SAND2013-1951C

Informing Macroscale Constitutive Laws through Peridynamic Modeling of Grain-Scale Mechanisms in Plutonium Oxide

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Workshop on Nonlocal Damage and Failure

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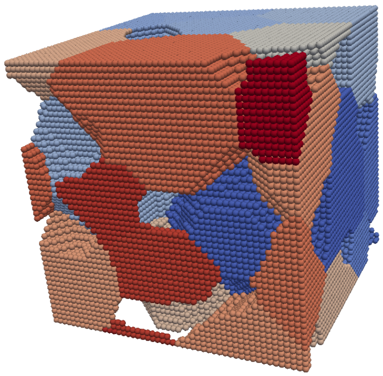
Motivation

Mechanical properties of $^{238}PuO_2$ fuel pellets are controlled by their microstructure and composition

WHAT FACTORS DETERMINE THE MICROSTRUCTURE AND COMPOSITION?

- Fabrication conditions (powder compaction & sintering)
- Storage conditions
- Pre-use annealing
- Service conditions



PuO_2 grain / void structure

CAN WE MODEL THE LINK BETWEEN MICROSCALE AND MACROSCALE?

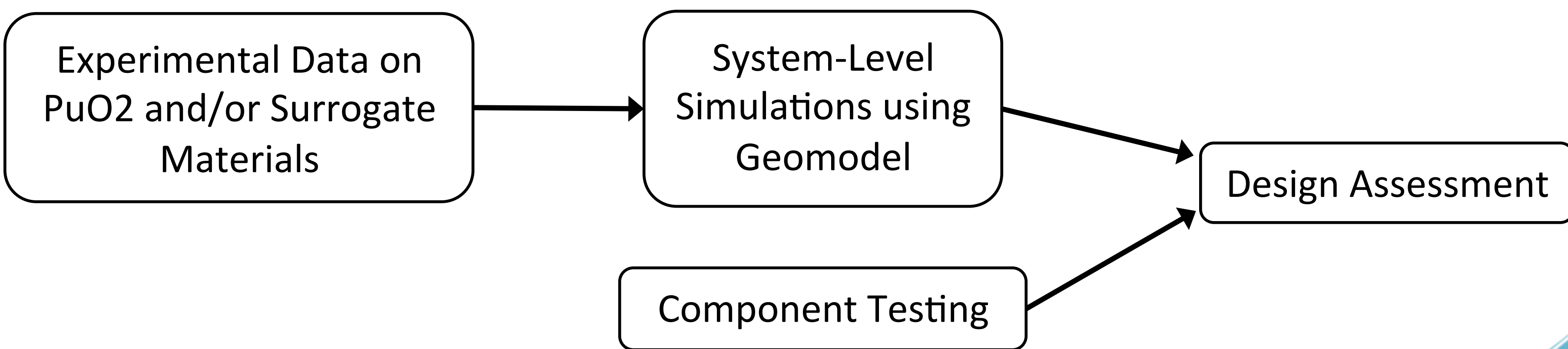
- Critical features at the grain scale
  - Grain size / grain shape / void volume
  - Material failure along grain boundaries and subsequent void collapse
- Response of representational volume can inform macro-scale constitutive law

➡ We propose **peridynamics** as a means to capture grain-scale response

Design Assessment Based on Experiments and Simulations

KEY ROLE FOR COMPUTATIONAL SIMULATION

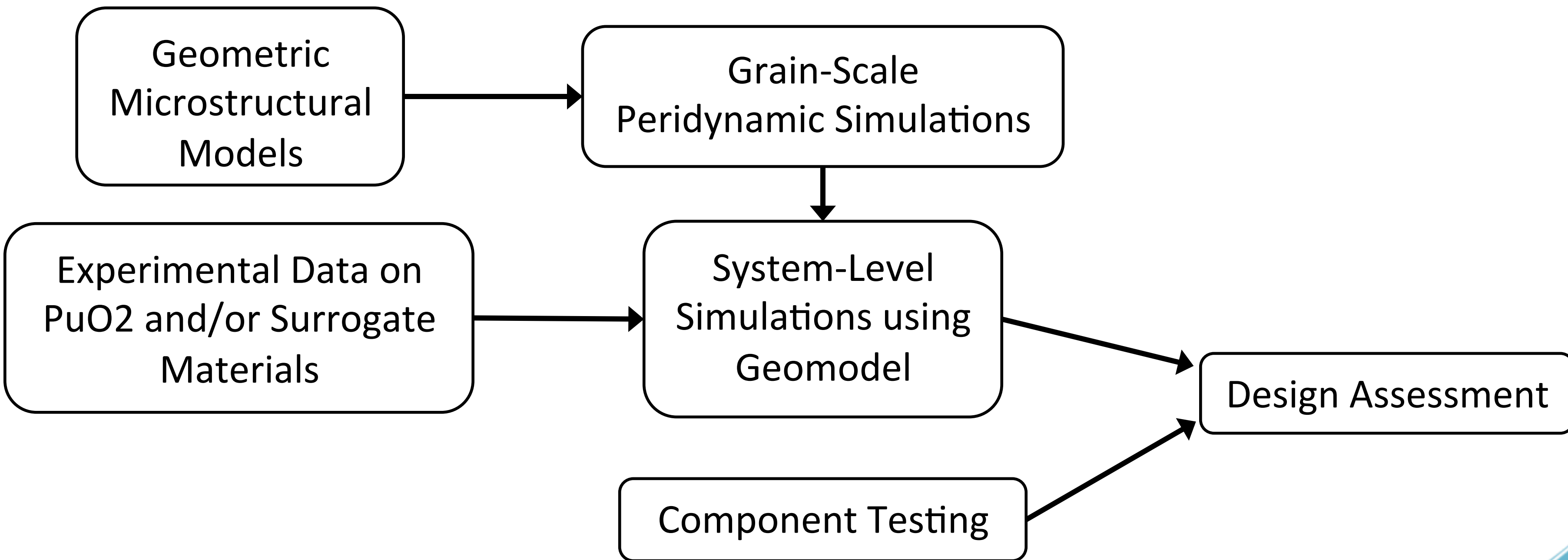
- Performing experiments on PuO_2 is difficult / expensive
- Limited experimental data in the literature
  - Material characterization
  - Calibration of material models
- Modeling performed at the system level
  - Classical FEM
  - Continuum geomodel
- Limited component testing



Enrich Simulation Effort with Grain-Scale Models

UTILIZE PERIDYNAMICS AT THE MESOSCALE

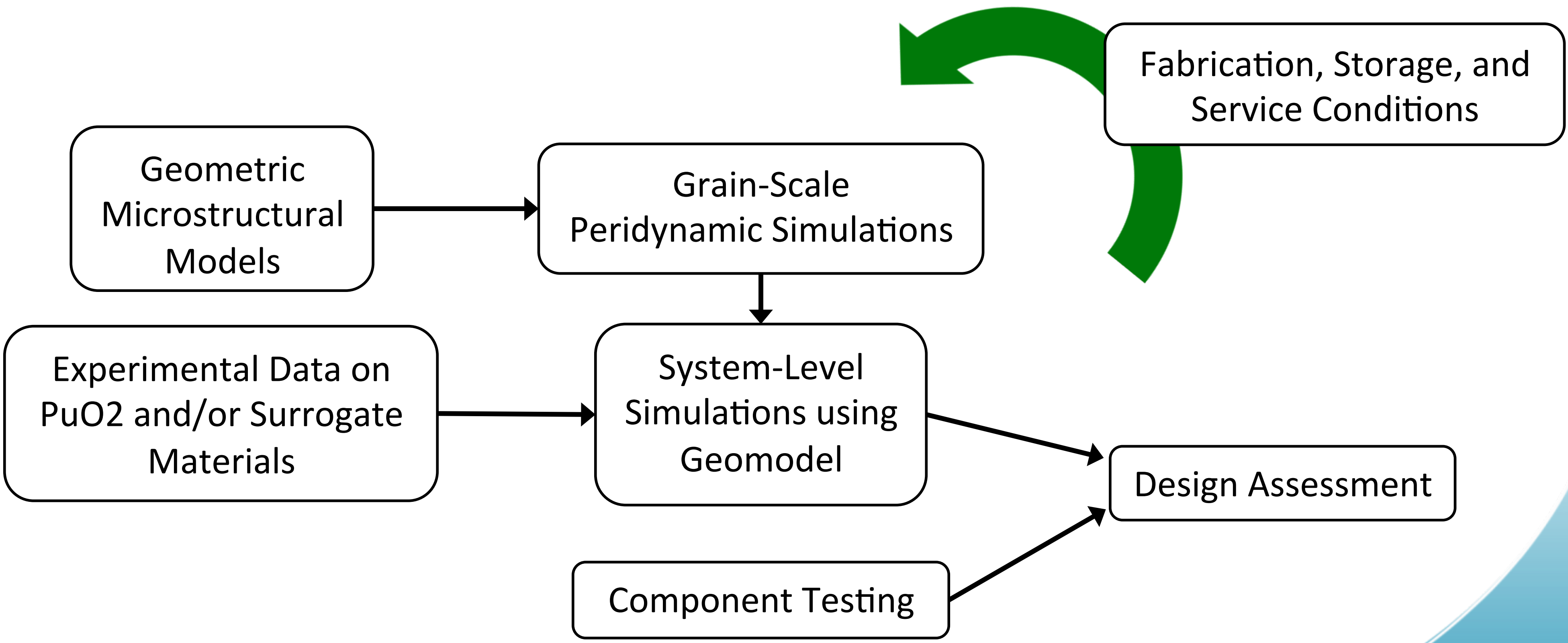
- Generate representative grain-scale models
- Peridynamic modeling of grain structure
  - Failure mechanisms occur at the grain scale
- Inform constitutive models at component / system level
  - Resolving the grain structure in system-level analyses is computationally intractable



Potential to Improve Mechanical Performance

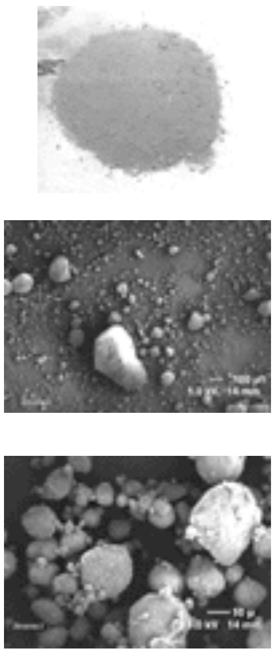
MOVING BEYOND DESIGN ASSESSMENT

- The grain structure is dictated by fabrication, storage, and service conditions
- Mechanical response is largely determined by the grain structure
- There is potential to alter fabrication, storage, and service conditions for improved mechanical performance based on simulation results

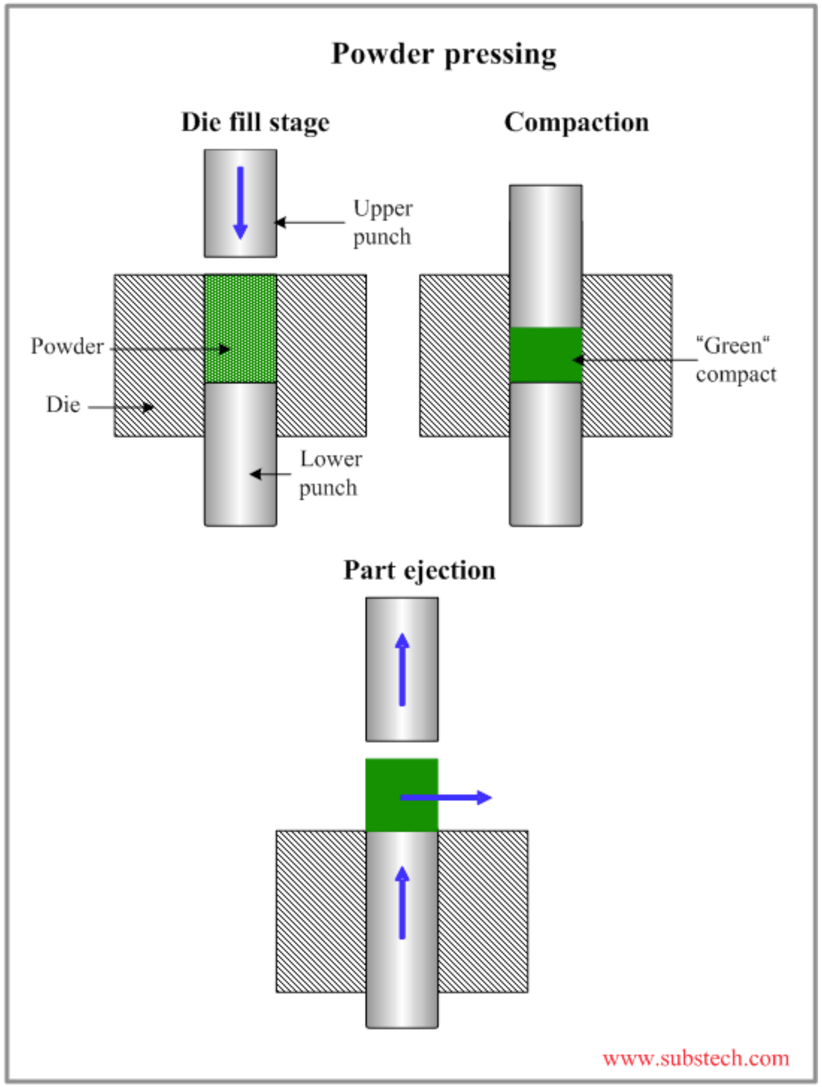


PuO_2 Fuel Pellet Fabrication

FINAL MICROSTRUCTURE IS CONTROLLED BY PROCESSING

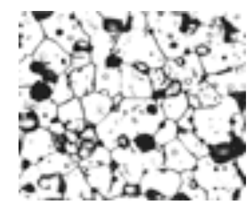


PuO_2 powder



Pressed PuO_2 pellet

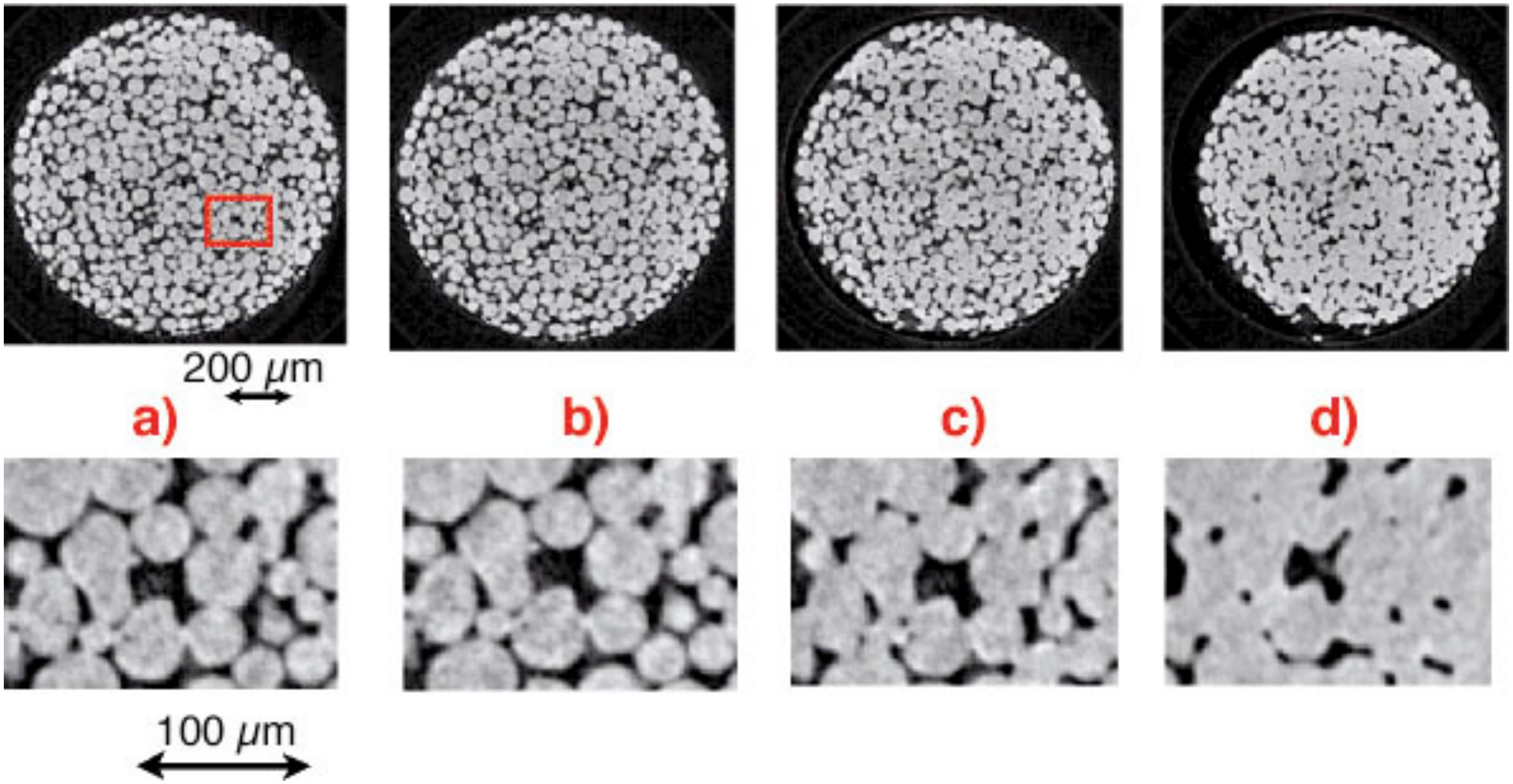
Sintered pellet at 1400 °C



Sintered pellet at 1700 °C

http://www.lanl.gov/source/orgs/nmt/nmtdo/AQarchive/96spring/fuel_fabrication.html

Microstructural Evolution During Sintering



- 2D slices perpendicular to the cylindrical axis
  - a) Before sintering
  - b) At 1000°C
  - c) At 1050°C
  - d) Final microstructure

http://www.esrf.eu/UsersAndScience/Publications/Highlights/2002/Materials/MAT3

Experimental Results of Stout, Ellis, and Pereyra

UNCONFINED COMPRESSION TESTS OF $^{238}UO_2$, $^{238}PuO_2$, and $^{239}PuO_2$

- Hypothesized that deformation is roughly elastic-perfectly-plastic due to dislocation motion
- Localized intergranular and/or transgranular failure
- Important variables: porosity, grain size, temperature, strain rate
- Significant variability in experimental data

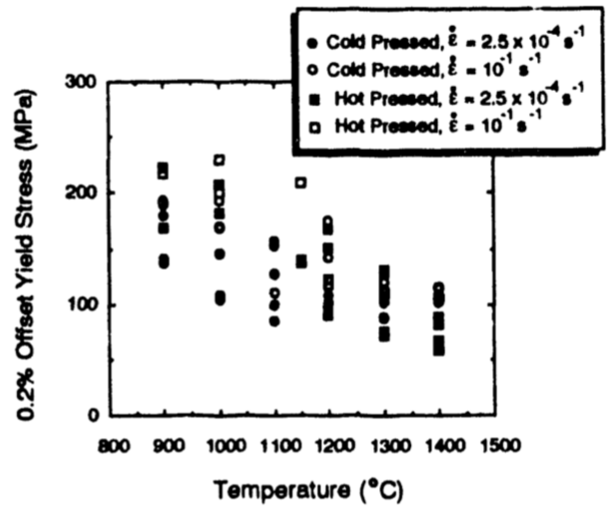


Figure 7 A combination of the yield strength data for both the hot- and cold-pressed urania, ε = 0.1 s^{-1} and 2.5 x 10^{-4} s^{-1}.

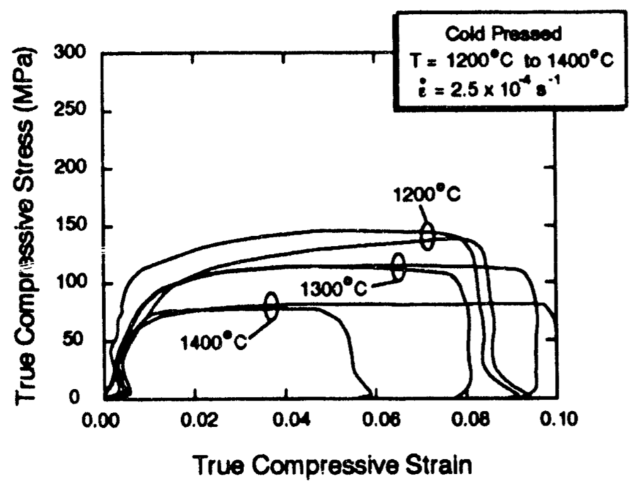


Figure 9d Stress/strain behavior of the cold-pressed and sintered urania at temperatures of 1200, 1300, and 1400°C and a strain rate of ε = 2.5 x 10^{-4} s^{-1}.

M.G. Stout, R.W. Ellis, R.A. Pereyra, Mechanical Behavior of $^{238}UO_2$, $^{238}PuO_2$, and $^{239}PuO_2$ as a Function of Strain Rate and Temperature, *LA-12811-MS*, 1994.

Experimental Results of Stout, Ellis, and Pereyra

MATERIAL FAILURE WAS PREDOMINATLY TRANSGRANULAR

- Unconfined compression tests of $^{238}UO_2$, $^{238}PuO_2$, and $^{239}PuO_2$
- Dominant vertical cracks were typically transgranular
- Non-vertical, intergranular cracks also observed, believed to be artifacts of fabrication process

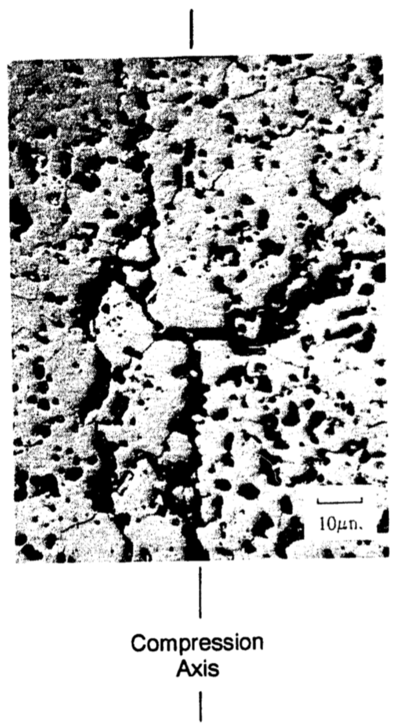


Figure 14a Intergranular fracture in a specimen deformed at 1000°C and a strain rate of $\epsilon = 2.5 \times 10^{-4}\ s^{-1}$.

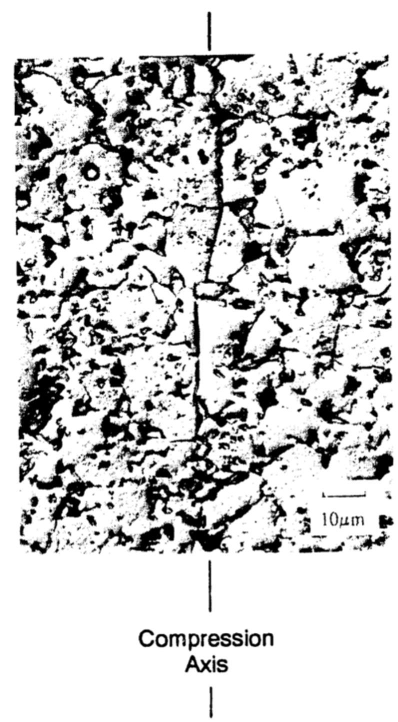


Figure 14b Transgranular fracture in a specimen deformed at 1000°C and a strain rate of $\epsilon = 2.5 \times 10^{-4}\ s^{-1}$.

M.G. Stout, R.W. Ellis, R.A. Pereyra, Mechanical Behavior of $^{238}UO_2$, $^{238}PuO_2$, and $^{239}PuO_2$ as a Function of Strain Rate and Temperature, *LA-12811-MS*, 1994.

Macroscale Constitutive Model for Classical FEM

CLASSICAL CONTINUUM GEOMODEL APPLIED IN SYSTEM MODEL

- `SOIL_FOAM` constitutive model in *Sierra/SolidMechanics*
  [Krieg 1978, Swenson and Taylor 1983, Taylor and Flanagan 1989, SAND2011-7597]
- Response is decomposed into volumetric and deviatoric components
  - Yield surface defined in principal stress space: confinement determines yield stress

$$\sigma_{yd} = a_0 + a_1 p + a_2 p^2$$

  - Arbitrary user-provided function specifies pressure as a function of volume

```
BEGIN PARAMETERS FOR MODEL SOIL_FOAM
  YOUNGS MODULUS =
  POISSONS RATIO =
  A0 =
  A1 =
  A2 =
  PRESSURE CUTOFF =
  PRESSURE FUNCTION =
END
```

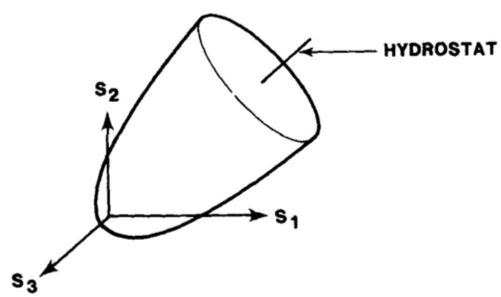


Figure 3. Yield surface in principal stress space

[Swenson and Taylor, 1983]

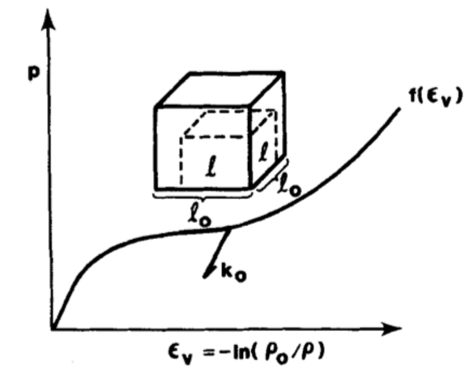


Figure 4. The pressure versus finite volume strain behaviour

[Swenson and Taylor, 1983]

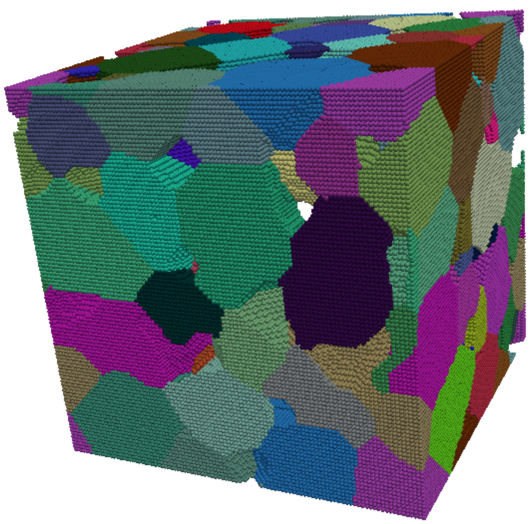
Peridynamic RVE models can inform continuum model

Creation of Representational Volume Elements

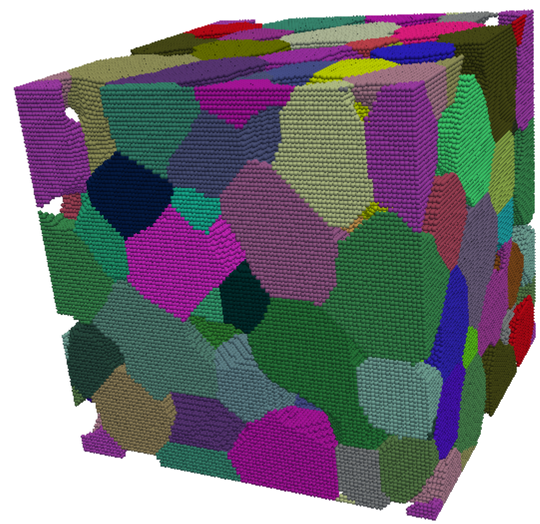
MODEL SIMULATES MICROSTRUCTURAL EVOLUTION DURING SOLID STATE SINTERING

- Simulates densification by annihilation, curve-driven grain growth and pore coarsening by surface diffusion
- Generates topologically correct microstructures given the processing variables
- The size and shape of stress concentrators (pores) are topologically correct
- Can generate correct microstructures over a wide range of processing conditions and starting powder characteristics.

MICROSTRUCTURAL MODELS



15% void volume



20% void volume

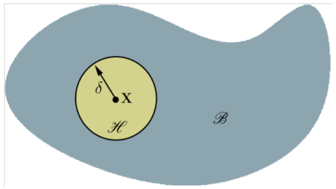
Tikare et al., Comp. Mat. Sci., 2010, 48 317

Peridynamic Modeling of PuO_2 Microstructures

Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

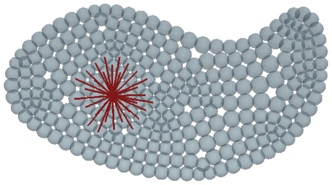
- Peridynamics is a *nonlocal* extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an *integral equation:*

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \underbrace{\int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}' \rangle \right\} \, \mathrm{d}V_{\mathbf{x}'}}_{\text{Divergence of stress replaced with integral of nonlocal forces.}} + \mathbf{b}(\mathbf{x},t)$$



- Peridynamic *bonds* connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds
- *Material failure* is modeled through the breaking of peridynamic bonds
- A peridynamic body may be discretized by a finite number of elements:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}_i' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}_i',t]\langle \mathbf{x} - \mathbf{x}_i' \rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x},t)$$



S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.

Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics. *Advances in Applied Mechanics* 44:73-168, 2010.

Peridynamic Modeling of PuO_2 Microstructures

GOALS

- Demonstrate that peridynamics can reproduce experimental data
  - Unconfined compression data of Stout, Ellis, and Pereyra
- Inform macro-scale constitutive model
  - Pressure as a function of volume
  - Yield stress as a function of pressure

CONSTITUTIVE MODELS

- State-based linear peridynamic solid
- Bond-based microelastic
- State-based elastic-plastic
- Non-ordinary state-based elastic-plastic
- Modified critical stretch bond failure law

SANDIA COMPUTING RESOURCES

- *Sierra/SolidMechanics* analysis code
- *Peridigm* analysis code
- RedSky compute cluster

Bond Failure Law

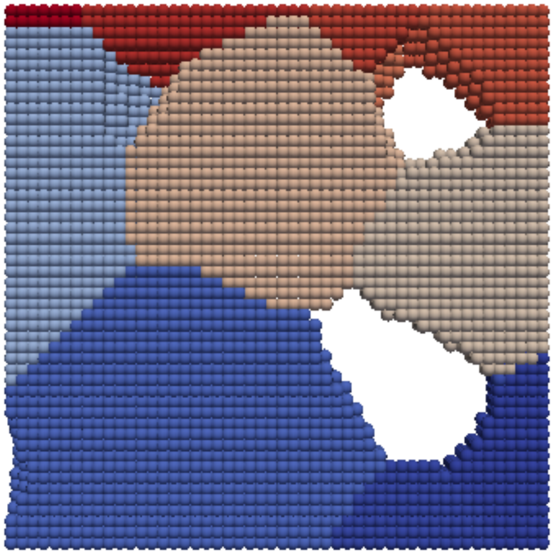
CRITICAL STRETCH BOND FAILURE RULE

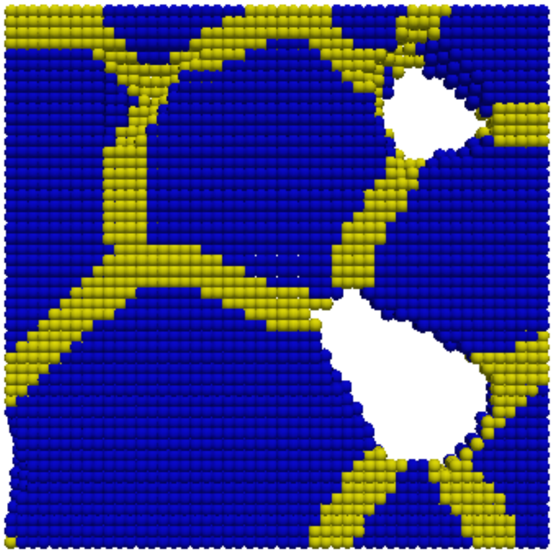
- Bonds fail when their extension exceeds a critical value
- Bond failure is irreversible

$$\phi = \begin{cases} 0 & \text{if} \quad s_{\max} < s_{\text{crit}} \\ 1 & \text{if} \quad s_{\max} \geq s_{\text{crit}} \end{cases}$$

$$s_{\max} = \frac{||\underline{e}||_{\max}}{||\underline{x}||}$$

- Bond failure law is applied only in direct vicinity of grain boundaries
- Contact algorithm controls material interactions after bonds are broken





S.A. Silling and E. Askari, A meshfree method based on the peridynamic model of solid mechanics, *Computers and Structures*, 83, 2005.

Linear Peridynamic Solid Constitutive Model

$\mathcal{H}$	Family	m	Weighted volume
$\underline{x}$	Bond (reference config.)	θ	Dilatation
$\underline{\omega}$	Influence function	k	Bulk modulus
$\underline{e}$	Bond extension	μ	Shear modulus
$\underline{e}^d$	Deviatoric bond extension		

$$m = \int_{\mathcal{H}} (\underline{\omega}\,\underline{x}) \cdot \underline{x}\, dV$$

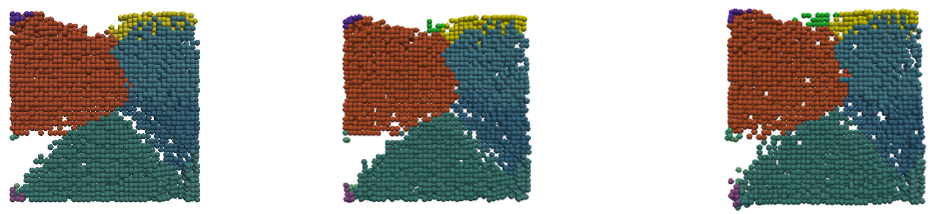
$$\theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega}\,\underline{x}) \cdot \underline{e}\, dV \qquad \underline{e}^d = \underline{e} - \frac{\theta\, \underline{x}}{3}$$

$$\underline{t} = \frac{3k\theta}{m}\,\underline{\omega}\,\underline{x} + \frac{15\mu}{m}\,\underline{\omega}\,\underline{e}^{\mathrm{d}}$$

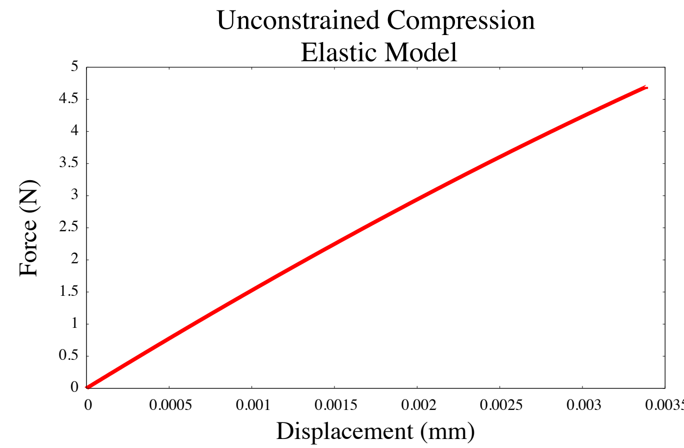
S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

Unconfined Compression: State-Based Elastic Model

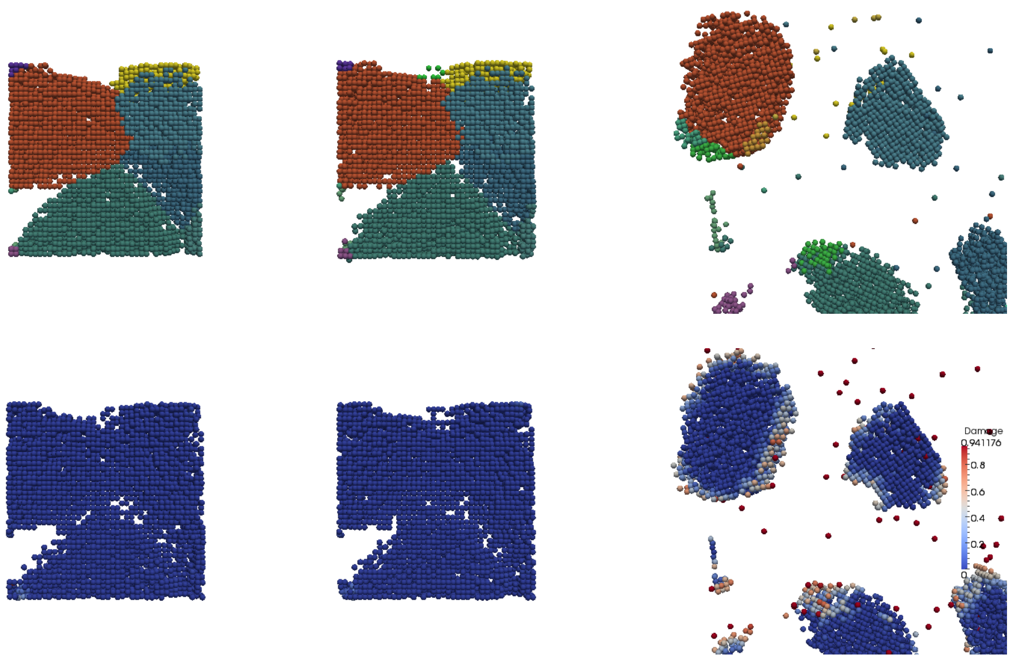
No bond failure

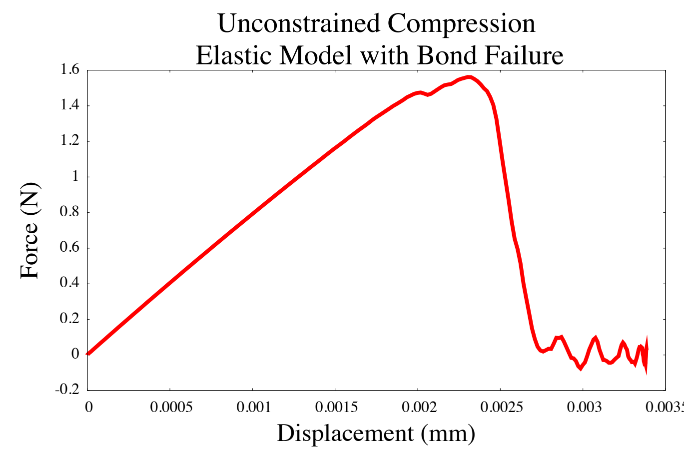


Cross section perpendicular to load



Bond failure





Bond-based Microplastic Constitutive Model

k	Bulk modulus	δ	Horizon
s	Bond stretch	s_p	Plastic bond stretch
s_Y	Yield stretch		

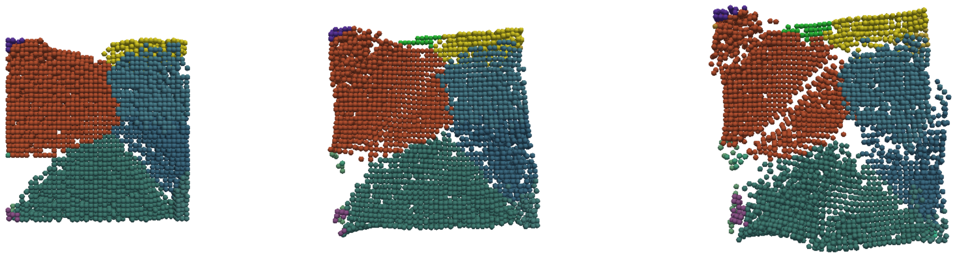
$$s_p(0) = 0, \qquad \dot{s}_p = \begin{cases} \dot{s} & \text{if } |s - s_p| \geq s_Y, \\ 0 & \text{otherwise.} \end{cases}$$

$$\Rightarrow \quad \underline{t} = \frac{18k}{\pi\delta^4}\left(s - s_p\right)$$

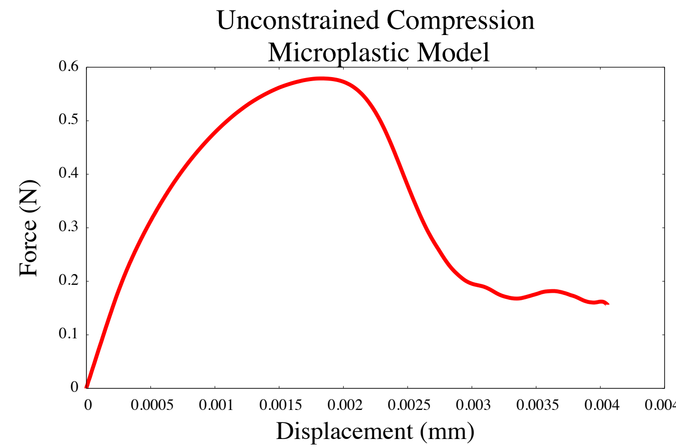
R.W. Macek and S.A. Silling, Peridynamics via Finite Element Analysis, *Finite Elements in Analysis and Design*, 43, 2007.

Unconfined Compression: Microplastic Model

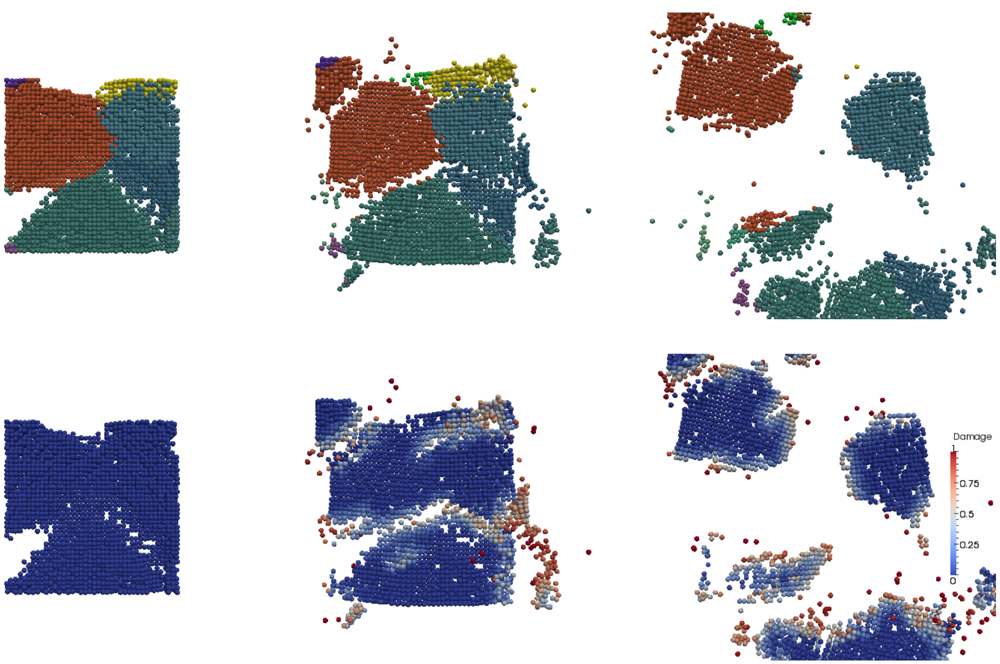
No bond failure

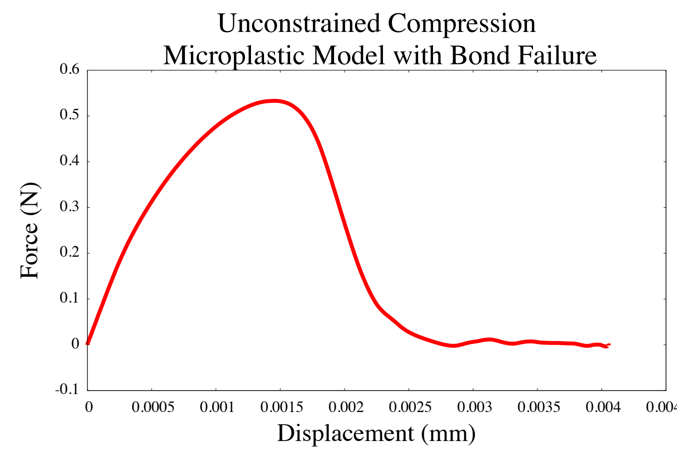


Cross section perpendicular to load



Bond failure





State-Based Elastic-Plastic Constitutive Model

$\mathcal{H}$	Family	m	Weighted volume
$\underline{x}$	Bond (reference config.)	θ	Dilatation
$\underline{\omega}$	Influence function	k	Bulk modulus
$\underline{e}$	Bond extension	μ	Shear modulus
$\underline{e}^d$	Deviatoric bond extension		

$$m = \int_{\mathcal{H}} (\underline{\omega}\, \underline{x}) \cdot \underline{x}\, dV \qquad \theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega}\, \underline{x}) \cdot \underline{e}\, dV$$

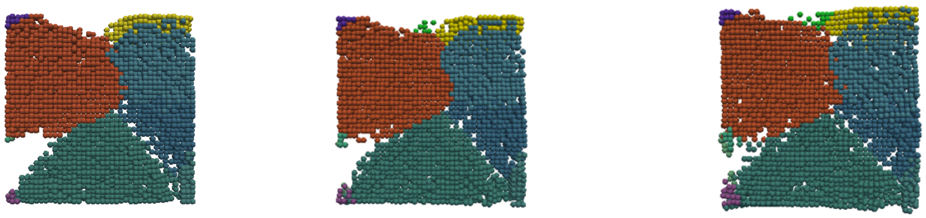
$$\underline{e}^d = \underline{e} - \frac{\theta\, \underline{x}}{3} = \underline{e}^{de} + \underline{e}^{dp} \qquad \dot{\underline{e}}^{dp} = \lambda\, \nabla^d \psi$$

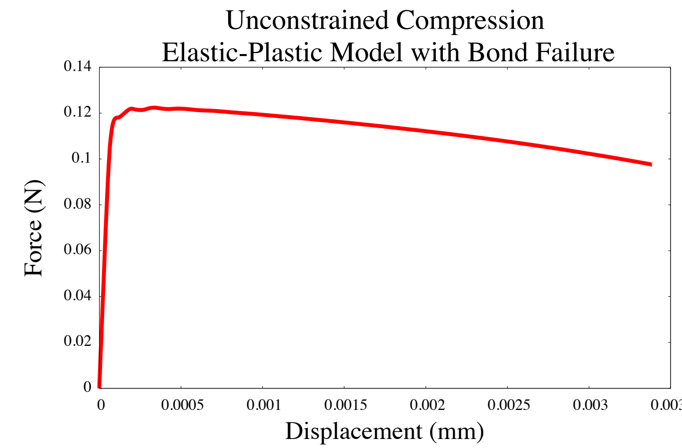
$$\underline{t} = \frac{3k\theta}{m}\, \underline{\omega}\, \underline{\mathrm{x}} + \frac{15\mu}{m}\, \underline{\omega}\, \left(\underline{e}^{\mathrm{d}} - \underline{e}^{\mathrm{dp}}\right)$$

J.A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. Sandia Report SAND2011-3166, 2011.

Unconfined Compression: Elastic-Plastic Model

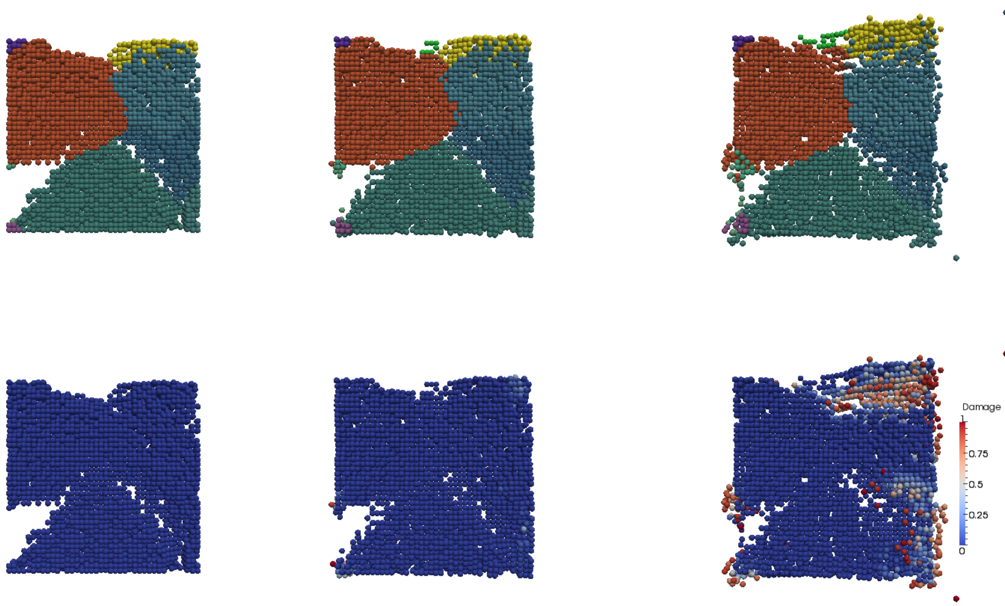
No bond failure

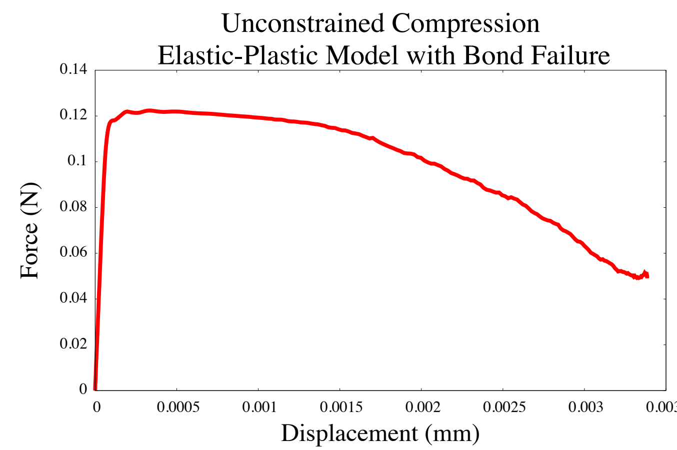




Cross section perpendicular to load

Bond failure





Non-Ordinary State-Based Material Models

APPLICTION OF CLASSICAL (LOCAL) MATERIAL MODELS WITHIN PERIDYNAMICS

- Approximate deformation gradient based on initial and current locations of material points in family

<u>Approximate Deformation Gradient</u>

$$\bar{\mathbf{F}} = \left(\sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{Y}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i} \right) \mathbf{K}^{-1}$$

<u>Shape Tensor</u>

$$\mathbf{K} = \sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i}$$

- Kinematic data passed to classical material model
- Classical material model computes stress
- Stress converted to pairwise forces

$$\underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle = \underline{\omega} \, \sigma \mathbf{K}^{-1} \langle \mathbf{x}' - \mathbf{x} \rangle$$

S. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari. Peridynamic states and constitutive modeling. *Journal of Elasticity*, 88(2):151-184, 2007.

Suppression of Zero-Energy Modes

APPROACH: PENALIZE DEFORMATION THAT DEVIATES FROM REGULARIZED DEFORMATION GRADIENT

Predicted location of neighbor

$$\mathbf{x}_n'^{\star} = \mathbf{x}_n + \bar{\mathbf{F}}_n \, (\mathbf{x}_o' - \mathbf{x}_o)$$

Hourglass vector

$$\mathbf{\Gamma}_{\mathrm{hg}} = \mathbf{x}_n'^{\star} - \mathbf{x}_n'$$

Hourglass vector projected onto bond

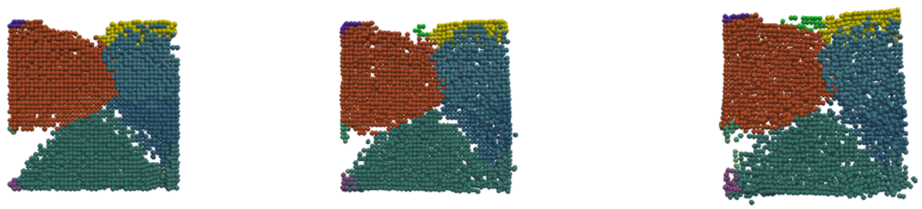
$$\gamma_{\mathrm{hg}} = \mathbf{\Gamma}_{\mathrm{hg}} \cdot (\mathbf{x}_n' - \mathbf{x}_n)$$

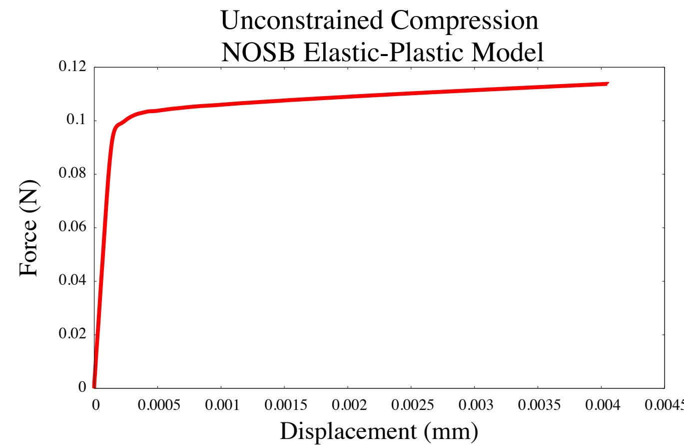
Hourglass force

$$\mathbf{f}_{\mathrm{hg}} = -\mathrm{C}_{\mathrm{hg}} \underbrace{\left(\frac{18k}{\pi\delta^4}\right)}_{\text{micro-modulus}} \underbrace{\frac{\gamma_{\mathrm{hg}}}{\|\mathbf{x}_o' - \mathbf{x}_o\|}}_{\text{hourglass stretch}} \underbrace{\frac{\mathbf{x}_n' - \mathbf{x}_n}{\|\mathbf{x}_n' - \mathbf{x}_n\|}}_{\text{bond unit vector}} \Delta V_{\mathrm{x}} \, \Delta V_{\mathrm{x}'}$$

Unconfined Compression: NOSB Elastic-Plastic Model

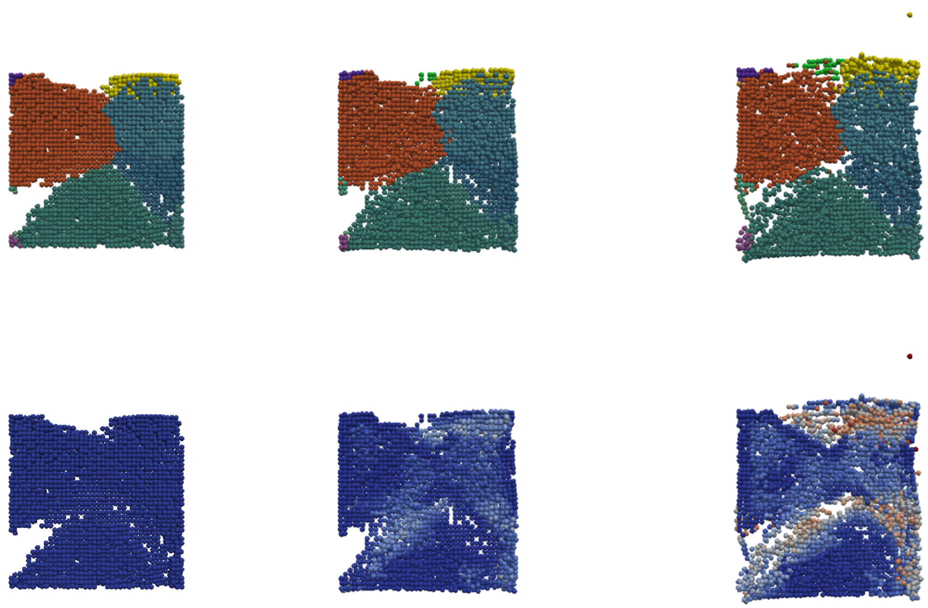
<u>No bond failure</u>

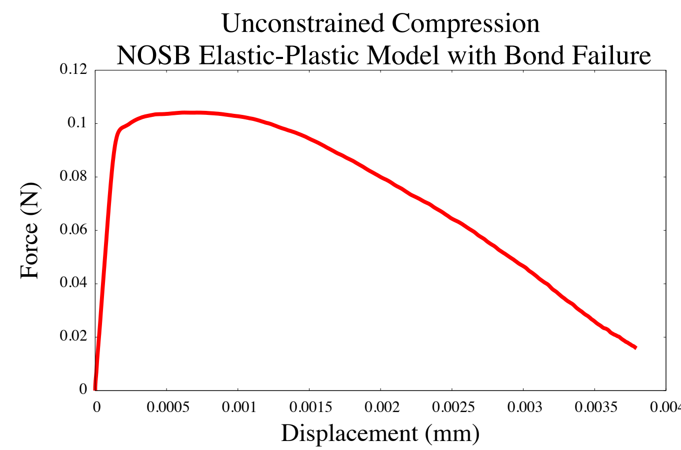




Cross section perpendicular to load

<u>Bond failure</u>





Unconfined Compression

COMPARISON TO EXPERIMENTAL DATA

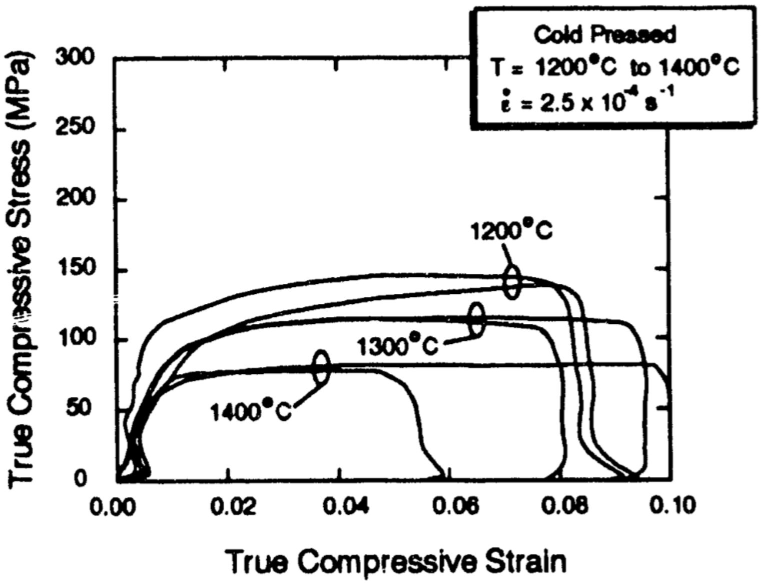
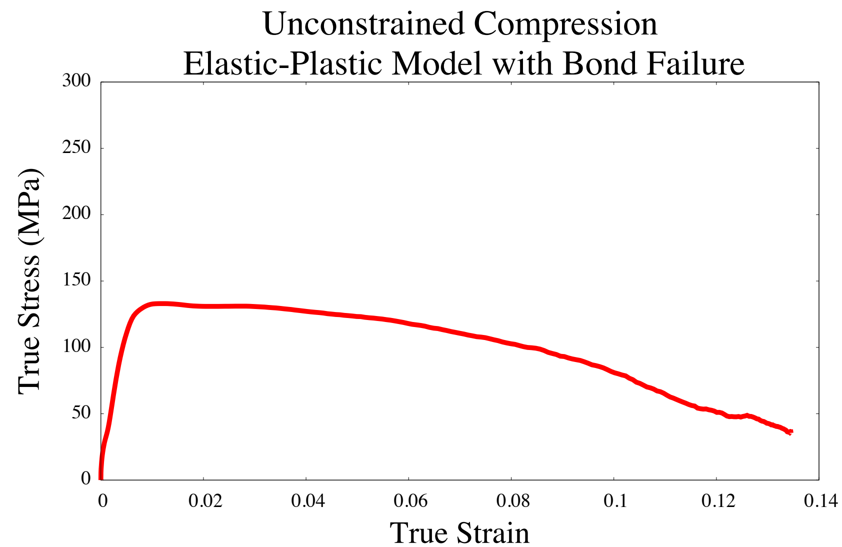


Figure 9d Stress/strain behavior of the cold-pressed and sintered urania at temperatures of 1200, 1300, and 1400°C and a strain rate of ε = 2.5 x 10^{-4} s^{-1}.

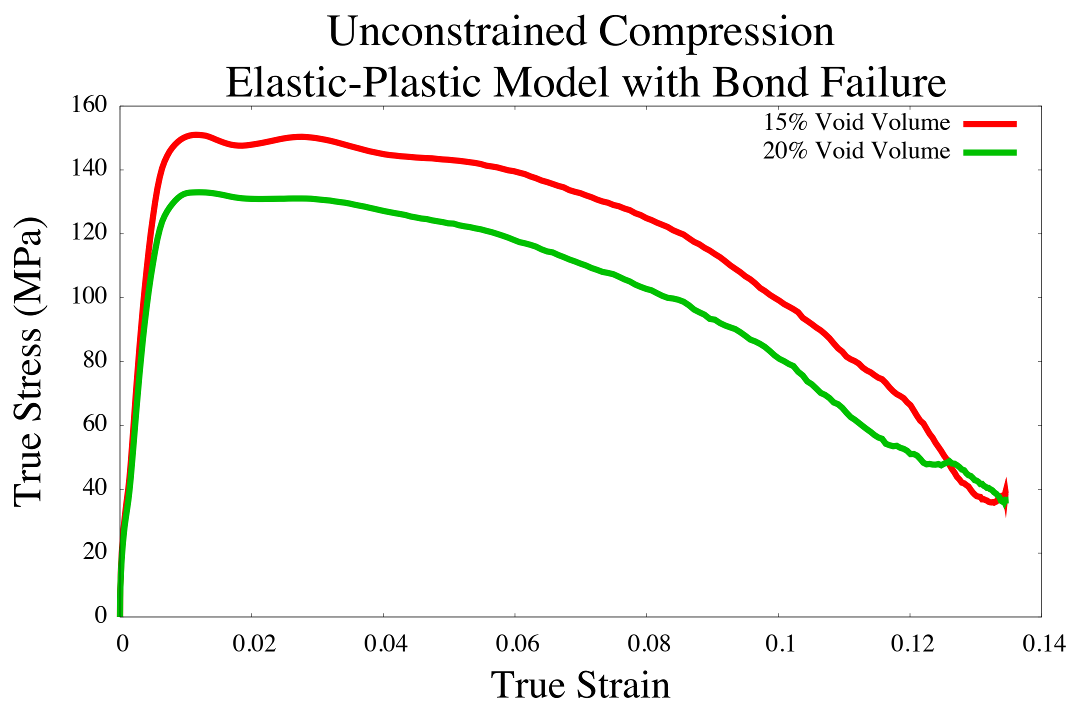
[Stout, Ellis, and Pereyra, 1994]

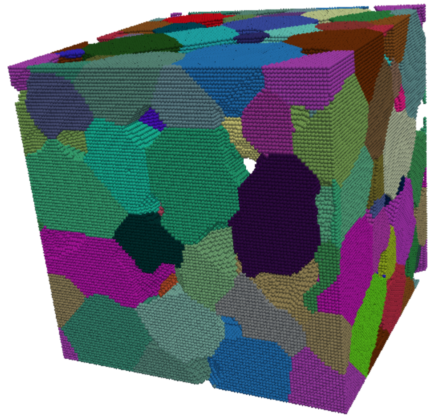


Unconfined Compression: Effect of Void Volume

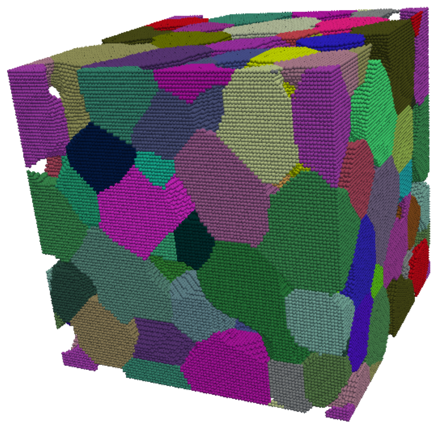
MICROSTRUCTURE AFFECTS MACROSCOPIC RESPONSE

- Reduced void volume leads to higher yield stress
- Inform macro-scale constitutive model





15% void volume

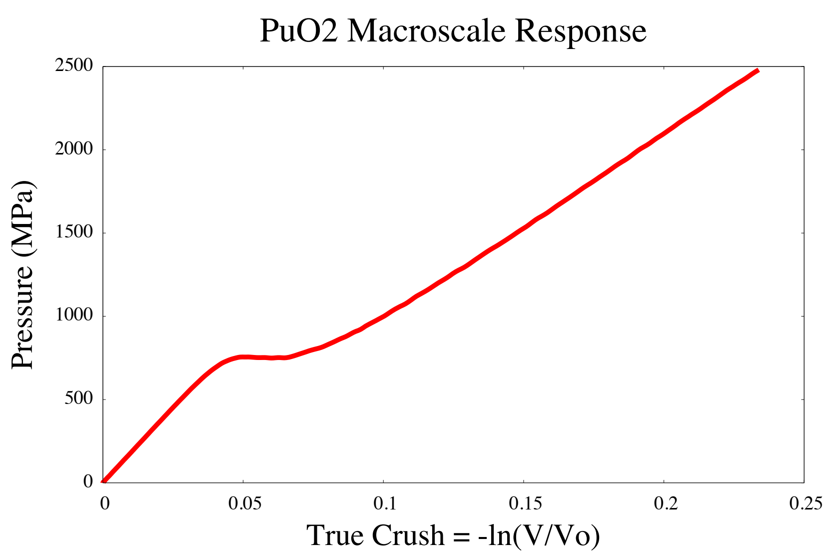


20% void volume

Pressure as a Function of Volumetric Strain

CLASSICAL CONTINUUM GEOMODEL APPLIED IN SYSTEM MODEL

- `SOIL_FOAM` constitutive model requires user-specified function describing the pressure response as a function of volumetric strain
- Peridynamic model predicts:
  - Initial elastic response
  - Macroscopic yielding due to void collapse
  - Re-stiffening of response following void collapse



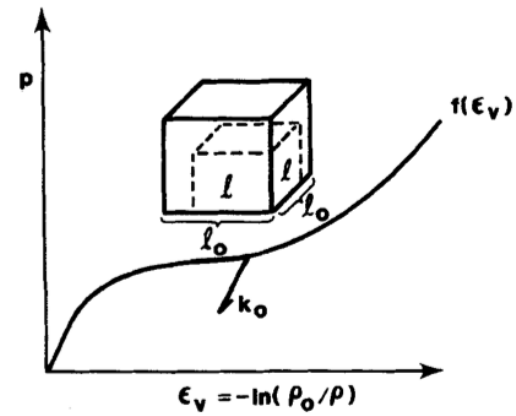
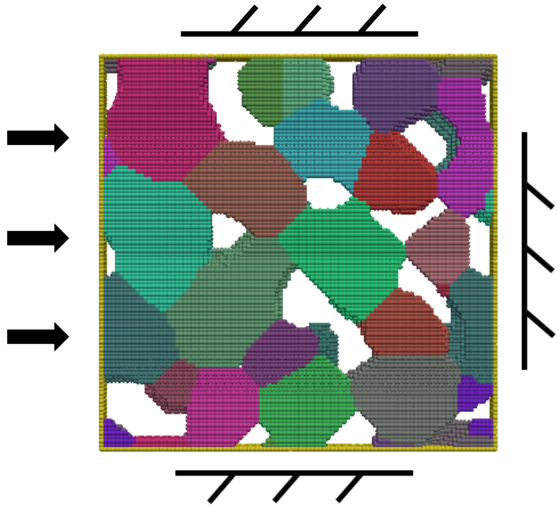
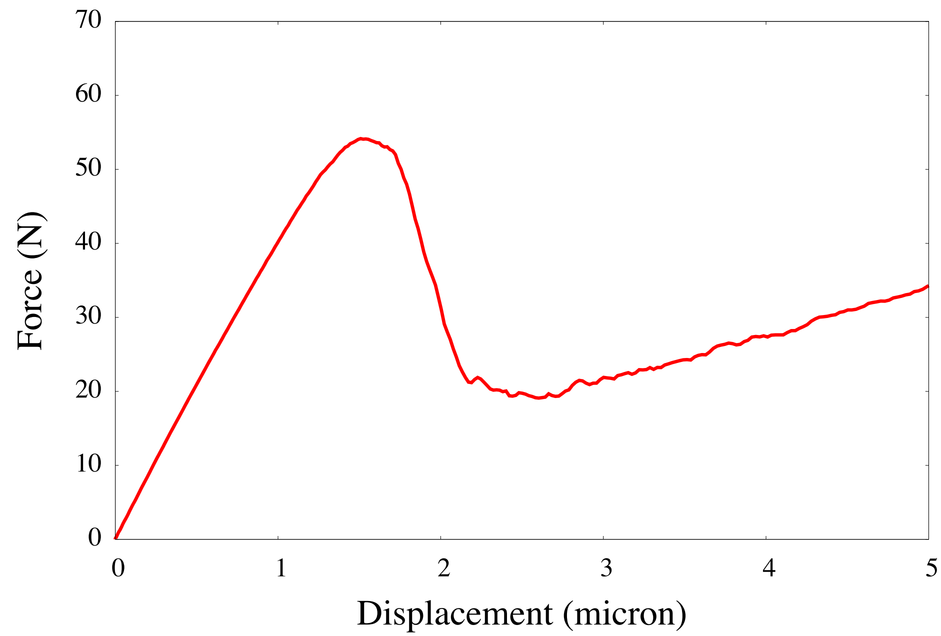


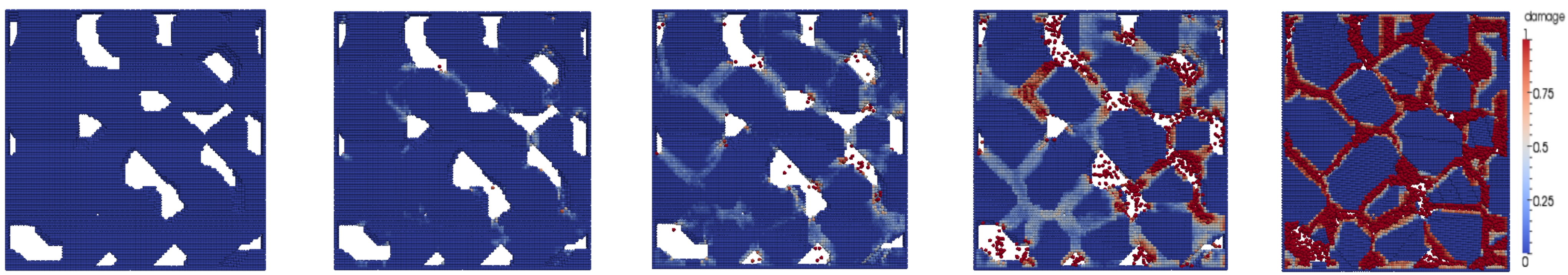
Figure 4. The pressure versus finite volume strain behaviour

[Swenson and Taylor, 1983]

Yield Stress as a Function of Confinement







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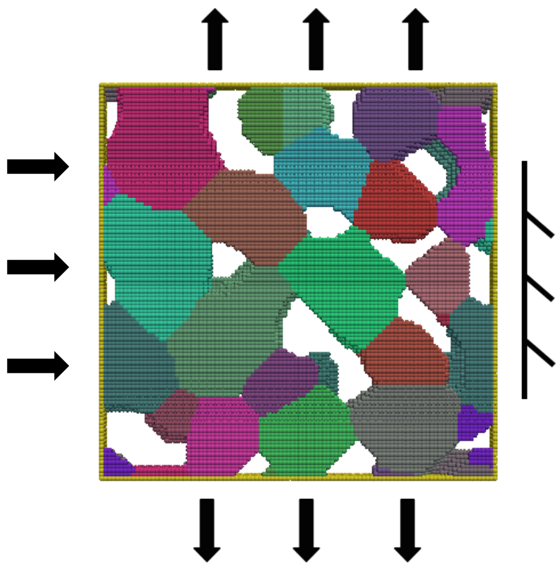
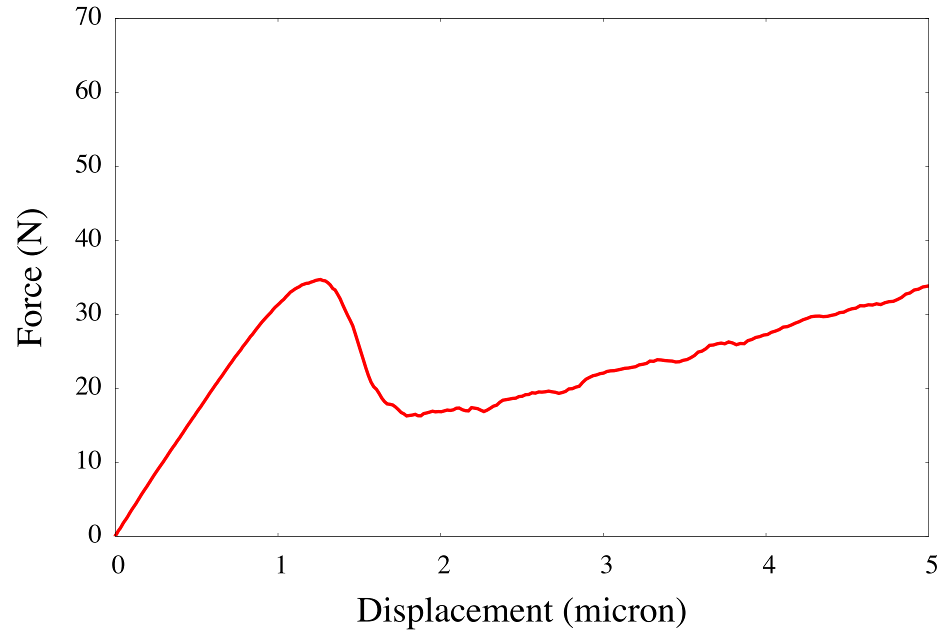
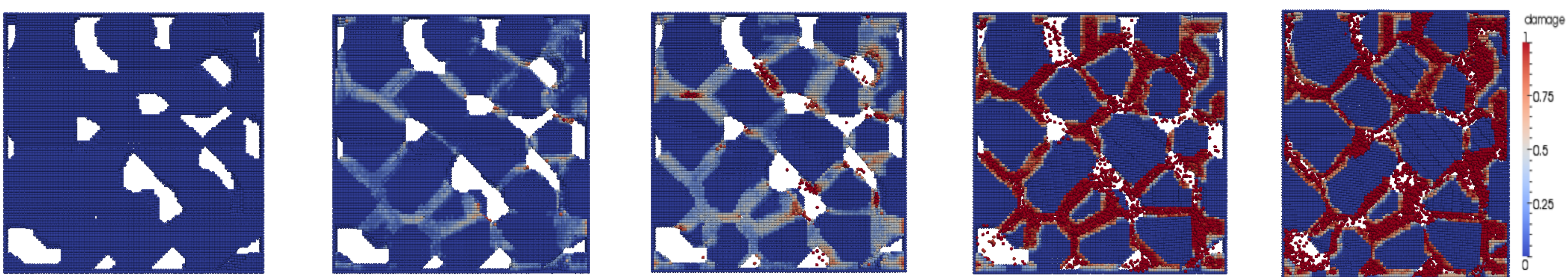
Reduced Confinement

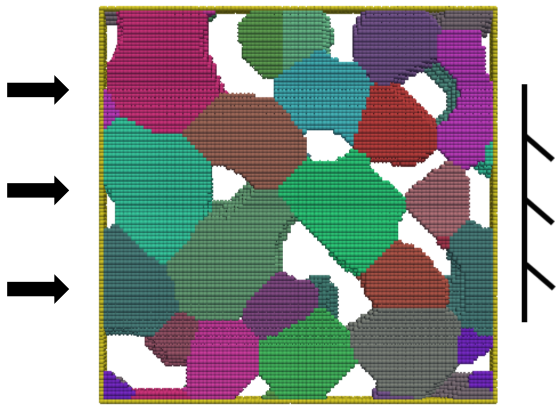


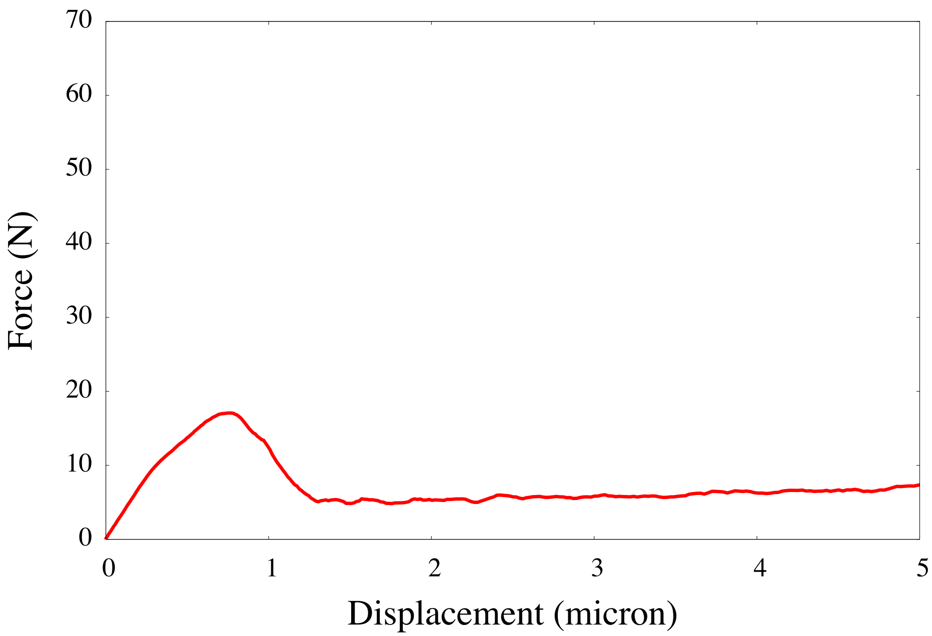


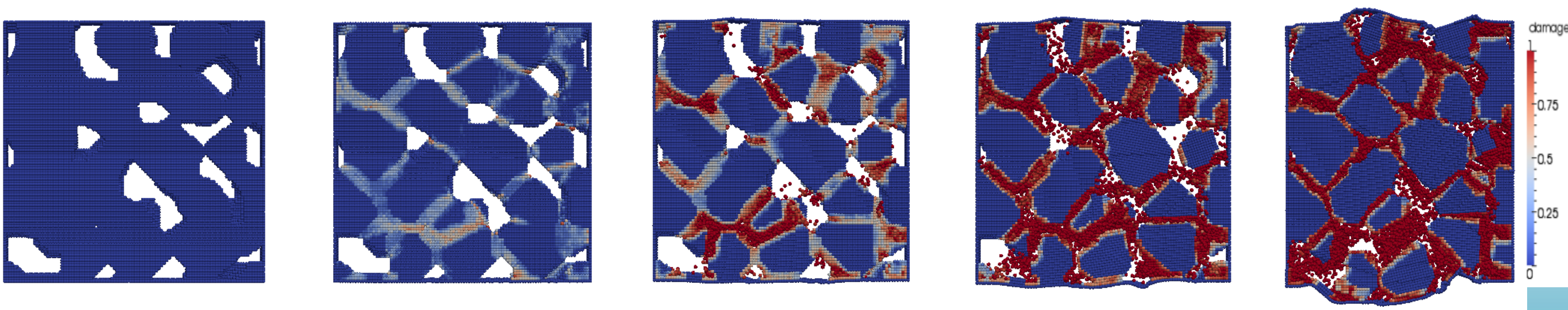
$$u_{\text{transverse}} = 0.15\, u_{\text{loading direction}}$$



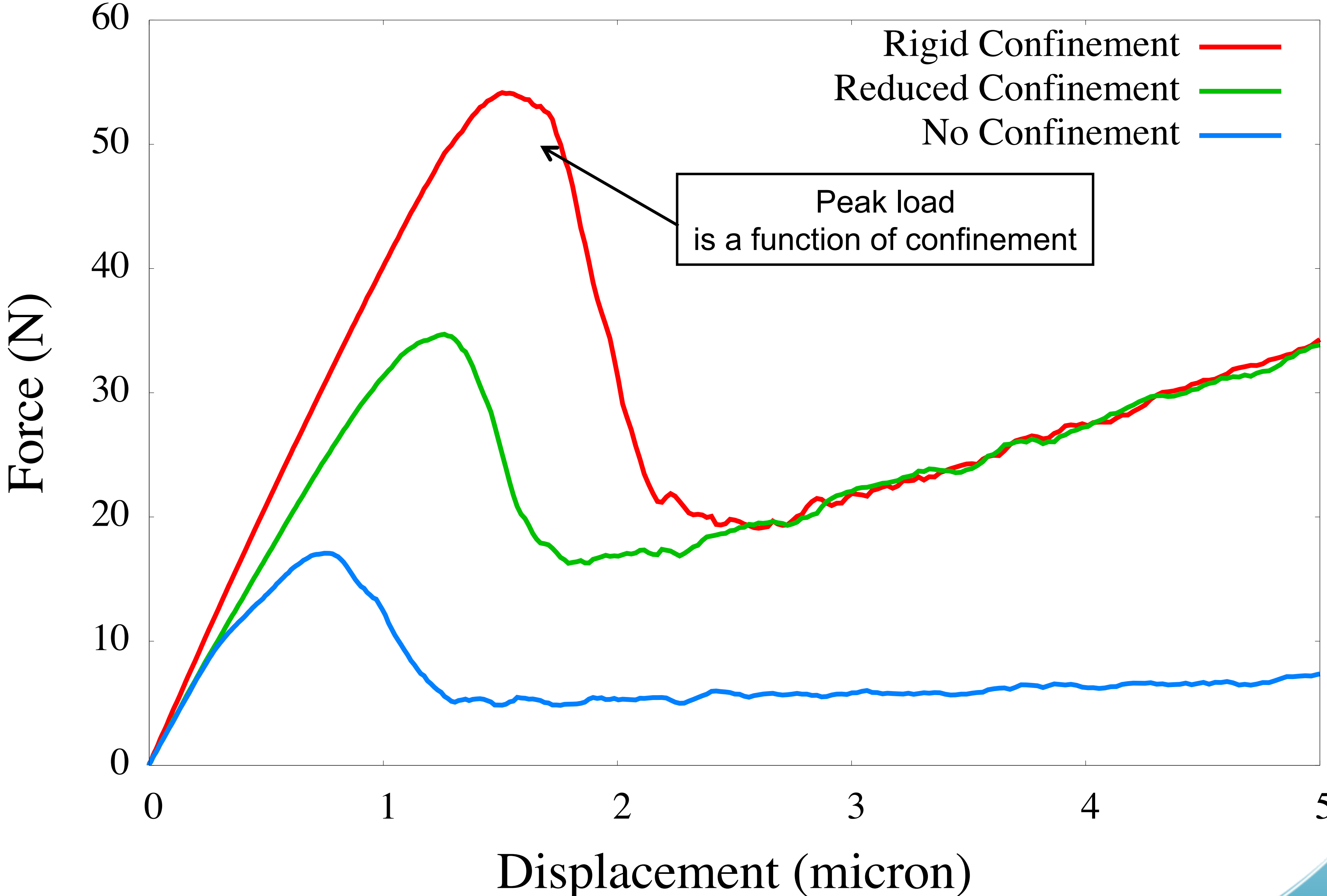
No Confinement



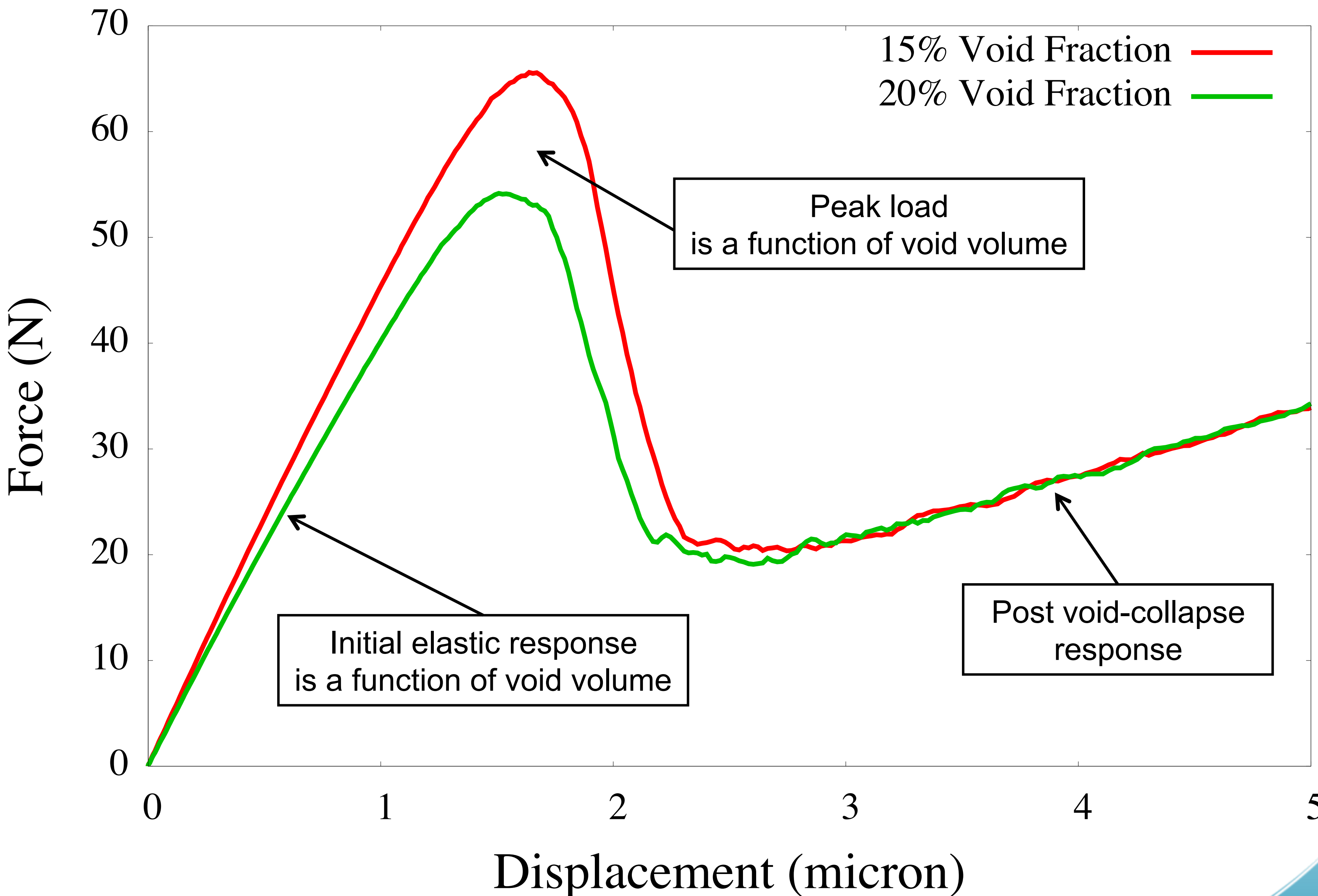




Macroscopic Response of Representational Volumes



Macroscopic Response of Representational Volumes



Conclusions and Ongoing Work

WHAT'S BEEN DONE

- Creation of representational volume element
  - Void fraction is a function of processing conditions
- Peridynamic model of representational volume mechanical response
- Macroscopic response tied to microstructure

WHERE WE ARE GOING

- Experimental validation of peridynamic representational volume model
- Calibration of macro-scale constitutive law base on meso-scale calculations
- Investigation of alternative models
  - Peridynamic constitutive model
  - Bond failure law

Questions?

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Radio Isotope Power Systems Launch Safety Program

RESOURCES

Advanced Simulation and Computing (ASC)

http://www.sandia.gov/asc/

Peridigm: A publicly-available peridynamics code

https://software.sandia.gov/trac/peridigm/

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