SAND2022-7768C

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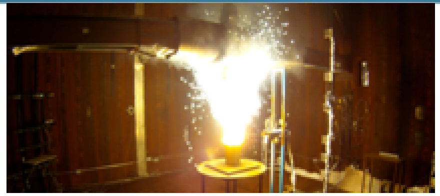
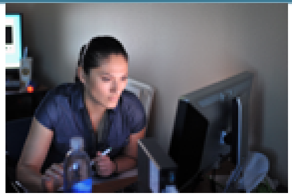
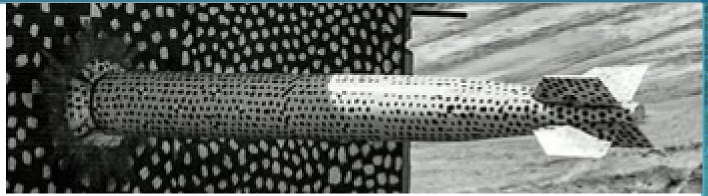
The role of pressure-dependent viscoplasticity and volumetric dilatation in energetic materials at intermediate strain rates

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

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U.S. DEPARTMENT OF ENERGY NNSA

International Explosives Conference

June 22-24, 2022, London, United Kingdom

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Mechanical Behavior of Energetics: A Modeling Challenge

- Why care about mechanical behavior? –Safety is key

  - Precursor to hot spot formation and High Explosive Violent Reaction (HEVR) events

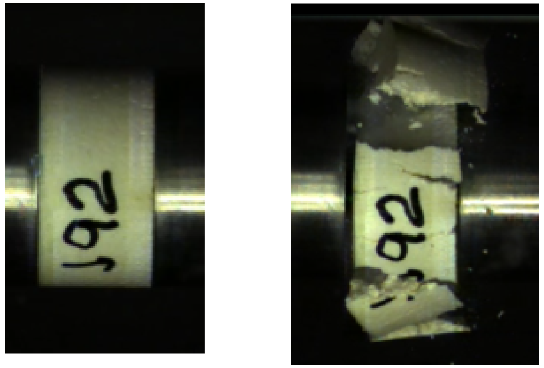
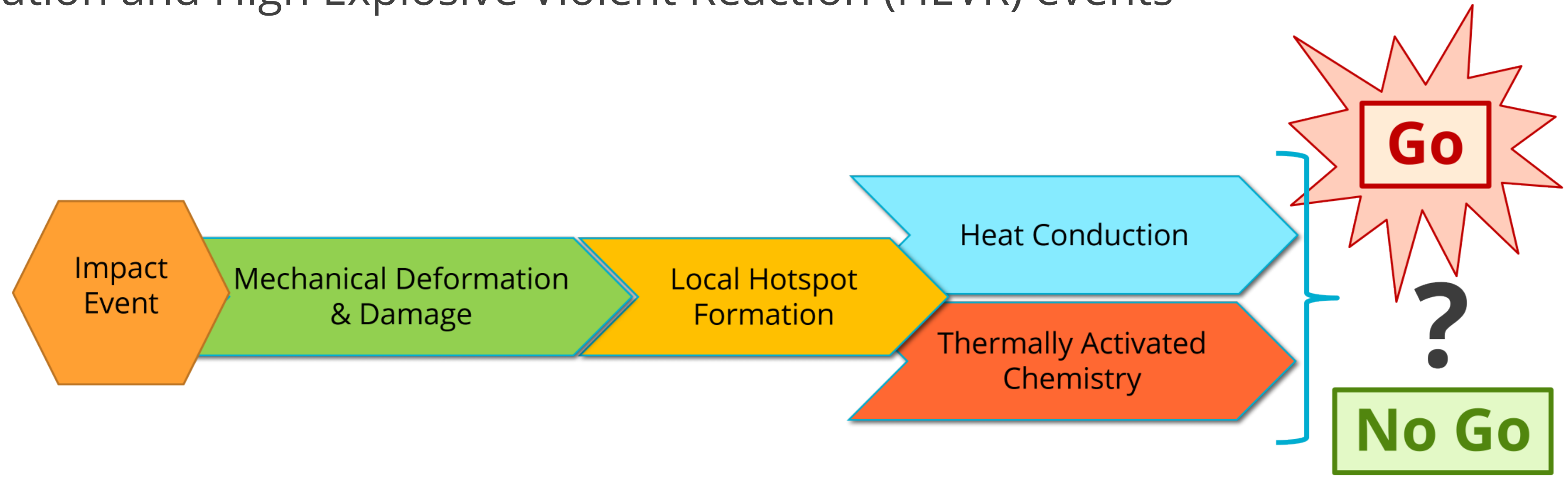


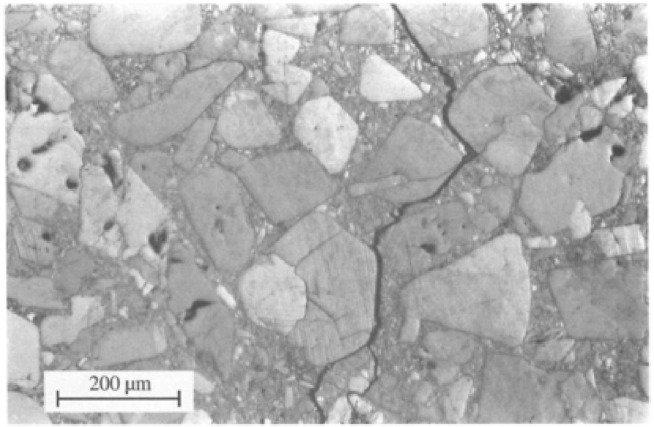
Image: courtesy Marcia Cooper



  - What is behavior of a mechanically deformed explosive exposed to other environments?—must first be able to predict the deformed state

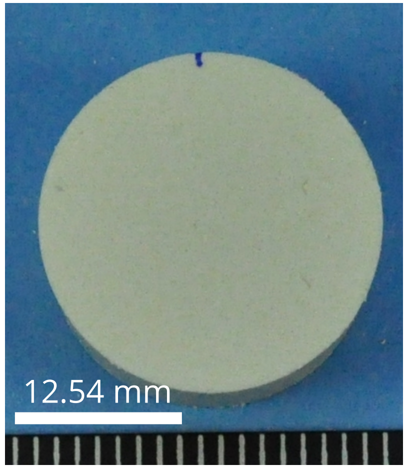
PBX Mechanical Behavior: A Modeling Challenge

- PBX Mechanical behavior is complex:
  - Strain rate dependent
  - Temperature dependent
  - Pressure dependence
  - Tension-Compression Asymmetry
  - Many inelastic deformation mechanisms: Viscoelasticity (binders), Cracking (intra- and inter-granular), Porosity opening, dislocation slip, twinning (some energetic crystals)



Plastic Bonded Explosive [Rae, 2002]

How to represent various inelastic mechanisms in a macroscale model?



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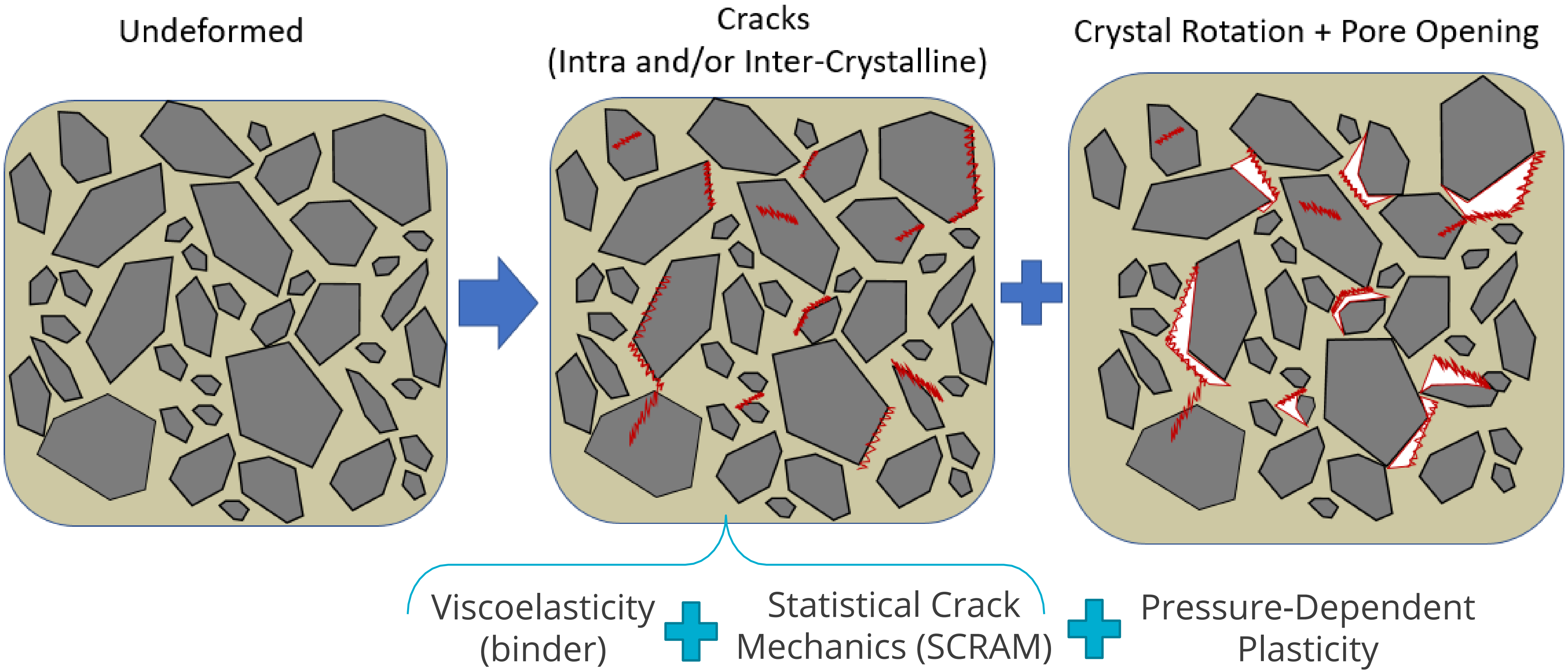
Hypothesized Mesoscale Deformation Mechanisms

- Simplified view of mesoscale processes and macroscale interpretation



ViscoPlastic-ViscoSCRAM Model Theory

- Kinematics:

$$\epsilon = e + \frac{1}{3}\epsilon_{\text{vol}} I \qquad \sigma_{\text{m}} = K\epsilon_{\text{vol}}$$

$$e = (e^{ve} + e^{D}) + e^{p}$$

- Viscoelasticity

$$\dot{s} = 2G^{\infty}\dot{e}^{ve} + \sum_{\kappa=1}^{N}\left(2G^{(\kappa)}\dot{e}^{ve} - \frac{s^{(\kappa)}}{\tau^{(\kappa)}}\right)$$

Prony series of shear moduli and relaxation times

$$\dot{s}^{(\kappa)} = 2G^{(\kappa)}(\dot{e} - \dot{e}^{p}) - \frac{s^{(\kappa)}}{\tau^{(\kappa)}} - \frac{G^{(\kappa)}}{G_0}\left[\frac{3}{a}\left(\frac{c}{a}\right)^2 \dot{c}s + \left(\frac{c}{a}\right)^3 \dot{s}\right]$$

- SCRAM Damage

$$e^{D} = \frac{1}{2G_0}\left(\frac{c}{a}\right)^3 s$$

$$\dot{c} = \begin{cases} v_{res}\left(\frac{K_I}{K_1}\right)^m & \text{for } K_I < K' \\ v_{res}\left[1 - \left(\frac{K_{0\mu}}{K_I}\right)^2\right] & \text{otherwise} \end{cases}$$

$$D = \frac{\left(\frac{c}{a}\right)^3}{1 + \left(\frac{c}{a}\right)^3}$$

- Drucker-Prager Plasticity

$$f(\sigma_{ij}) = \sigma_e + A \cdot \sigma_m - \sigma_y$$

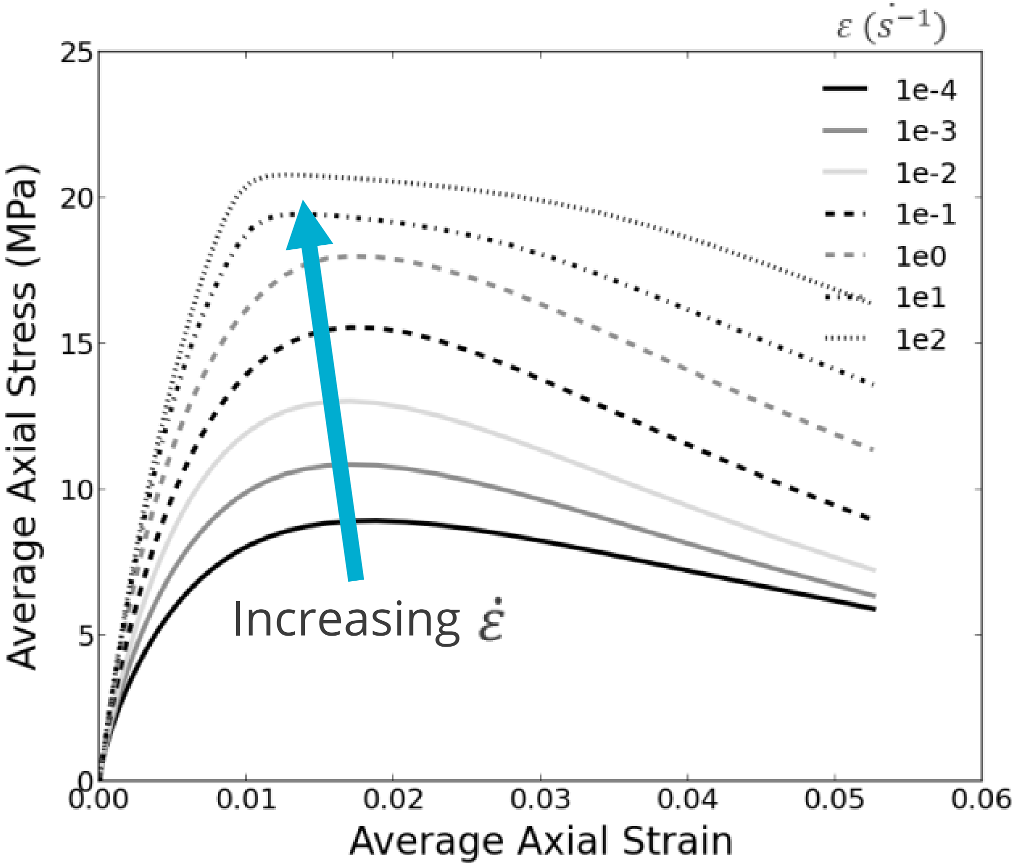
$$g(\sigma_{ij}) = \sigma_e + B \cdot \sigma_m - \sigma_y$$

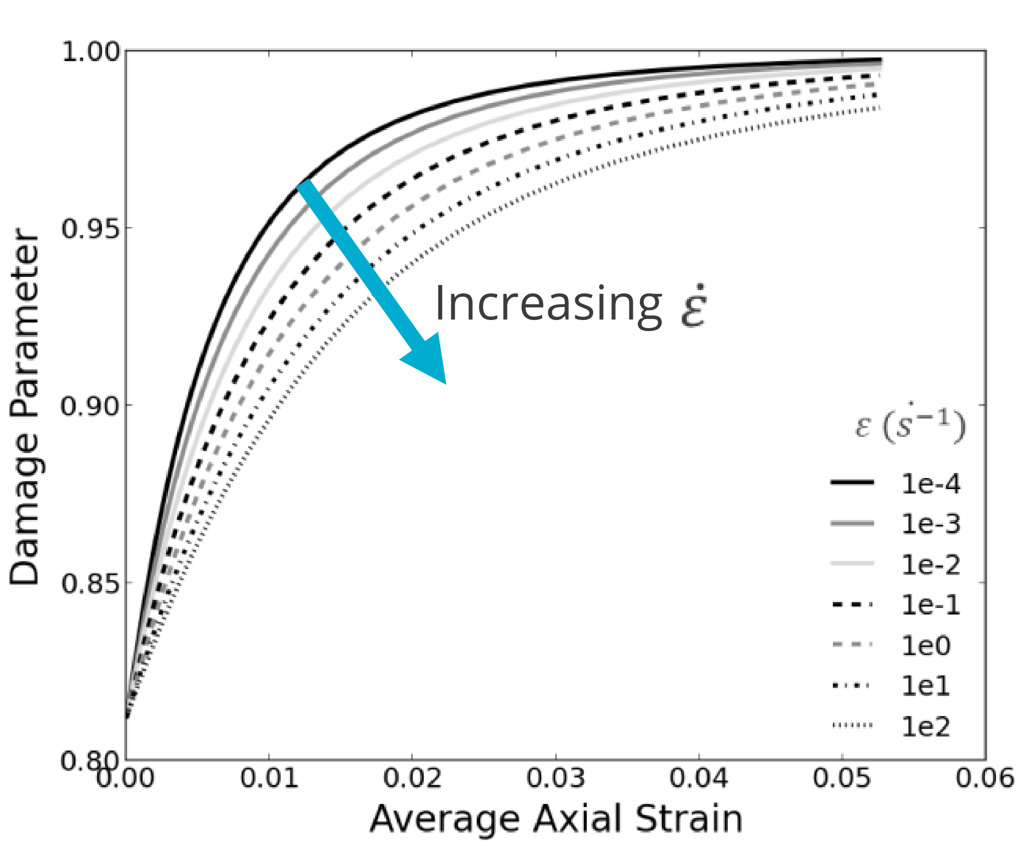
$$\dot{\epsilon}^{p} = \dot{\lambda}\frac{\partial g}{\partial \sigma}$$

$$\dot{\lambda} = \frac{1}{\tilde{\tau}}\langle\frac{f(\sigma_{ij})}{\sigma_0}\rangle^{\tilde{m}} \qquad \sigma_e = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$$

Uniaxial Compression

- Rate Dependence from Viscoelasticity and SCRAM mechanisms

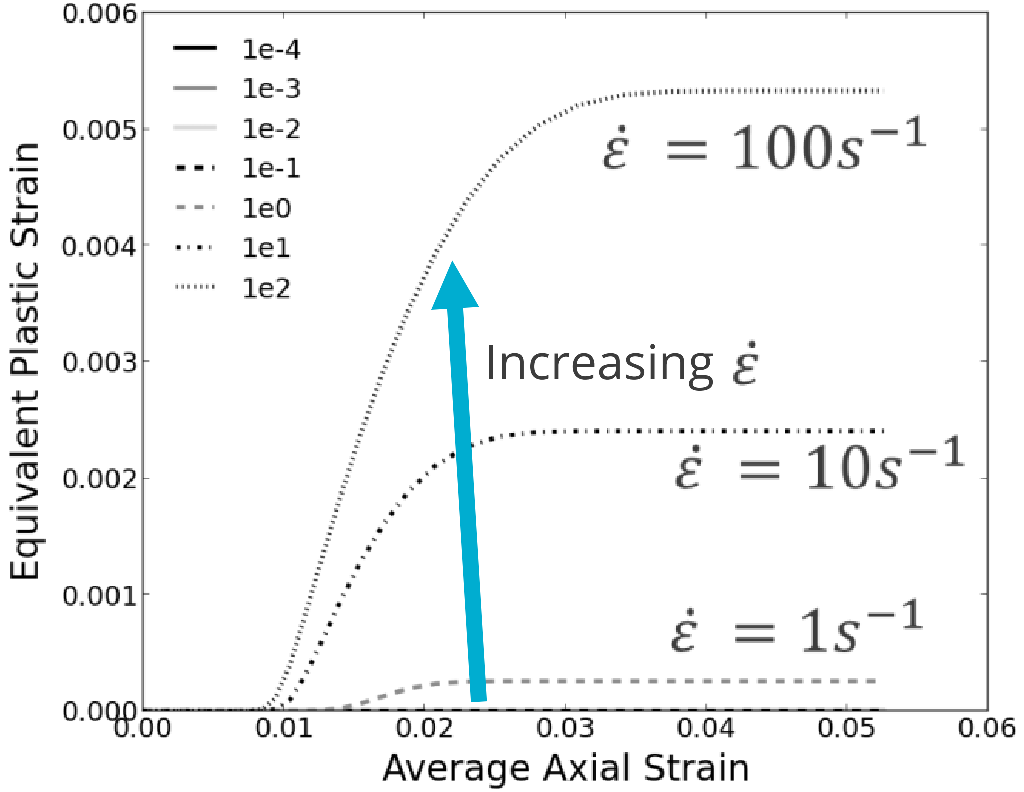


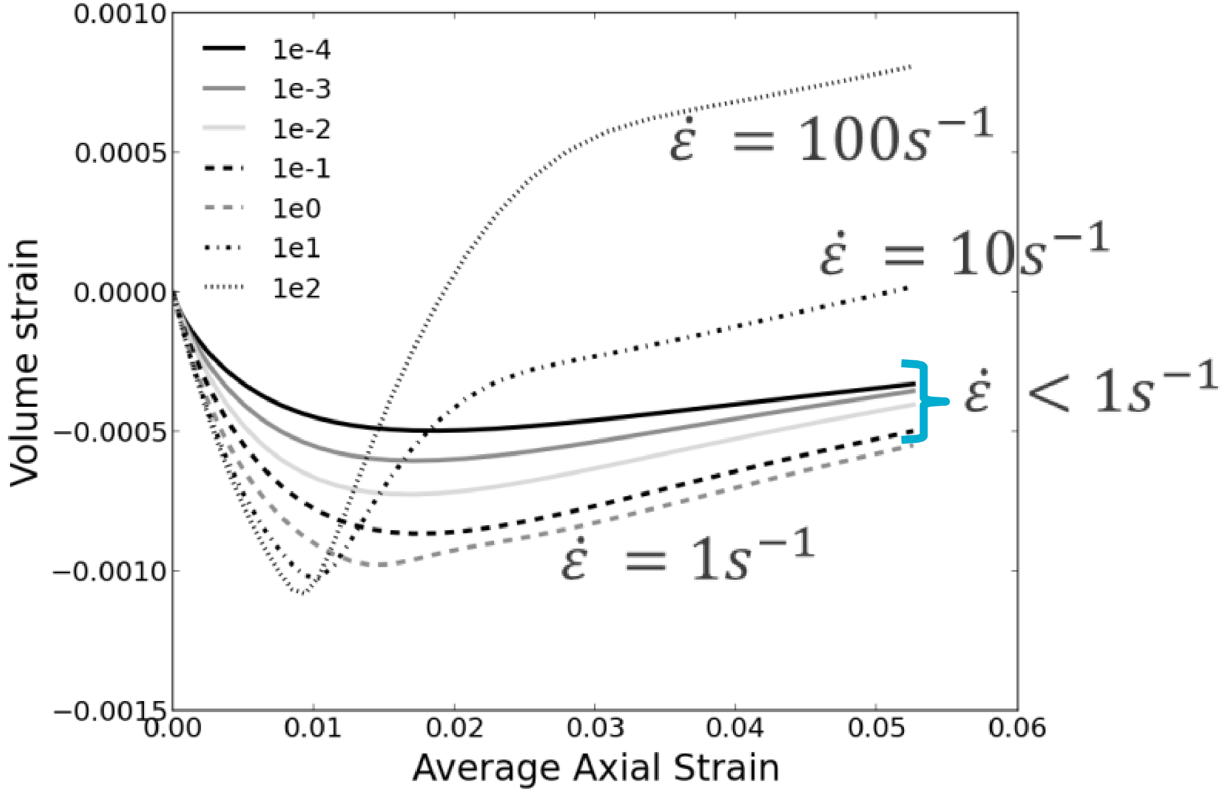


While increasing strain rate increases stiffness from the viscoelasticity, the damage evolution is reduced with increasing strain rate. Why?

Uniaxial Compression

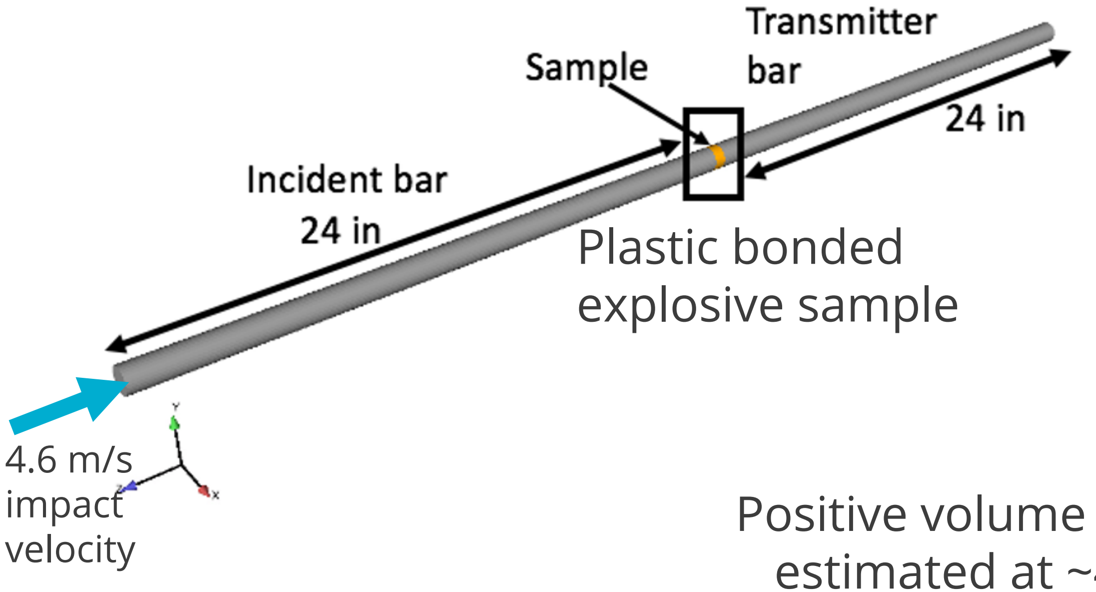
- Plasticity is a second inelastic mechanism, which is only active at strain rates $\dot{\varepsilon} \leq 1s^{-1}$



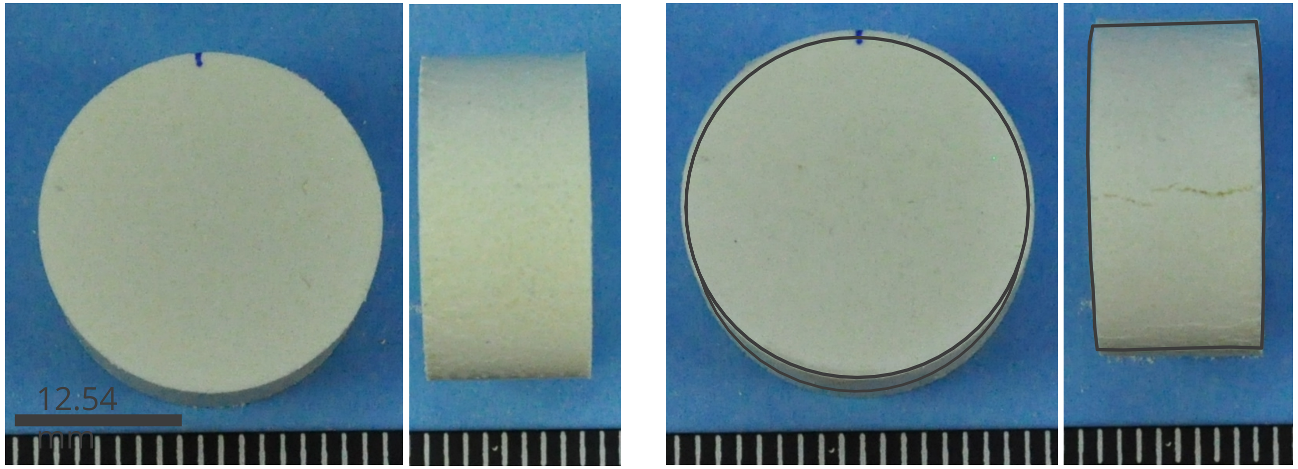


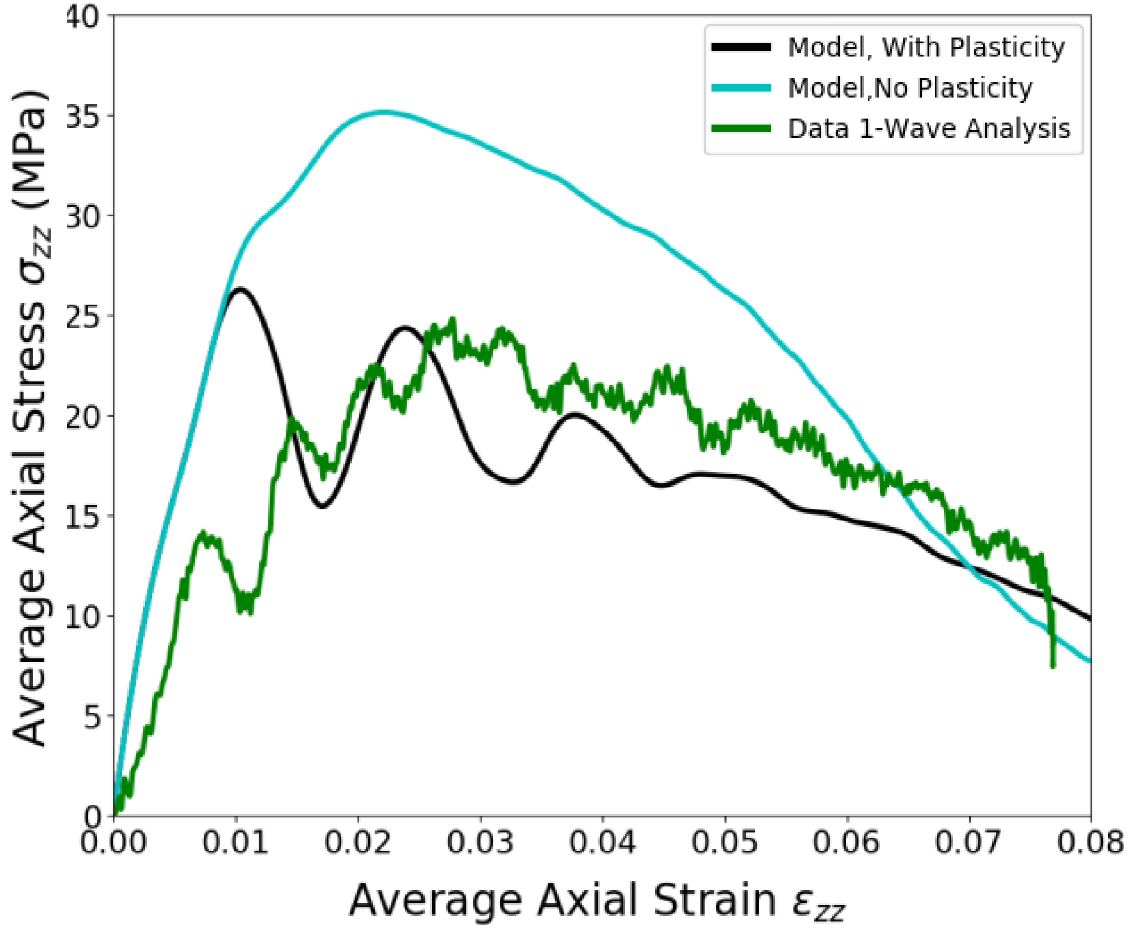
Plasticity limits stress development in the material which reduces the rate of damage and also produces positive volume strain (dilatation)

Intermediate Strain Rate Impact



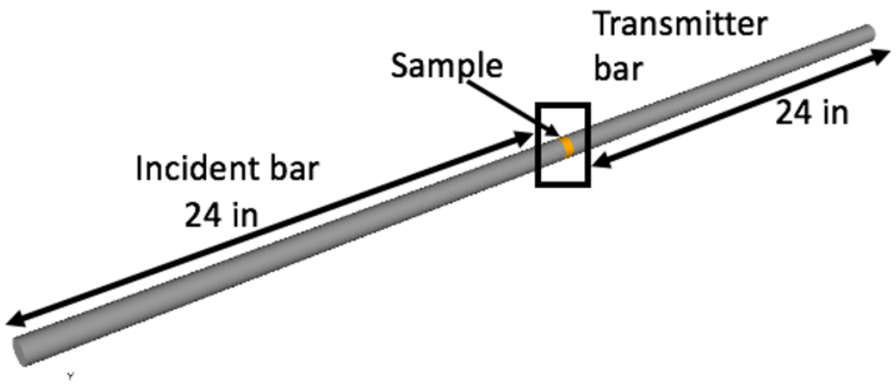
Positive volume strain:
estimated at ~4.6%

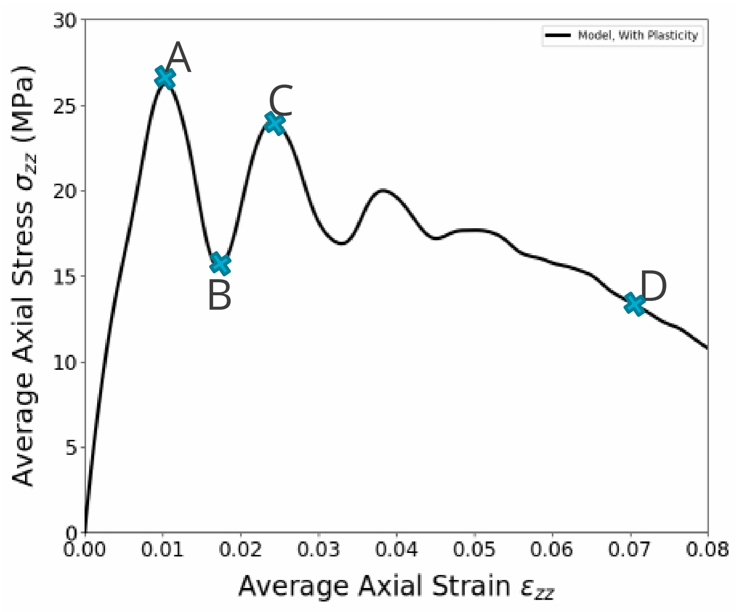


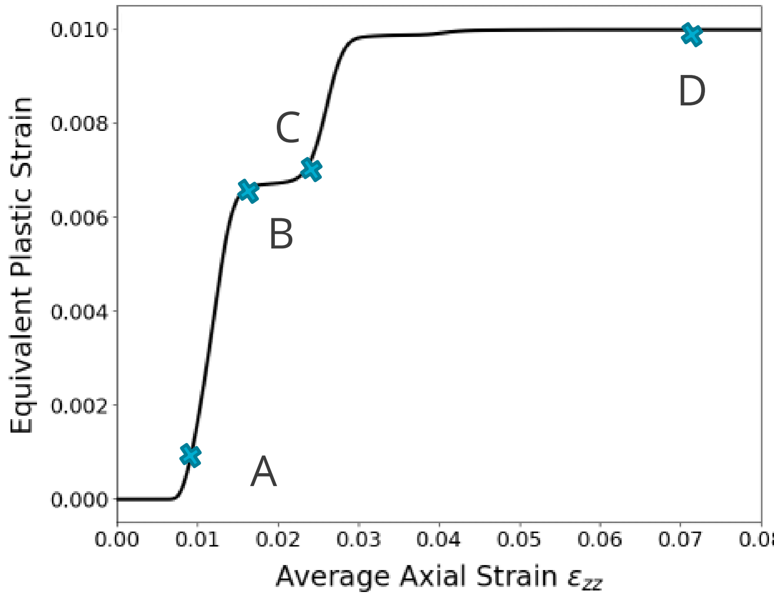


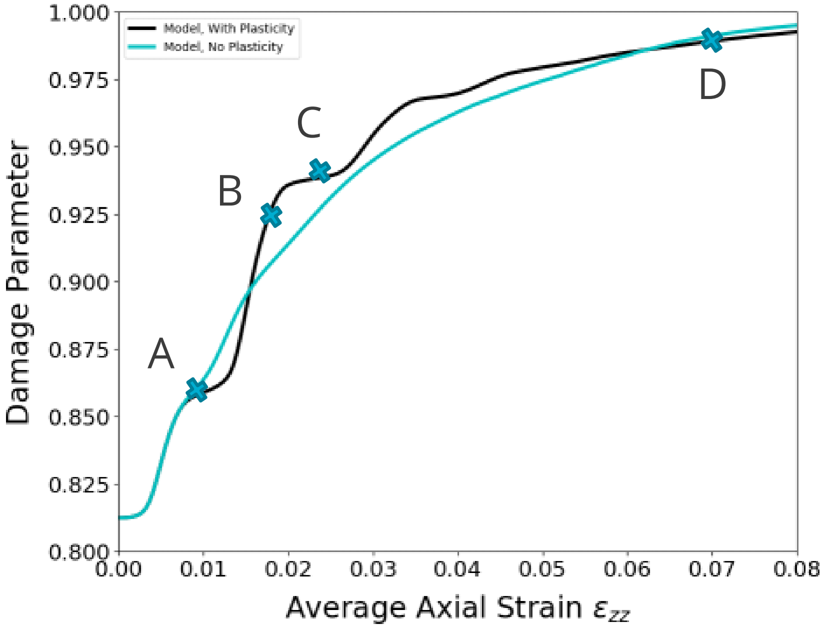
Evolution of SCRAM Damage and Plasticity

- Both SCRAM damage and plasticity are active simultaneously
- Final damage state is the same, but different evolution behavior
- Plastic flow occurs during stress wave oscillations

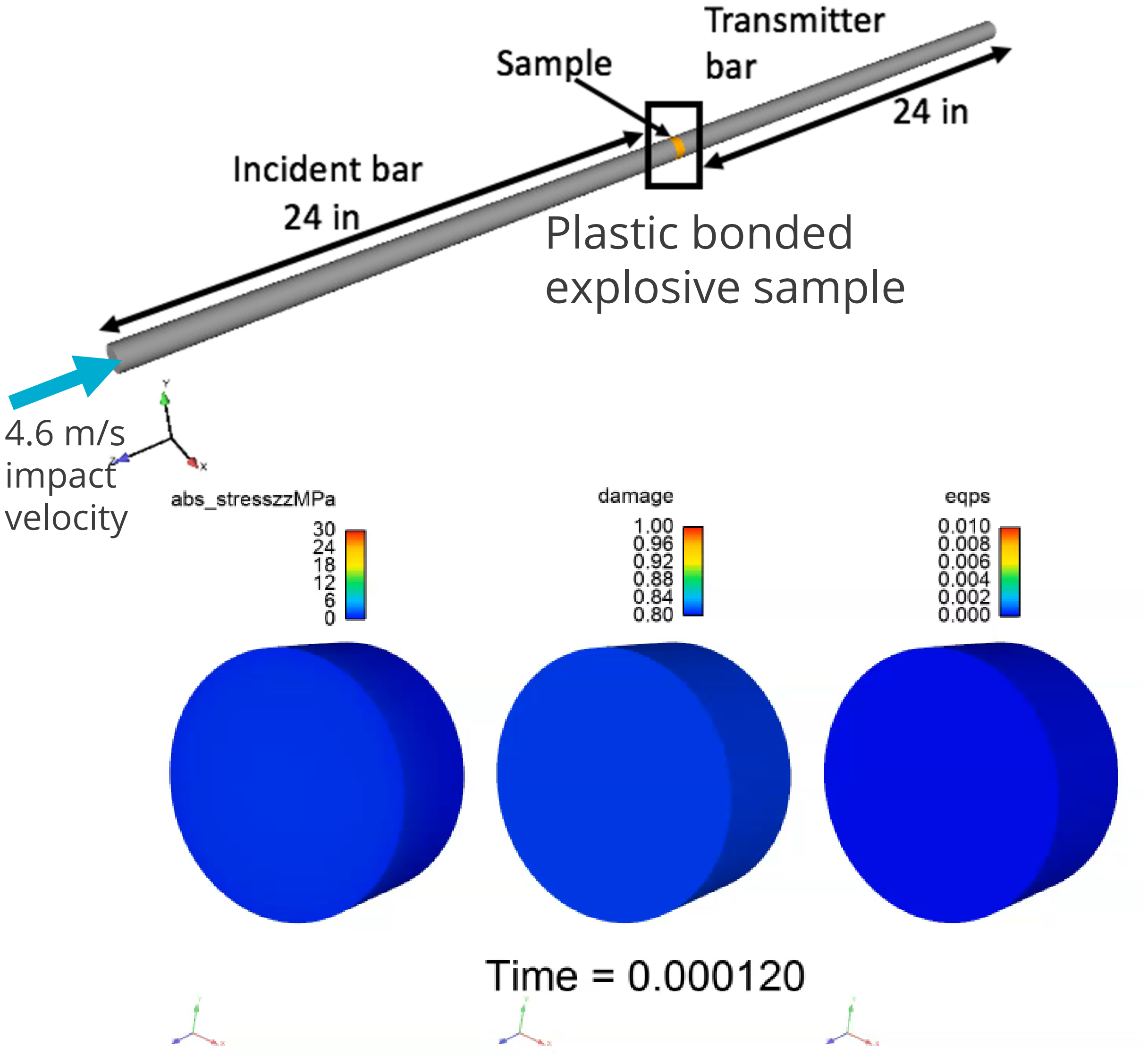


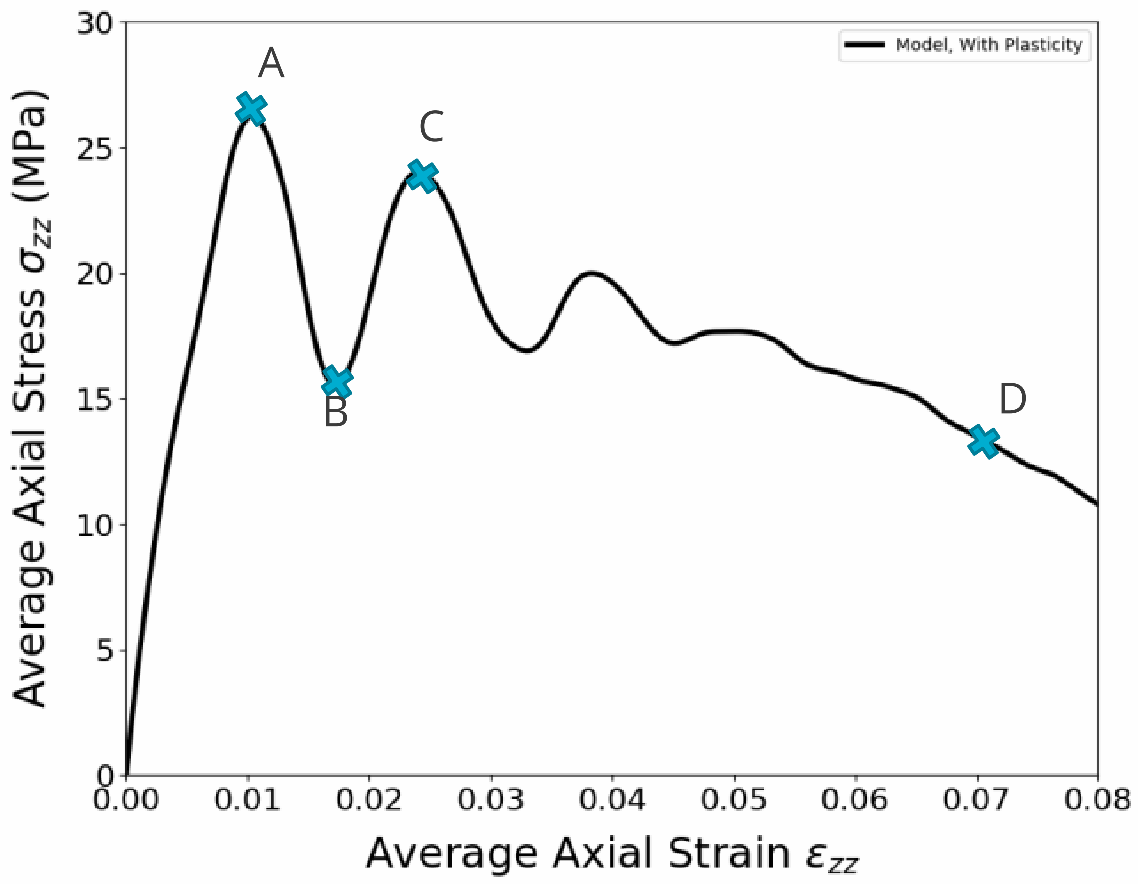




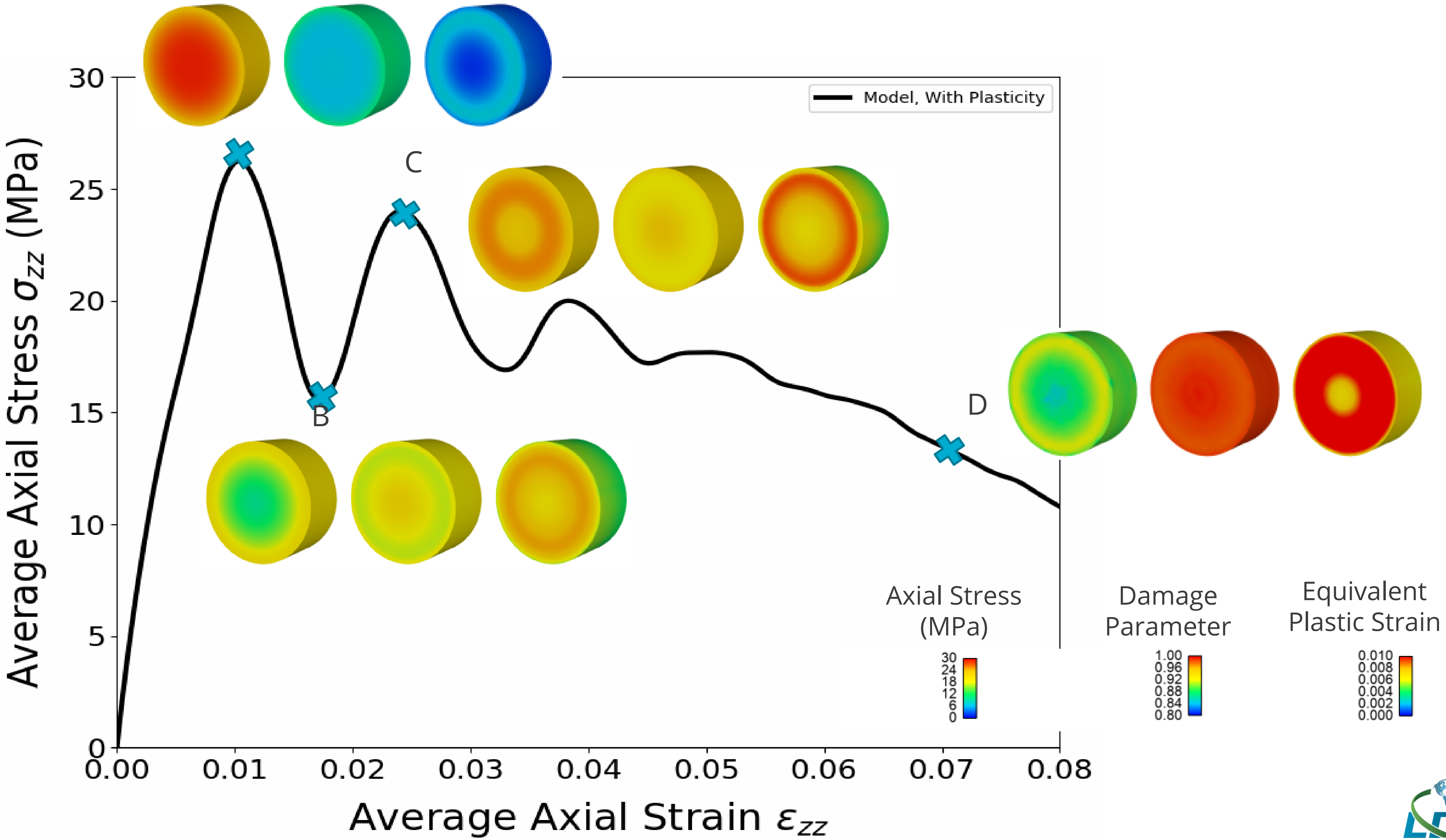


Evolution of SCRAM Damage and Plasticity



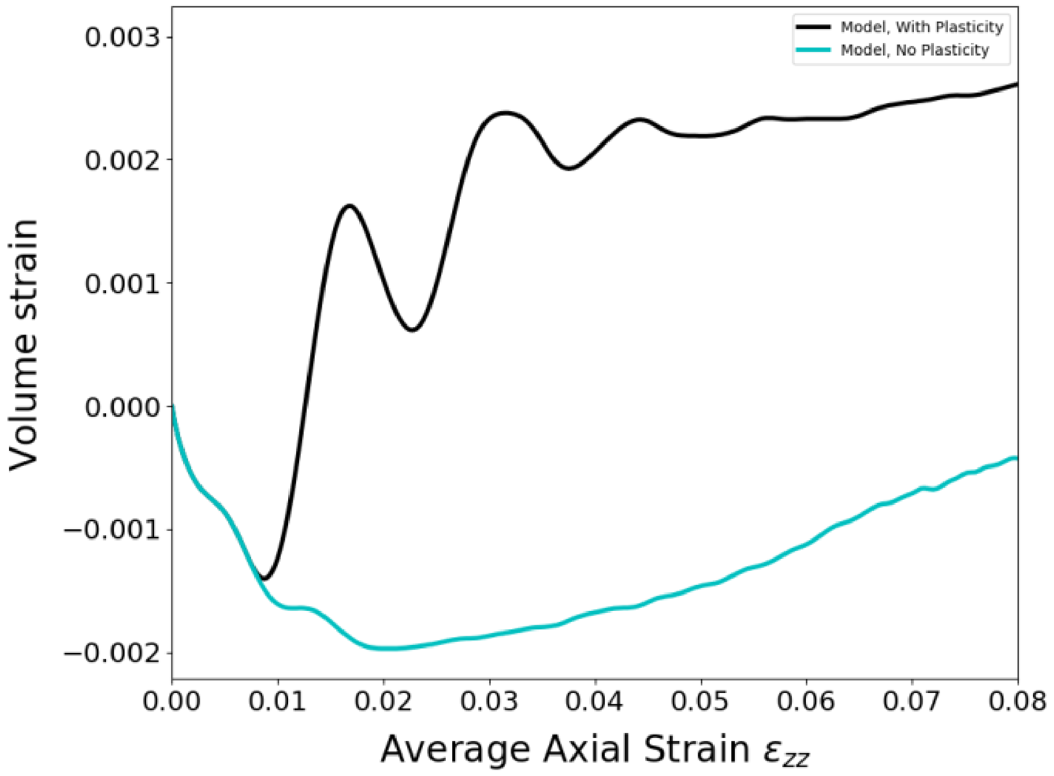


Evolution of SCRAM Damage and Plasticity

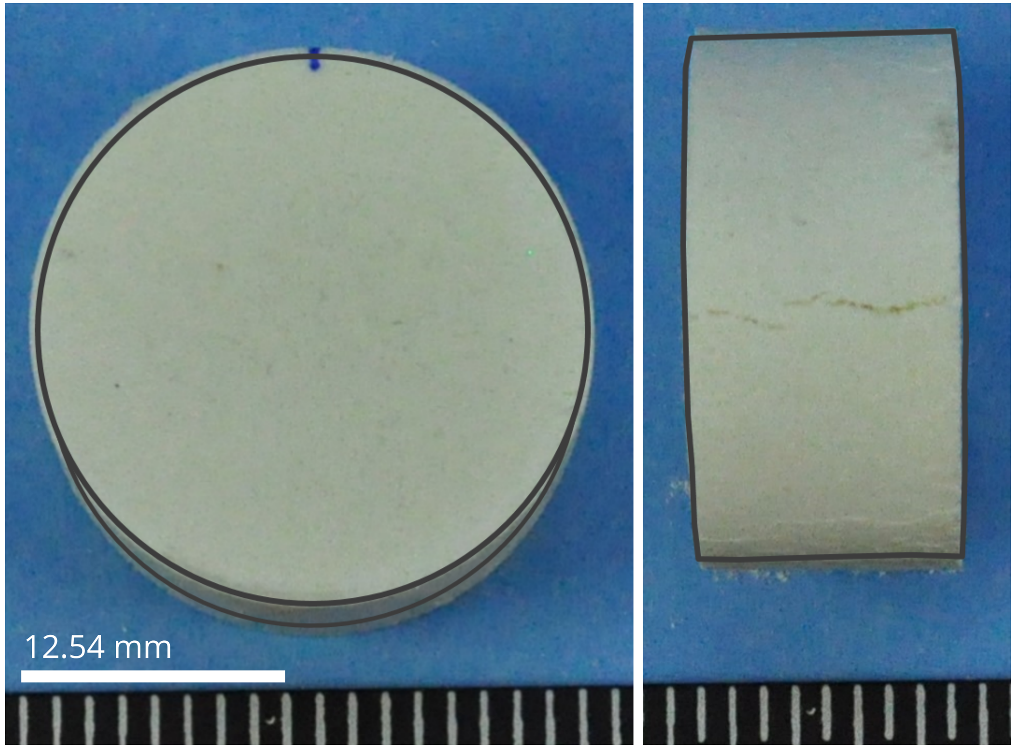


Plasticity allows predictions for net dilatation

- Net dilatation only predicted from model with plasticity
- Volume strain estimated from image analysis of pre- and post-mortem SHPB sample



Positive volume strain: estimated ~4.6%



Meshfree Mesoscale Models

Give insight to mechanical deformation and damage mechanisms under many different stress states

Bonded Particle Models (BPMs)

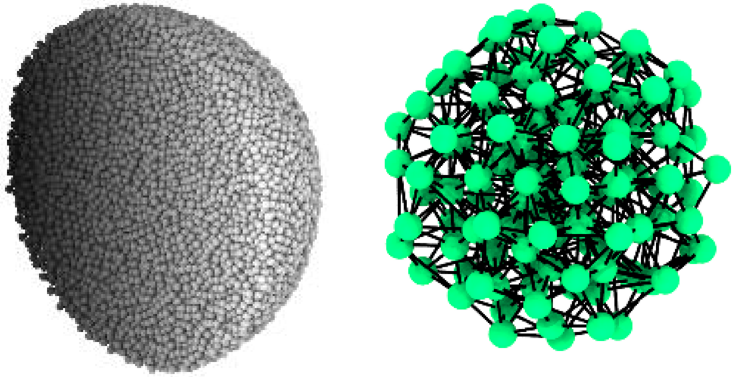
- BPMs are minimalistic particle-based models for fragmentation – ideal for studying trends/testing theories

- Very efficient, can simulate large systems, $\sim 10^3$ grains, at high resolutions, $\sim 10^4$ particles/grain

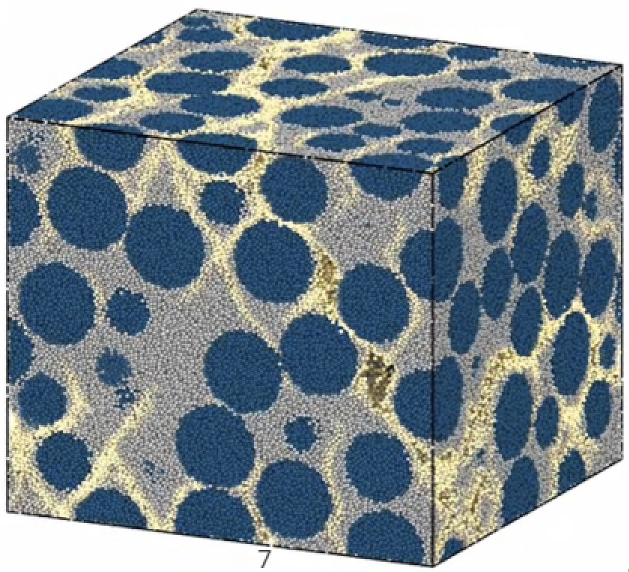
- In BPMs, grain = collection of repulsive particles connected by network of (typically) pairwise bonds
- Bonds break under specific criteria – e.g. stretch threshold
- Functional form of bond controls material properties: moduli, fracture toughness, plasticity, viscoelasticity, …

- Open-sourced models available in recently released LAMMPS package

Grain consisting of $\sim 10^2$ particles



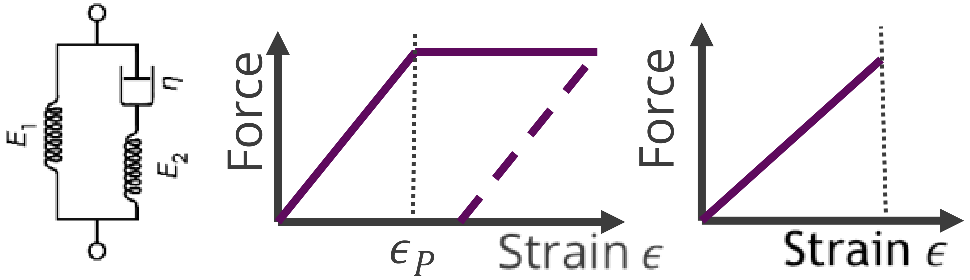
PBX-like composite

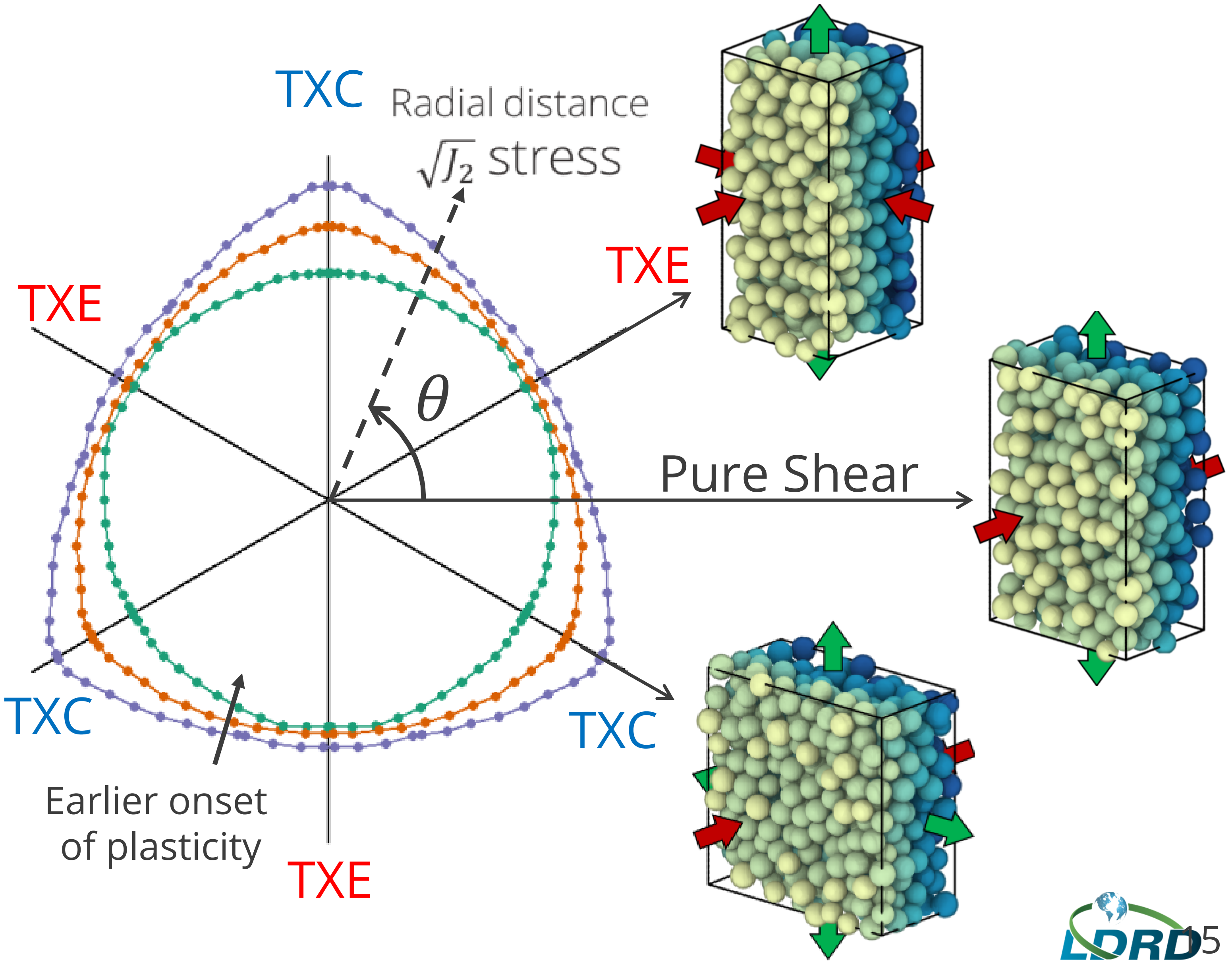


Identifying yield surface shape to inform continuum models

- Many possible loading paths, all have unique failure stress. Map out yield surfaces, often assumed to have simple shape (e.g. Drucker-Prager)

- **Testing how changes in binder's material properties impact yield surface**
  - better understanding of inelastic yielding for continuum models



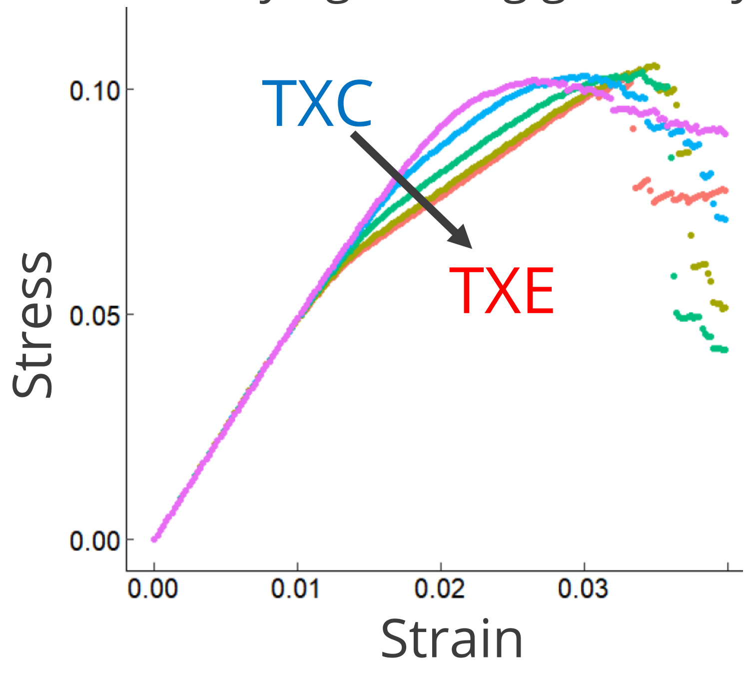


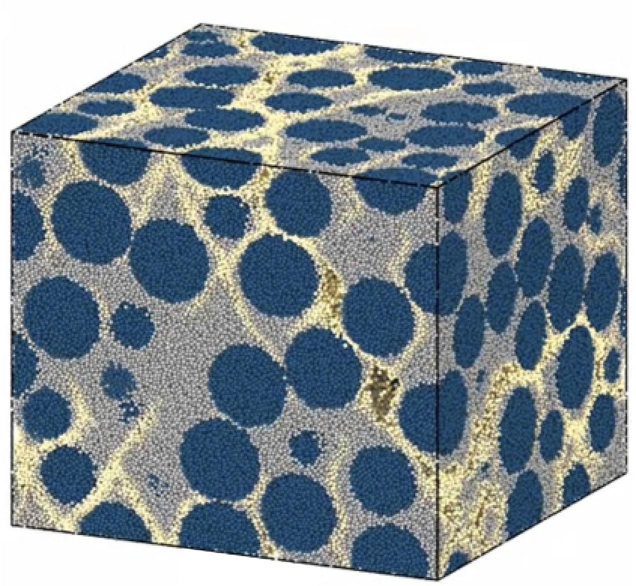
Extending framework to capture damage and crack percolation

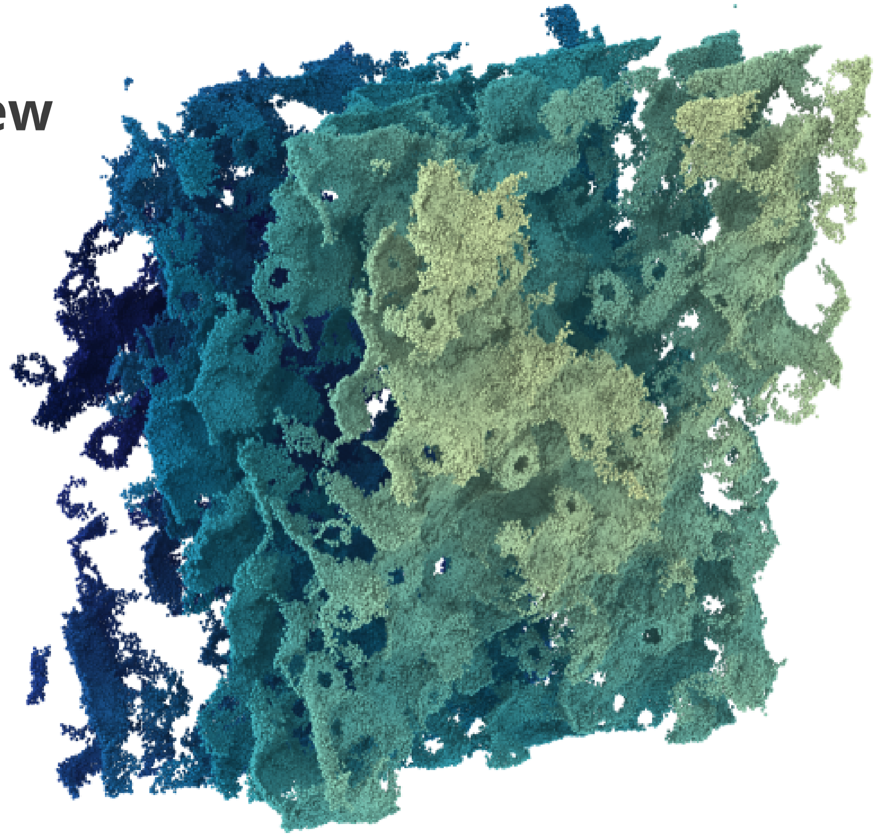
Simulations allow us to identify yield while simultaneously tracking crack growth in binder & quantifying damage

Complete spatial-temporal history of damage provides a new perspective on complex mechanical problems

See emergence of damaged modulus by varying loading geometry







Final percolating crack in binder in pure shear

Conclusions & Ongoing Work

- Multifaceted effort to understand and model mechanical behavior:
  - ViscoPlastic-ViscoSCRAM macroscale constitutive (strength) model with 3 key features: Viscoelasticity + SCRAM damage + viscoplasticity
  - Plasticity is an additional inelastic mechanism that limits stress development in the material which reduces the rate of damage and also produces positive volume strain (dilatation)
  - Improved agreement with intermediate strain rate SHPB test compared to model without plasticity

- Open Research Questions:
  - How best to capture coupling between the various deformation mechanisms (cracking, porosity opening, etc) in the macroscale model?
  - Best practices for calibration?
  - Material failure criterion—F(damage), F(plasticity), F(both)??
  - Mesoscale bonded particle models provide insight to deformation mechanisms, shape of yield surface, etc.

Thank You!

Extra Slides

ViscoPlastic-ViscoSCRAM Model Theory

- Solution Algorithm:

(1) After converging at time t_n, input:
  Time and strain increments: $\Delta t, \Delta\boldsymbol{\epsilon}$
  Stress state: $\boldsymbol{s}_n, (\sigma_m)_n, \boldsymbol{s}_n^{(\kappa)}$
  Damage variable: c_n
  Functions of the damage variable: $\psi_n, \theta_n, \boldsymbol{\Lambda}_n$
  History variable: $\boldsymbol{\epsilon}_n^p$

(2) Viscoelastic predictor:
  Initialize plastic flow increment: $\Delta\lambda = 0$
  Compute: $\boldsymbol{\sigma}_{n+1}^{TR}$ from (37), (34) and (24)
  Compute: $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{TR}$
  Compute: $\boldsymbol{\epsilon}_{n+1}^p = \boldsymbol{\epsilon}_n^p$

(3) Yield surface check:
  IF $f(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\epsilon}_{n+1}^p, D_n) > 0$, THEN GOTO (4)
  ELSE GOTO (5)
  ENDIF

(4) Viscoplastic corrector:
  Solve for $\{\boldsymbol{\sigma}_{n+1}, \boldsymbol{\epsilon}_{n+1}^p\}$. See Box 2 for return map algorithm.

(5) Damage variable, Maxwell stress, damage rate, and damage variable functions updates:
  Update: c_{n+1} from (27)
  Update: $\boldsymbol{s}_{n+1}^{(\kappa)}$ from (29)
  Update: $\dot{c}_{n+1}$ from (7)
  Update: ψ_{n+1} from (18)
  Update: θ_{n+1} from (19)
  Update: $\boldsymbol{\Lambda}_{n+1}$ from (20)