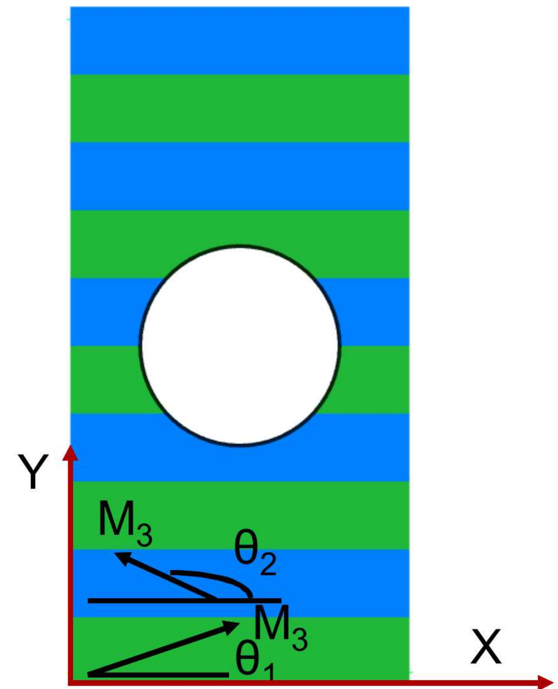
- Alternating angle for each layer





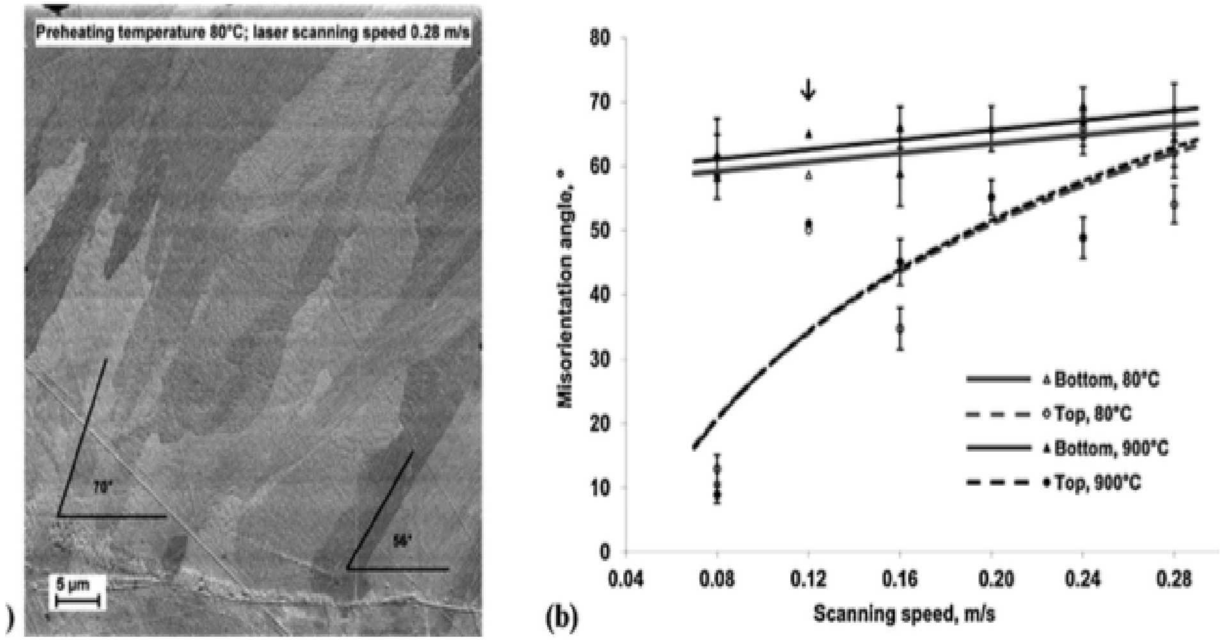
H.L. Wei, J. Mazumder, T. DebRoy, Scientific Reports 5:16446, (2015)

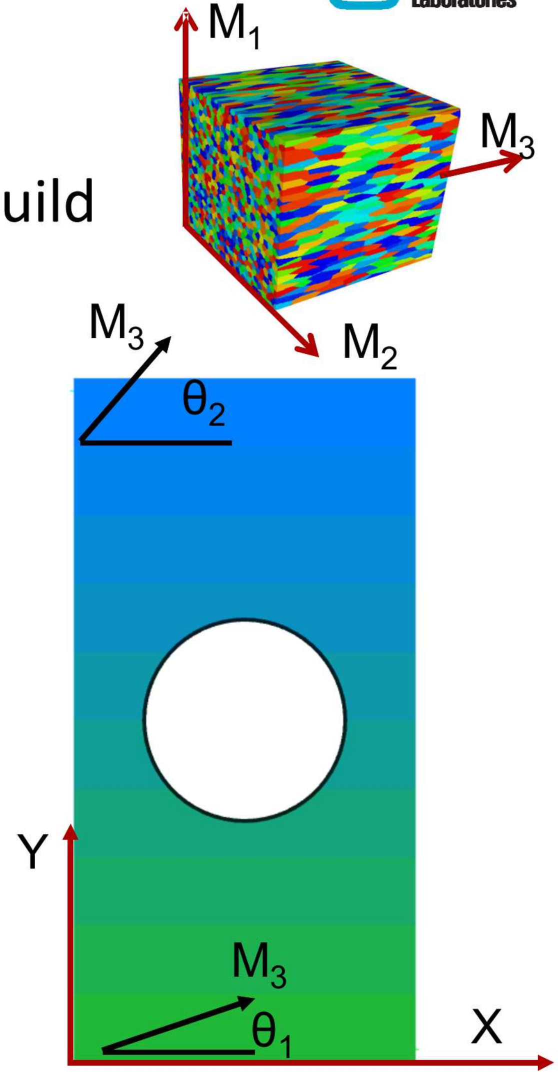




Literature-Based Library of Possible Microstructures

- Gradient angle between bottom and top of build

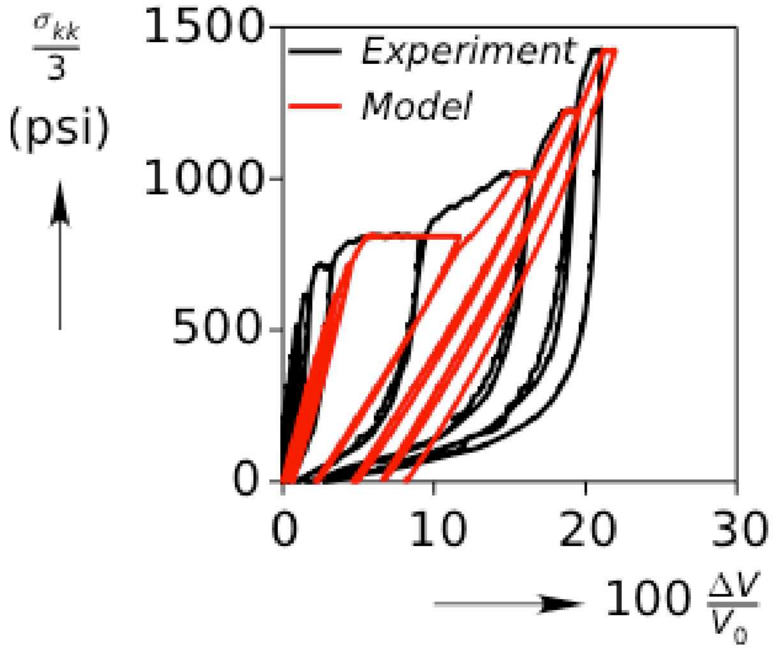


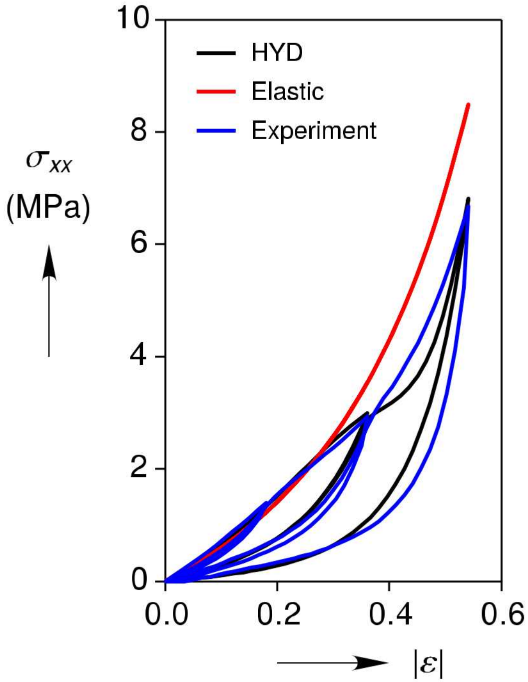


I. Yadroitsev, P. Krakhmalev, I. Yadroitsava, S. Johansson, I. Smurov, Journal of Materials Processing Technology 213 (2013) 606-613

Simple Macroscale Constitutive Modeling Is Unsuccessful

- Hyperelastic Yeoh Model with Isotropic-Kachanov Style Damage
- Quasi-Linear Viscoelasticity Does Not Help





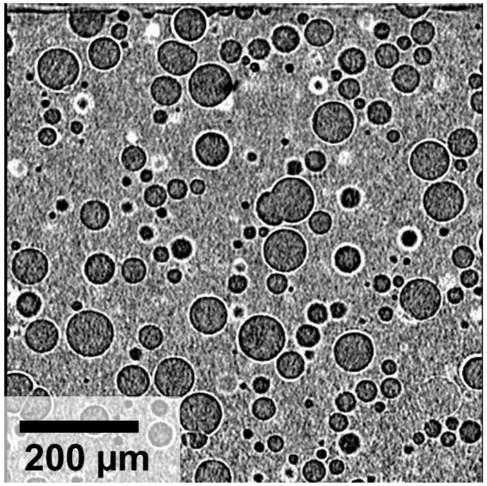
HYD model does not fit the hydrostatic pressurization data well

Model reasonably fits the uniaxial compression data (Mullins Effect)

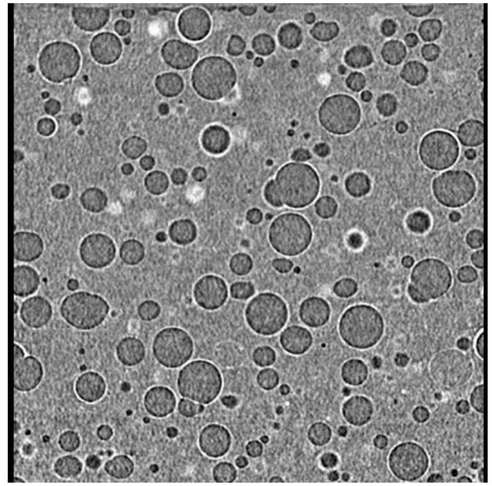
Simple phenomenological efforts fail to capture bulk behavior—We Need a Detailed Understanding of the Damage Behavior

High Magnification X-ray CT, in-situ Compression

0% Strain

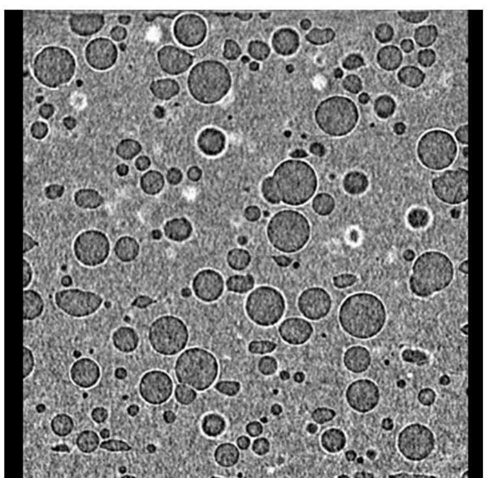


10% Strain

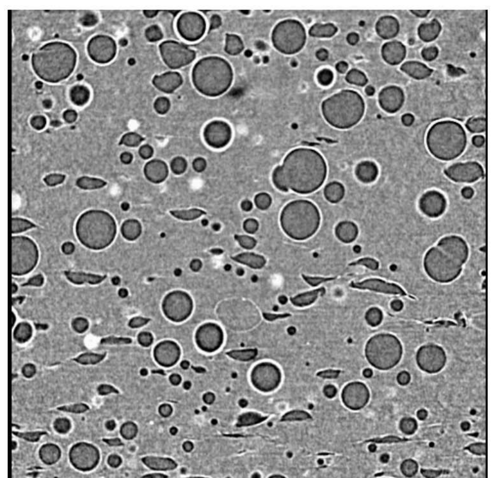


- Up to 10% strain, very few broken GMBs
- At 40% strain, some GMBs still intact!!

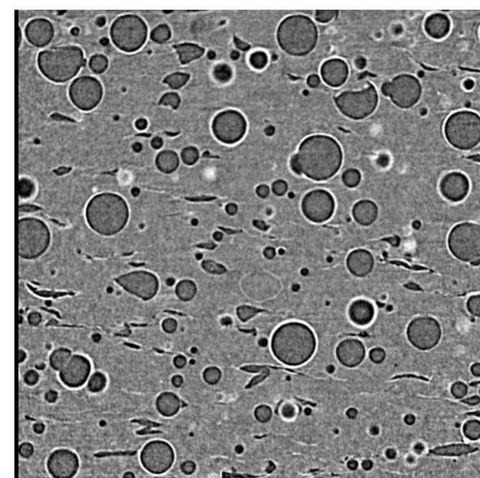
20% Strain



30% Strain



40% Strain



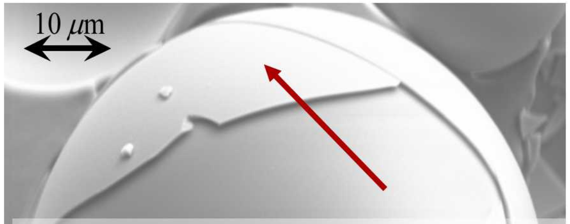
Failure Model for GMBs

Sandia National Laboratories

Borosilicate Glass Wall Material:

- Elastic Properties[1]:
  E_{glass} = 61 GPa, $\boldsymbol{\nu}_{glass}$=0.19

- Characteristic wall thickness
  - T_{wall} = 1 μm



Smooth GMB surface does not appear to have many flaws

Estimate flaw size ~ 0.2**μ**m

Failure Criteria Estimate:

- Fail individual shell elements (element death) when max principal stress = failure stress

  - LEFM approach to estimate failure stress

$$\sigma = \frac{K_{1c}}{\sqrt{\pi a}} \approx \frac{0.8MPa\sqrt{m}}{\sqrt{\pi(0.2x10^{-6})m}} \approx 1GPa$$

1.X. Nie and W.W. Chen. *Journal of the American Ceramic Society*, 90(8):2556–2562, 2007