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# Mesomechanics of Highly Filled, Polymer-Bonded Granular Composites

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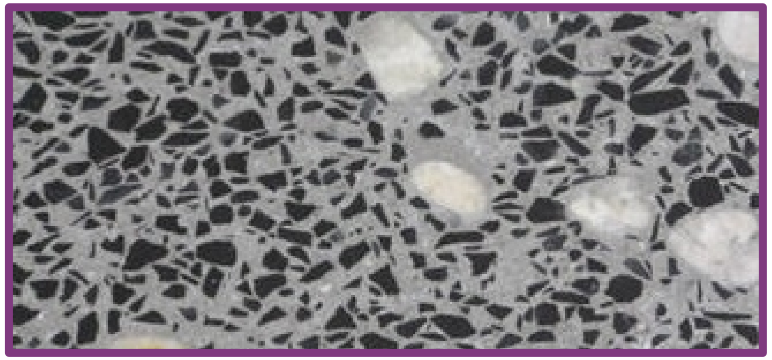
# Polymer bound granular composites

Many instances in industry:

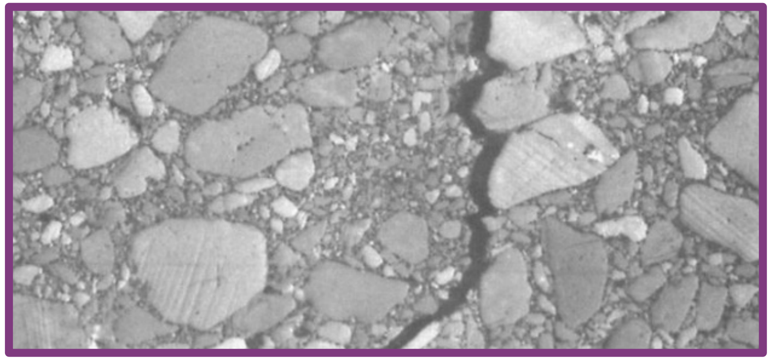
- Concrete, asphalt
- Polymer-bonded explosives
- 3D binder jet additive manufacturing
- Electrically conductive adhesives for soldering

Complex mechanics:

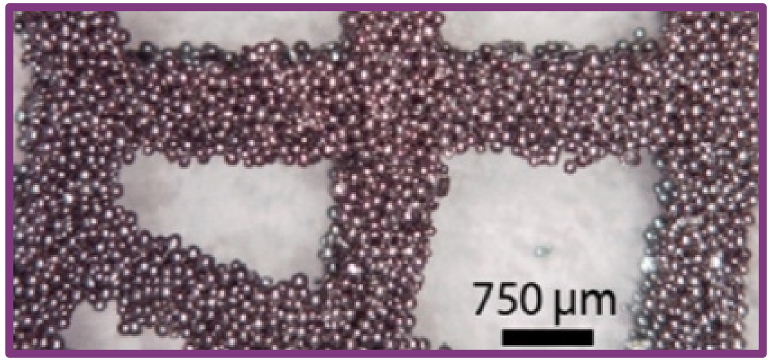
- Highly heterogeneous, granular vs. polymer
- Phases often have markedly different properties
- Length scale of each can be very different, $\sim 10^3\!:\!1$



Polished concrete (Wikipedia)



PBX microstructure $\sim 1\ \mathrm{mm}$
(PJ Rae *Proc. R. Soc. Lond. A.* 2002)



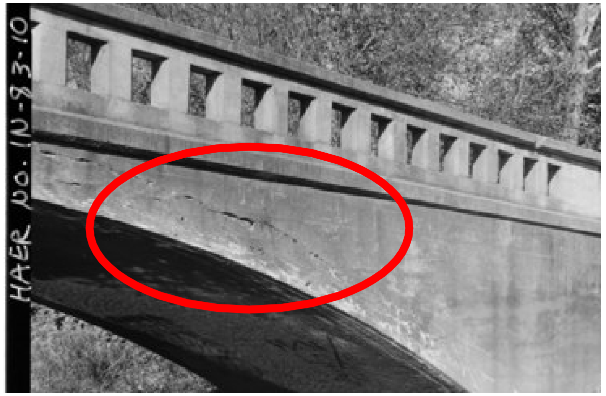

3D printed binder jet structure
(K. Lu *Powder Tech.* 2009)

# Predicting damage and failures is crucial

Transportation

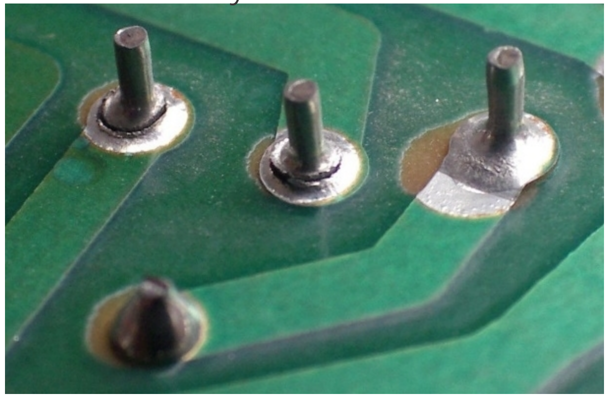
commons.wikimedia.org/wiki/File:Pothole_Big.jpg

Construction




www.loc.gov/pictures/item/in0447.photos.374550p/

Reliability of electronics



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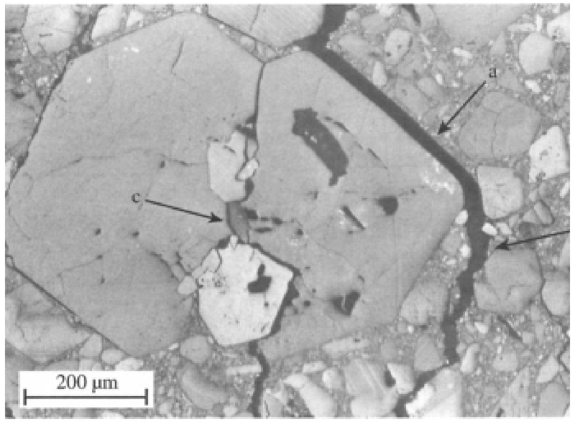
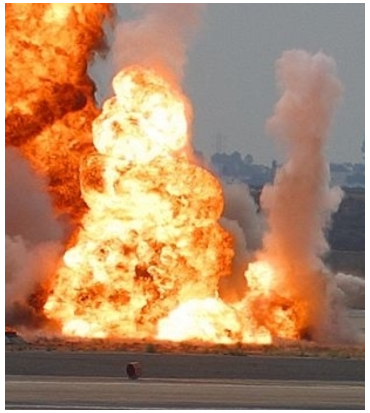
Food industry - tactile response

commons.wikimedia.org/wiki/File:Nestle-crunch-broken.jpg




PJ Rae *Proc. R. Soc. Lond. A.* (2002)

Safety in damaged components

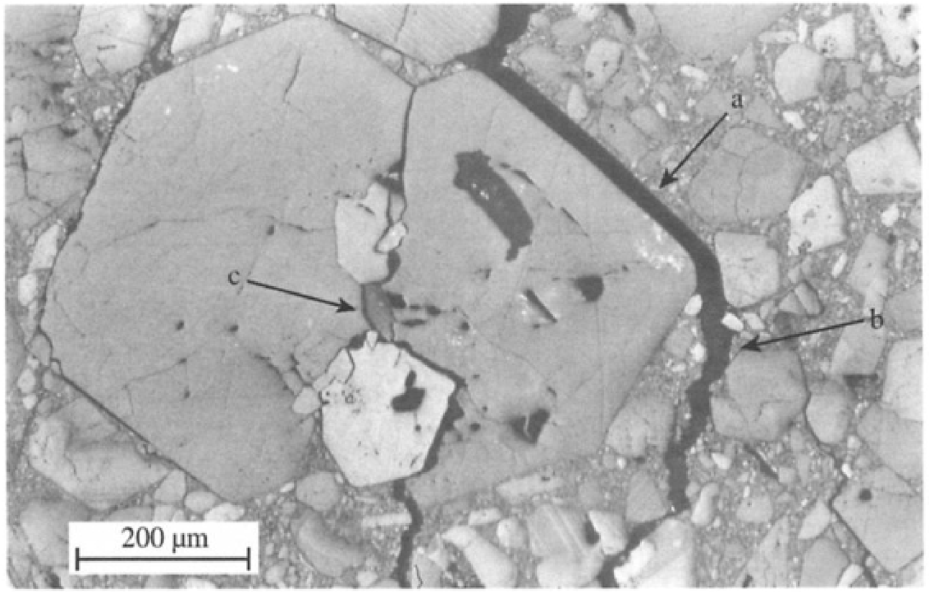


commons.wikimedia.org/wiki/File:Explosions_at_Miramar_Airshow.jpg

**How does manufacturing profess/design decisions affect mechanical response?**

**Goal**: Develop a robust computational micromechanics capability to simulate emergent macroscale phenomena from known microstructural and constituent material inputs

# Challenges in modeling failure




PJ Rae Proc. R. Soc. Lond. A. 2002

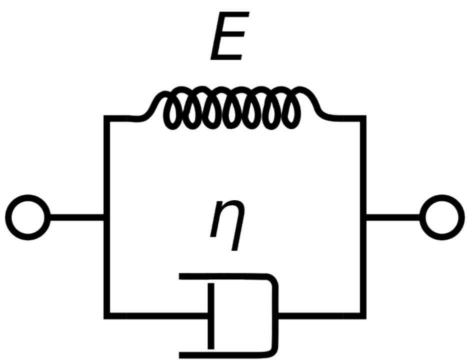
- Many physical mechanisms:
  - Plasticity/viscoelasticity in binder (or grains)
  - Rotation/delamination/friction in grains
  - Crack nucleation, growth, coalescence
- Variety of length scales
  - Failure often dominated by binder phase:
    Can be much smaller/thinner than grains
  - Macro response depends on 100s-1000s of grains
    Need to simulate an representative sample
- Mechanics of micron-sized grains may be dominated by defects, not well described by bulk material model
- Don’t always have material models for constituent phases
- Oodles of discontinuities

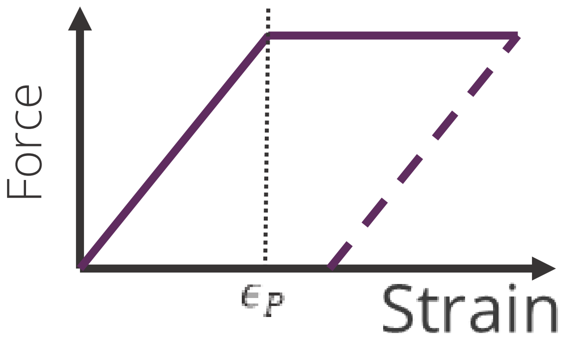
# Bonded Particle Model (BPM)

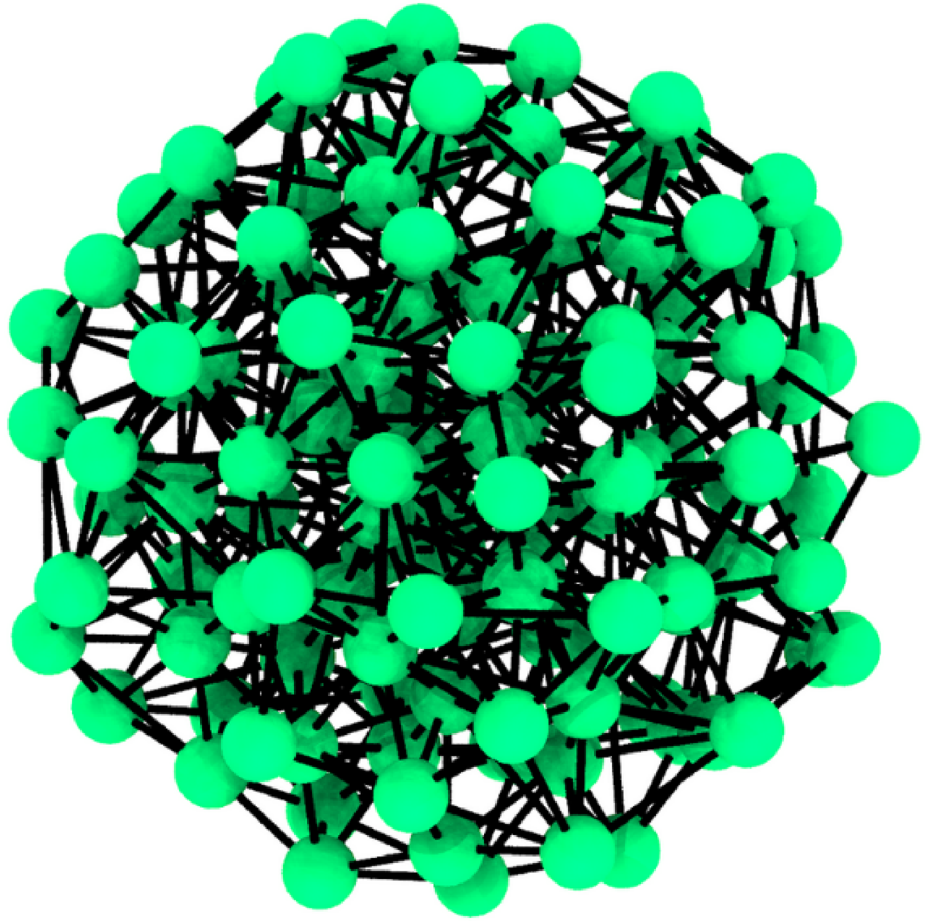
Lagrangian material points connected by a breakable network of bonds, AKA a spring network

Solve Newtonian equations while obeying symmetries
⇒ Physics-based approach, focus on emerging behavior

Ideal for studying trends in abstract material classes, vary details of bond forces to capture different physics



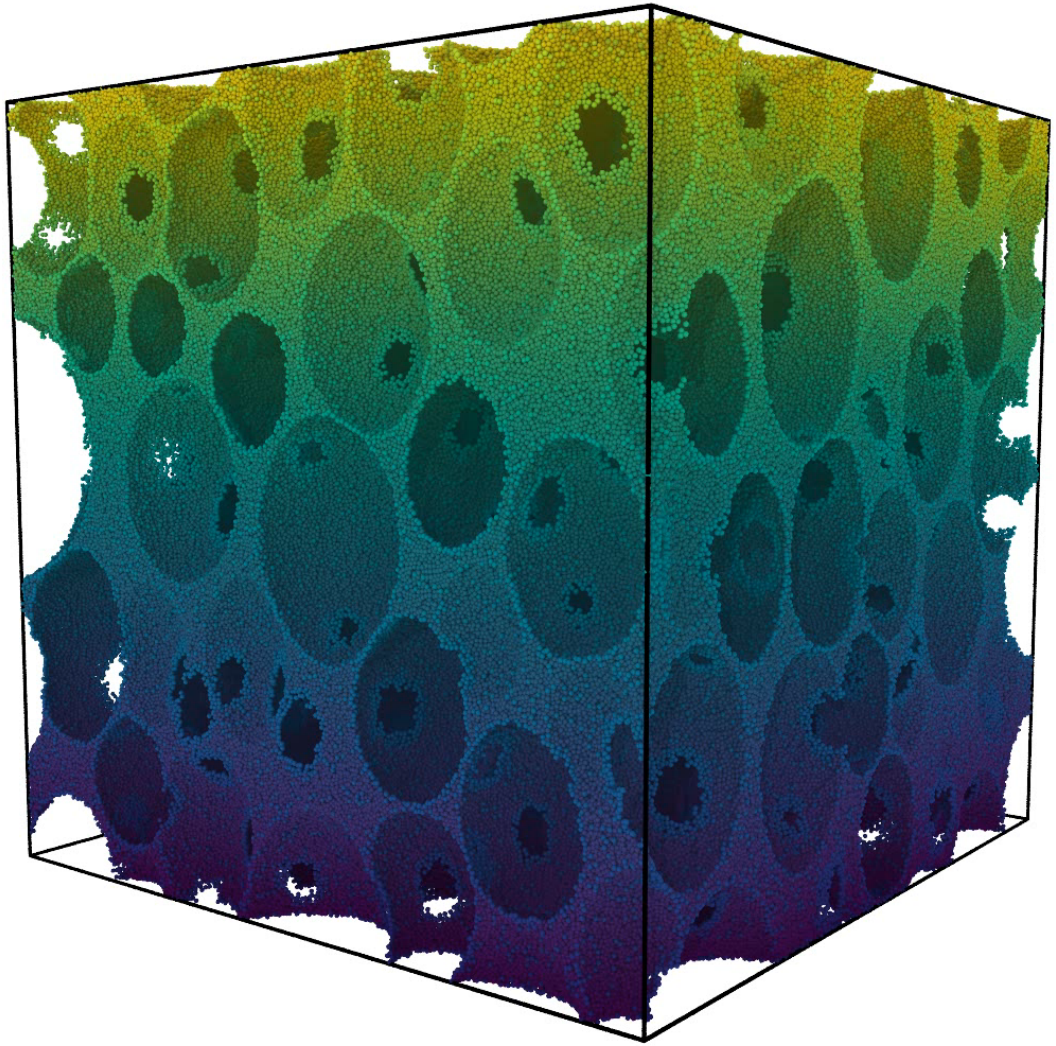
Unbonded particles repel with various contact forces

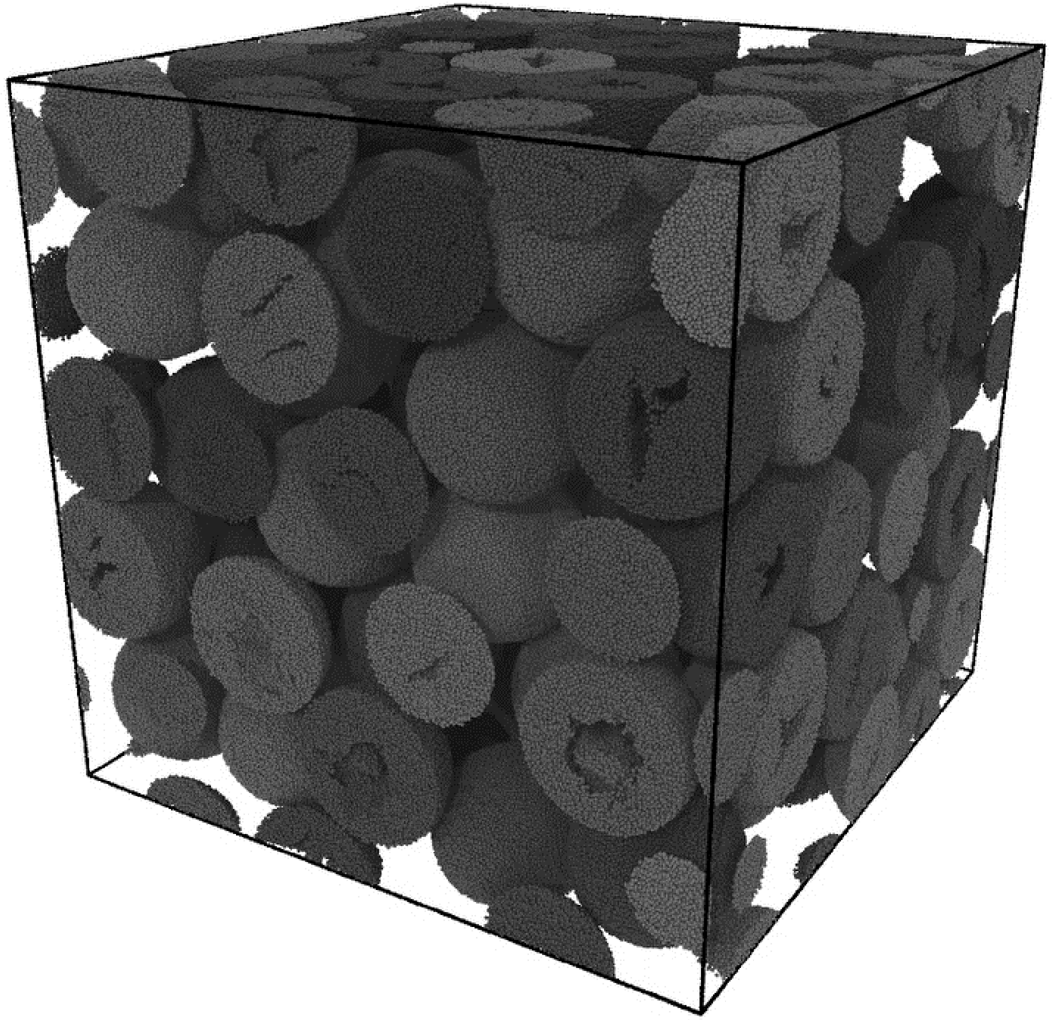
Implemented in LAMMPS, efficient and scales well

# Advantages of approach

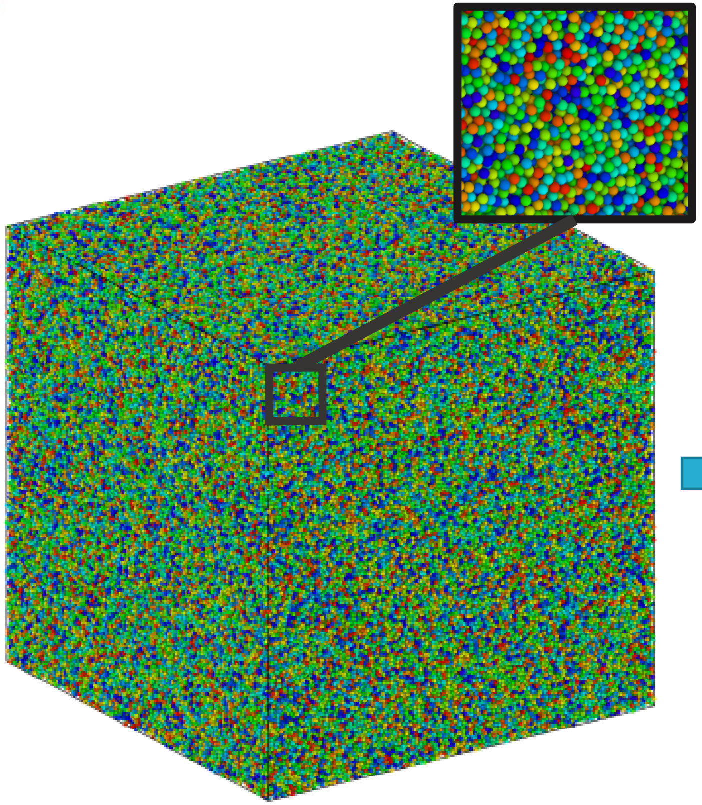
Simple and computationally cheap – can simulate large domains at high resolution

Stably handles large deformation, complex cracking/fragmentation, etc.

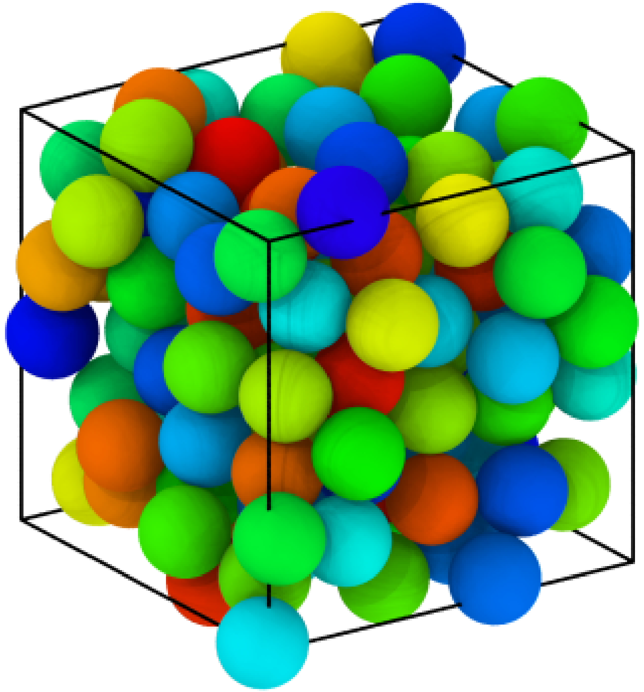




# Constructing composite mesostructures



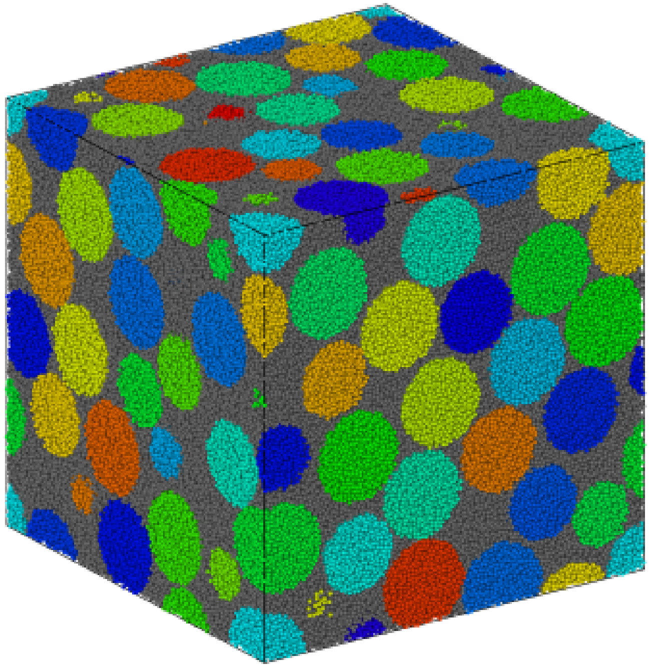
Create disordered packing of
~ $10^7$ BPM nodes/particles



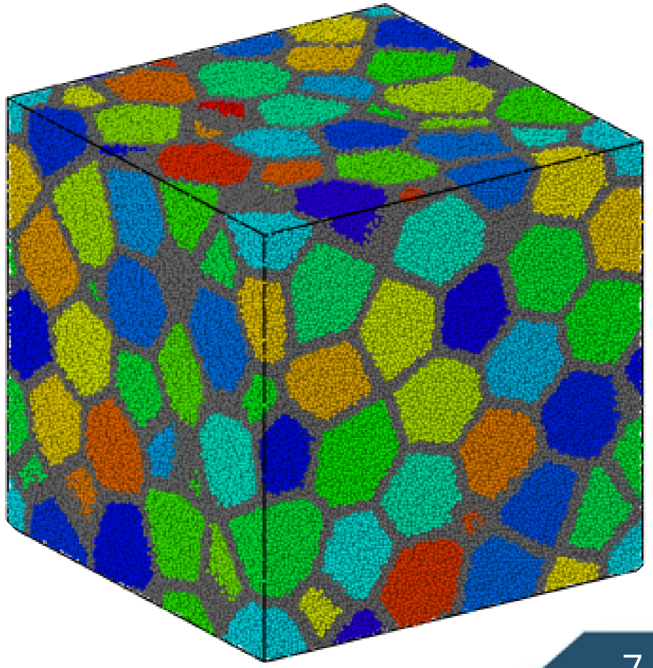
Generate locations of grains

Template for mesostructure

Spherical grains
64% vol fraction



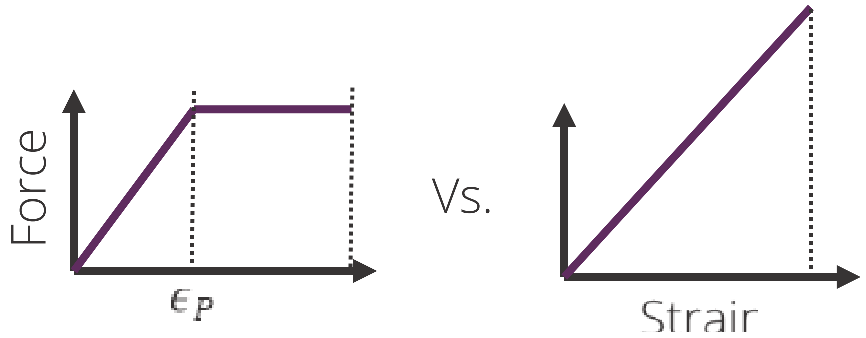
Voronoi cells
78% vol fraction



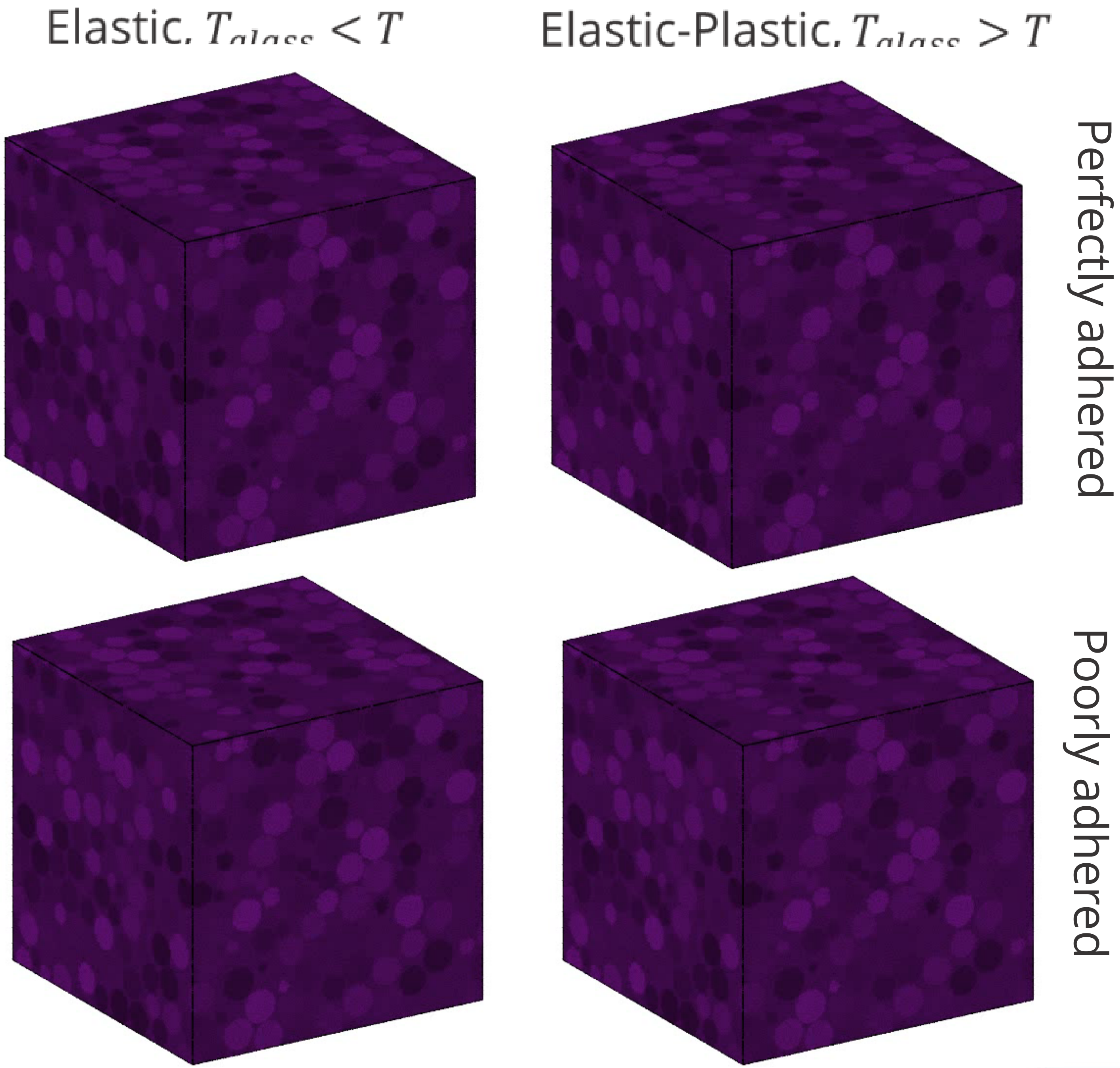
# Idealized material models

Consider 2 axes:

1. $T_{glass}$ of binder relative to operating temperature $T$
   I.e. adjust plasticity of binder bonds




1. Interfacial adhesion strength
   I.e. adjust strength of binder-grain bonds

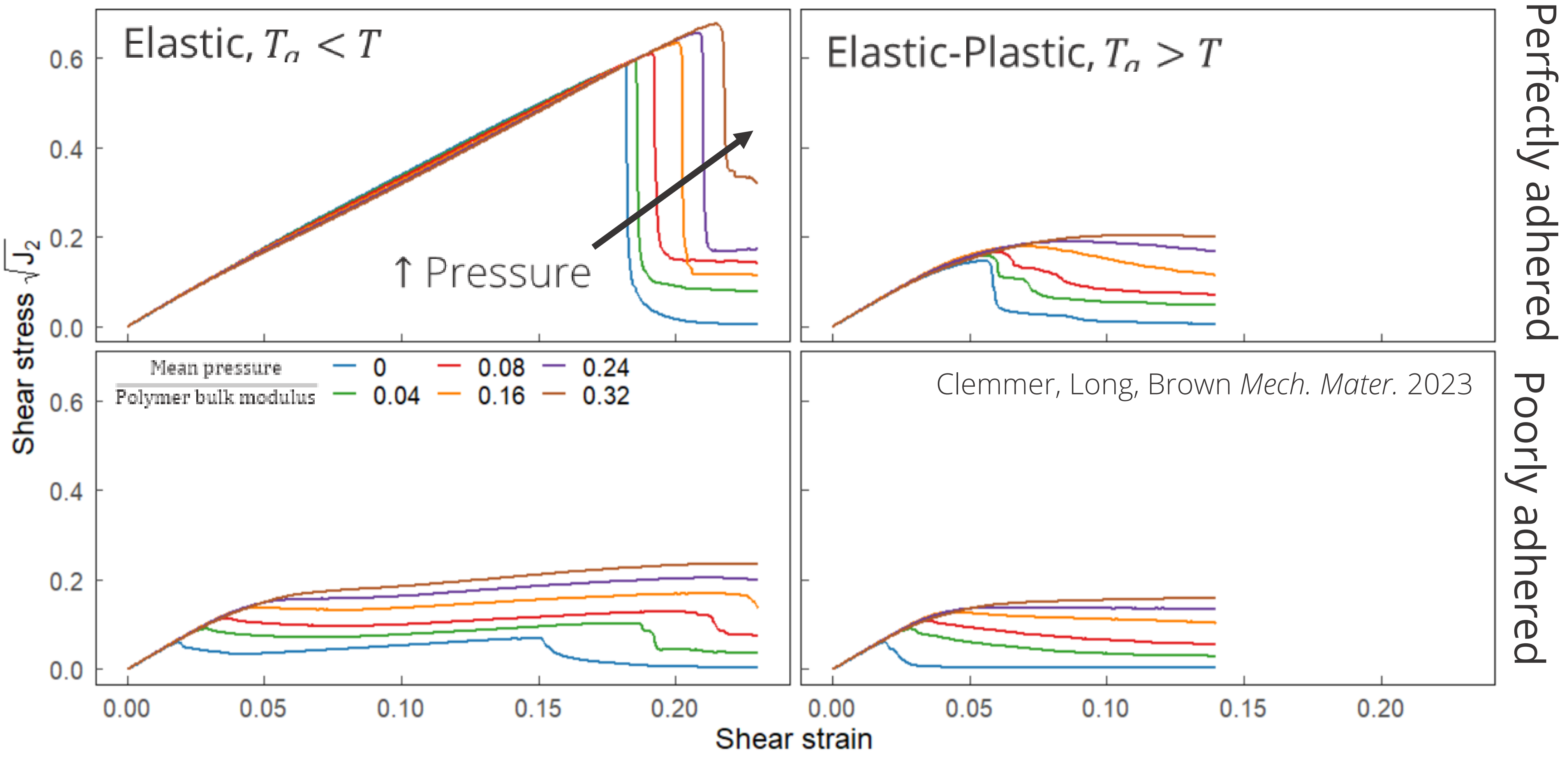



Color indicates # of broken bonds, ~Damage

# Pressure dependent mechanical response

Spherical grain systems, failure under triaxial compression at constant mean pressure

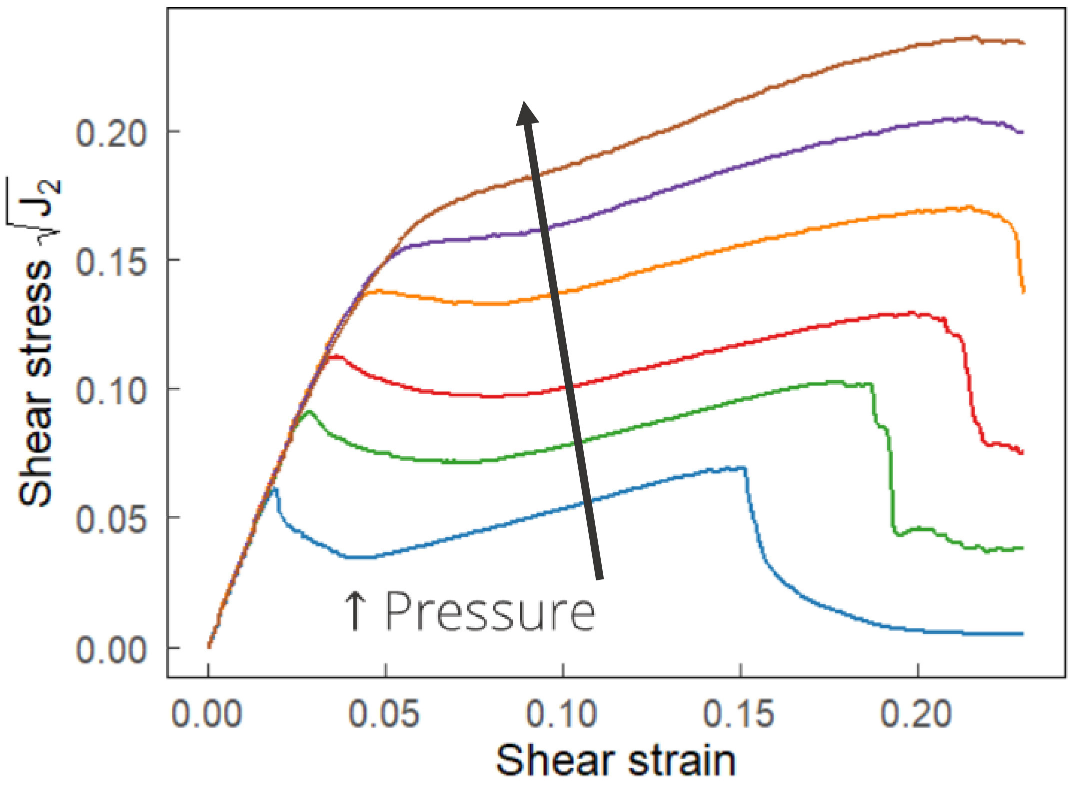
Can we explain how this complex behavior is governed by material inputs?



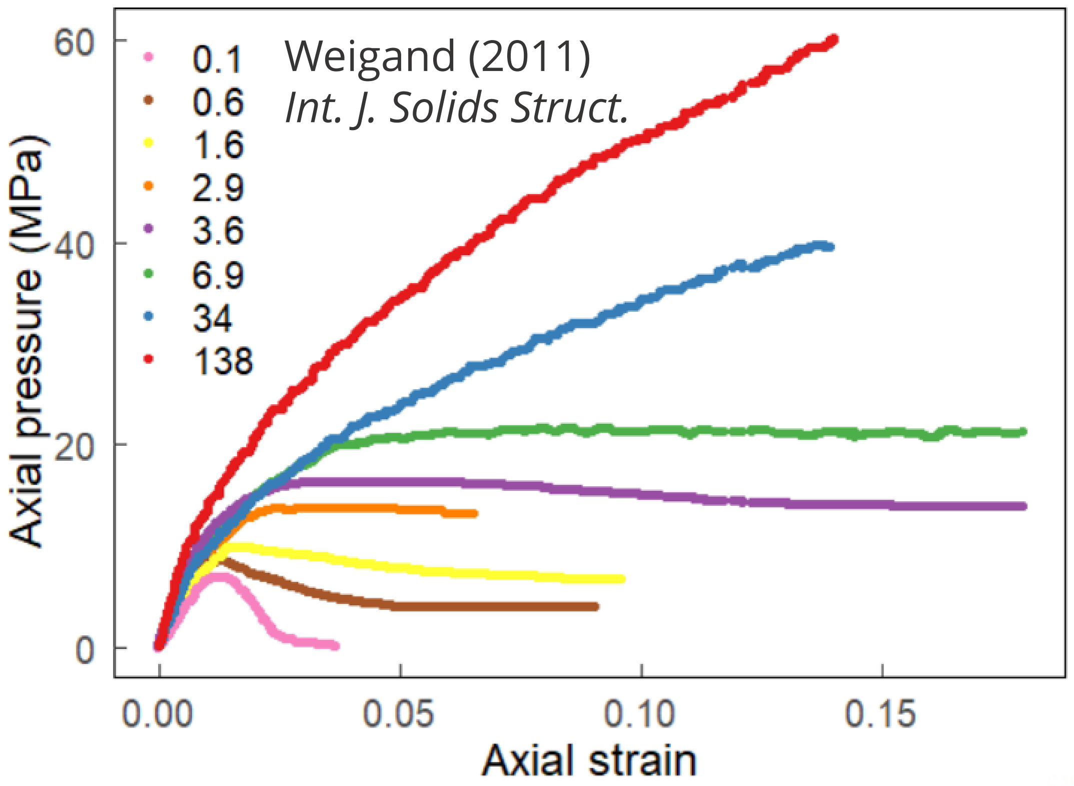
# Experimentally consistent results

In low$-T_{glass}$ limit, capture disappearance of strain-softening regime with increasing pressure

Elastic, $T_g < T$, poorly adhered

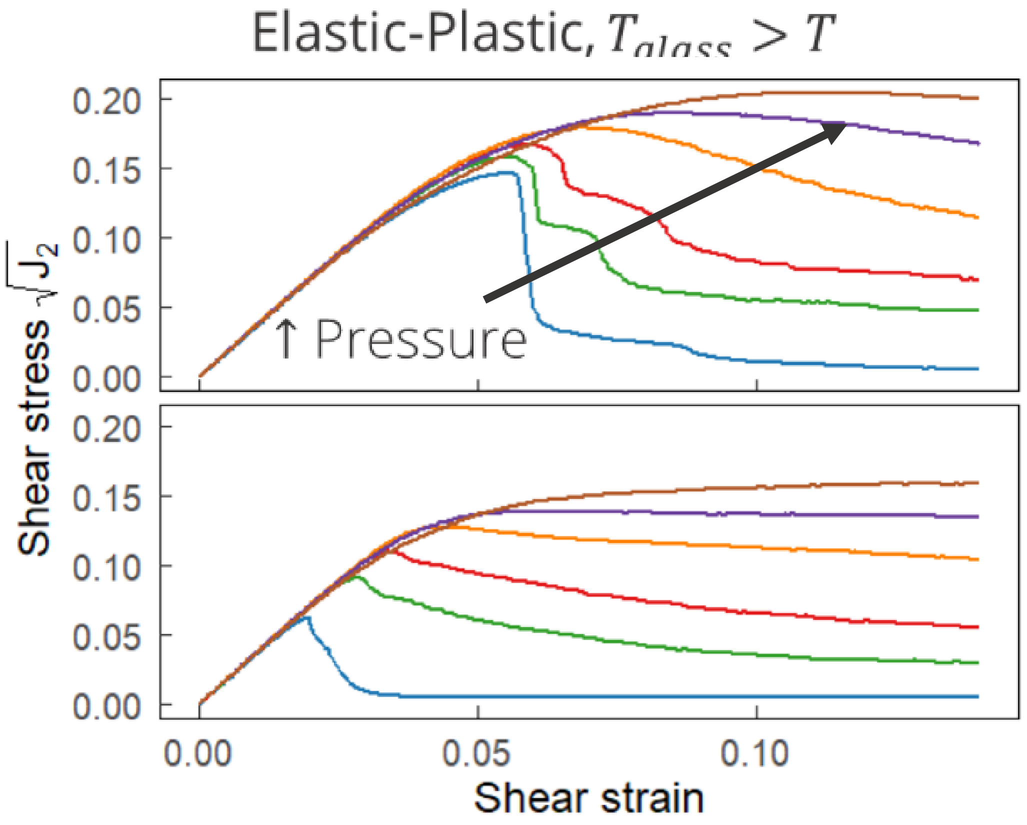


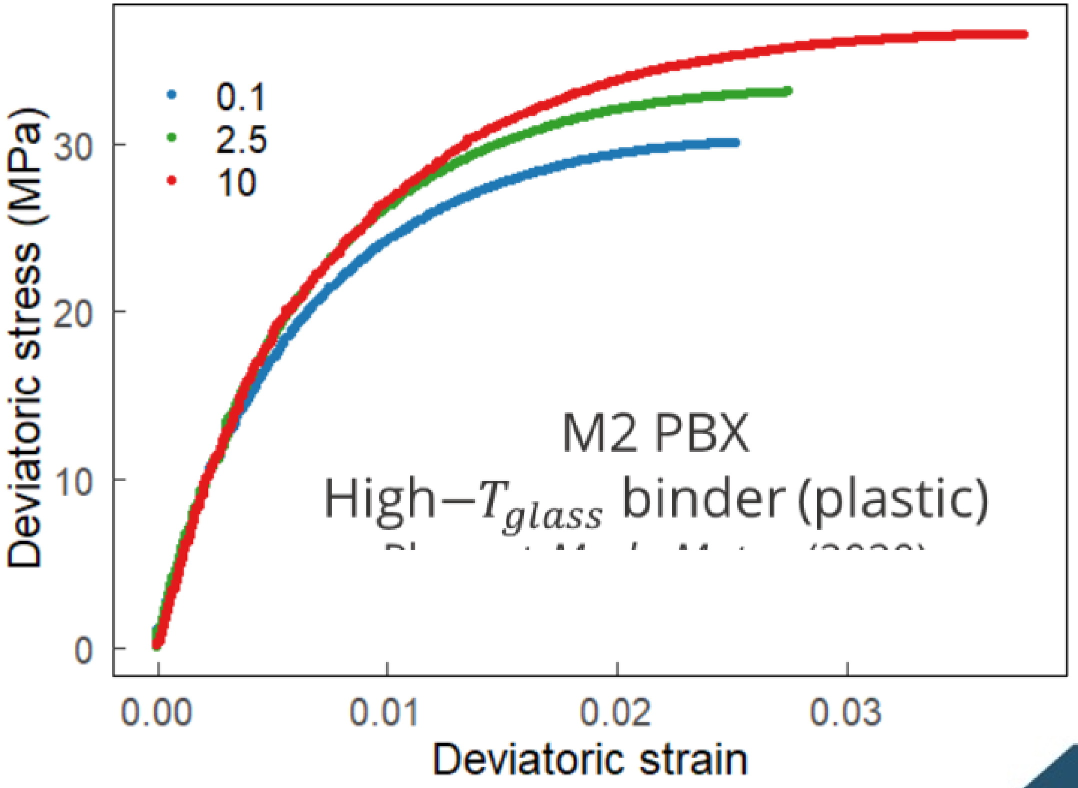

EDC PBX, low$-T_{glass}$ binder (elastic)



# Experimentally consistent results

In high$-T_{glass}$ limit, identify similar shift in yield/failure with increasing pressure, also capture transition from small-strain compressive volume strain to dilation post yield (not shown)



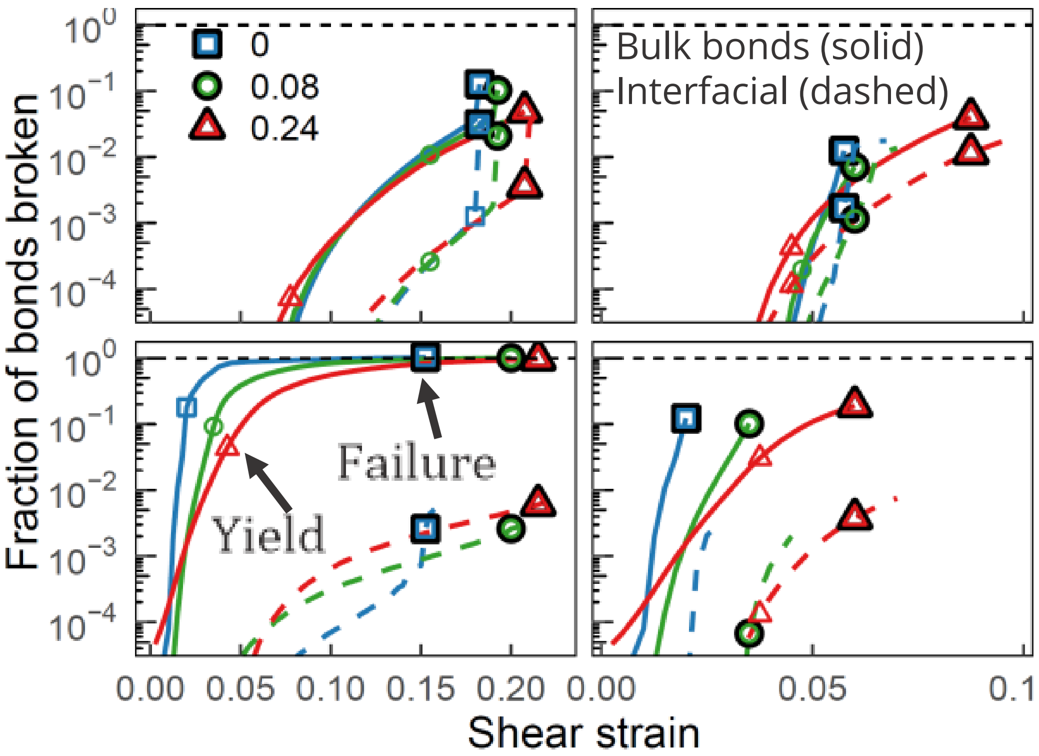



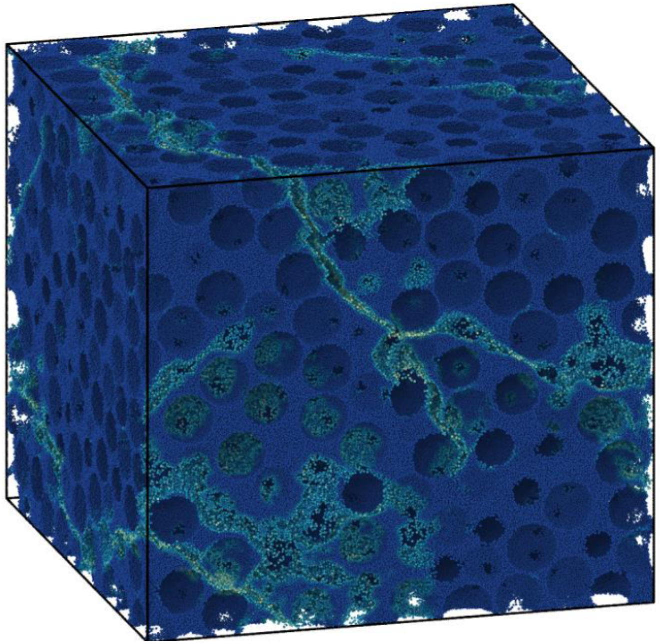
# Tracking microscopic activation of inelastic mechanisms

Demonstrated method reproduces key experimental findings

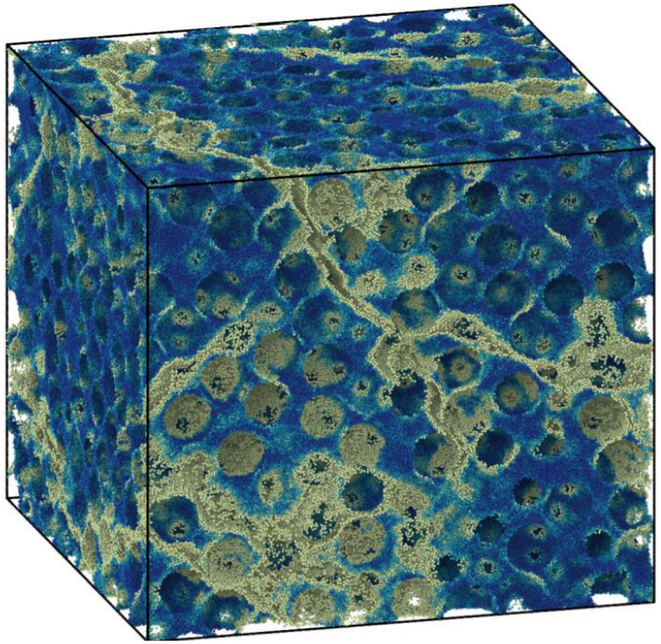
Use full access of microscopic dynamics to identify inelastic origin of key features/transitions on macroscopic stress strain curves

e.g. delamination of binder-grain interfaces leads to strain softening regime at low pressures



Broken bonds



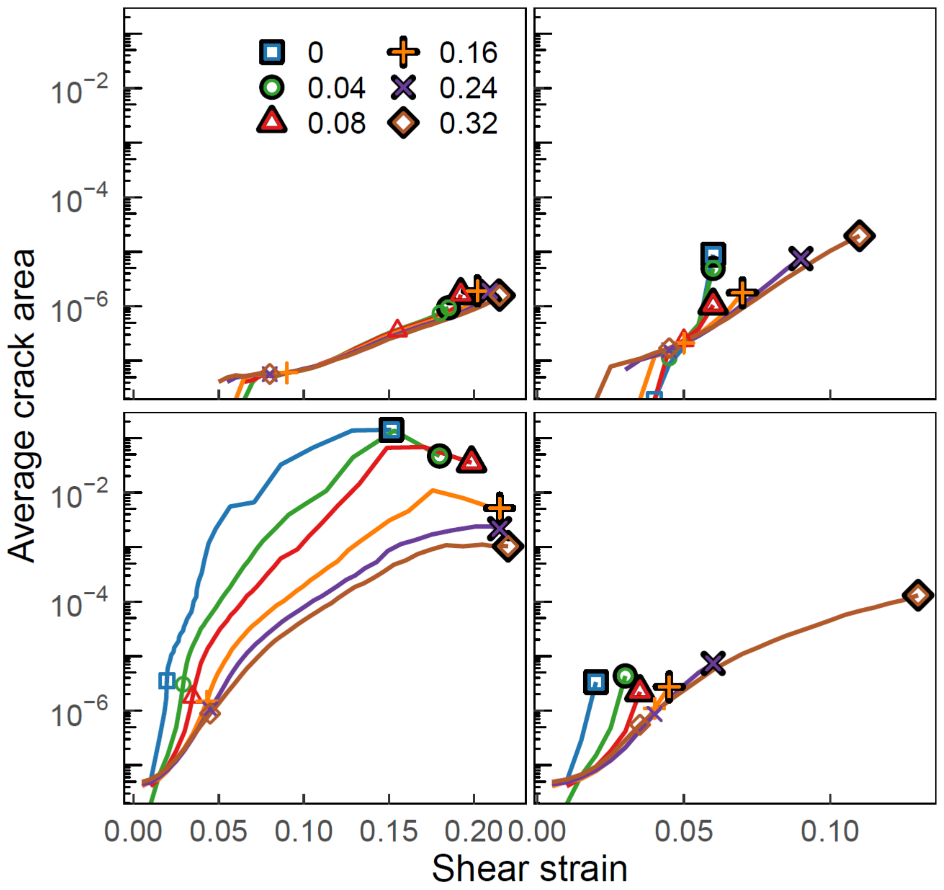
Plastically activation

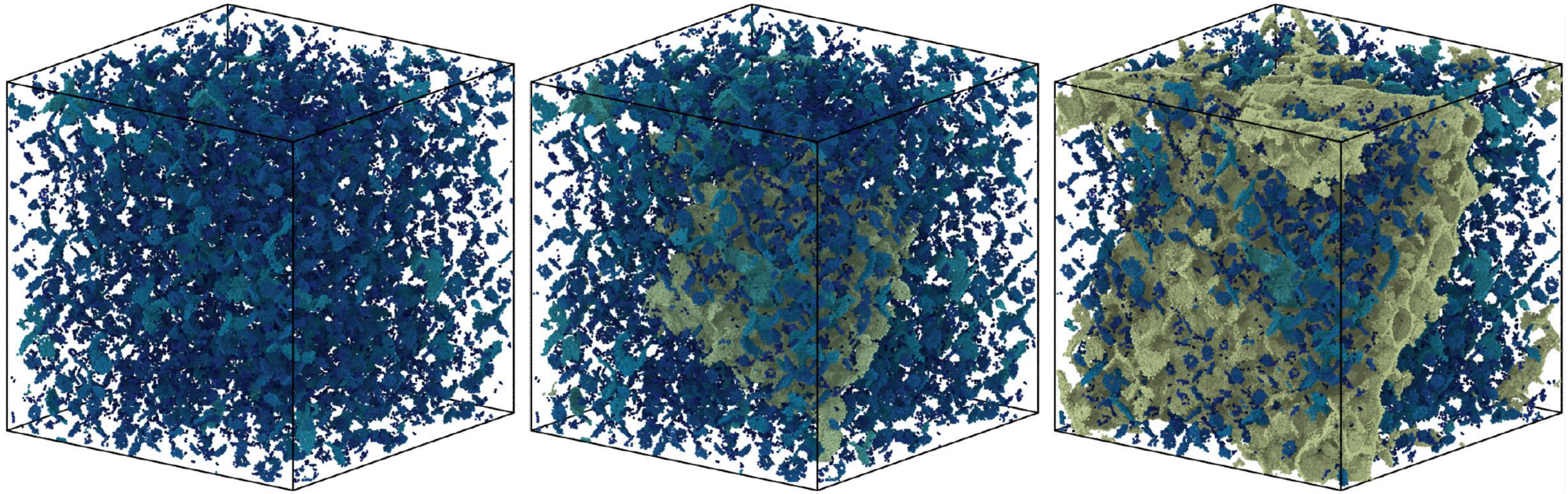
# Exploring mesoscopic crack dynamics

Continuum models of PBX utilize damage metrics to capture degradation in mechanical performance with deformation due to cracking

Long term goal to evaluate accuracy of such metrics by tracking evolution of crack-size distribution

Initially, see expected results: pressure suppresses crack growth



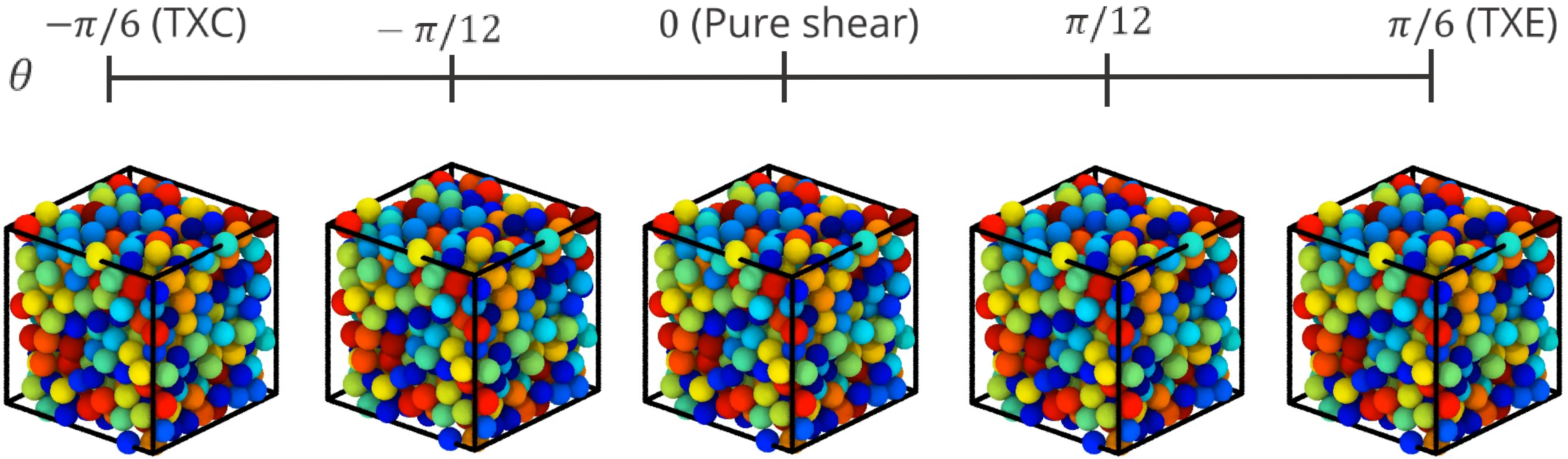
Identify distinct cracks by spatially clustering broken bond locations

Perform at regular strain intervals

# Current focus: yield/failure surface

Need to predict performance under diverse loading conditions

Continuum modeling often assumes no dependence on direction of applied shear (Drucker Prager)

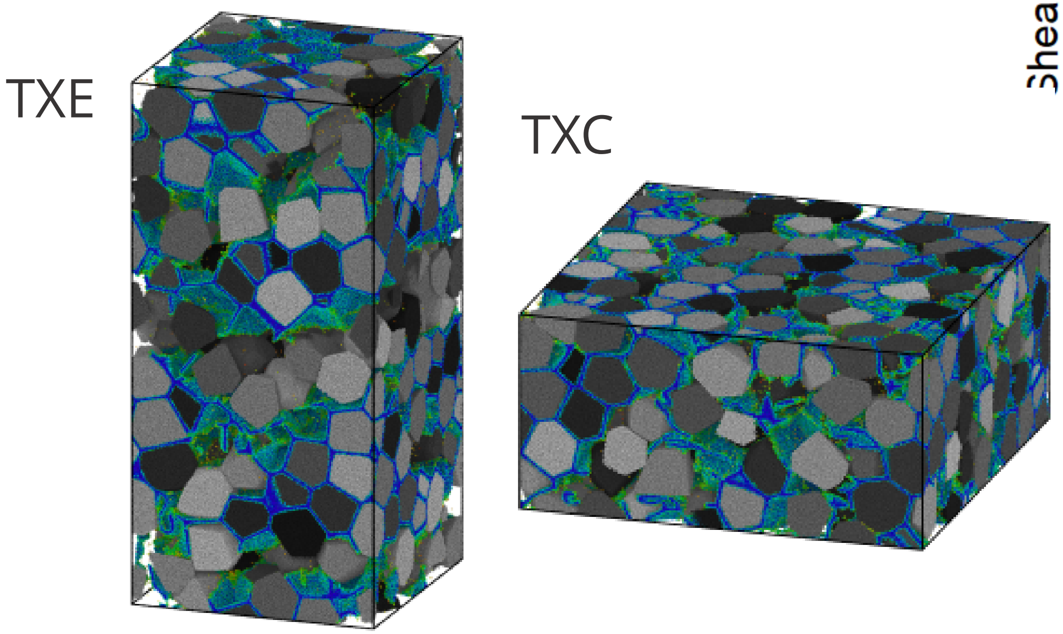


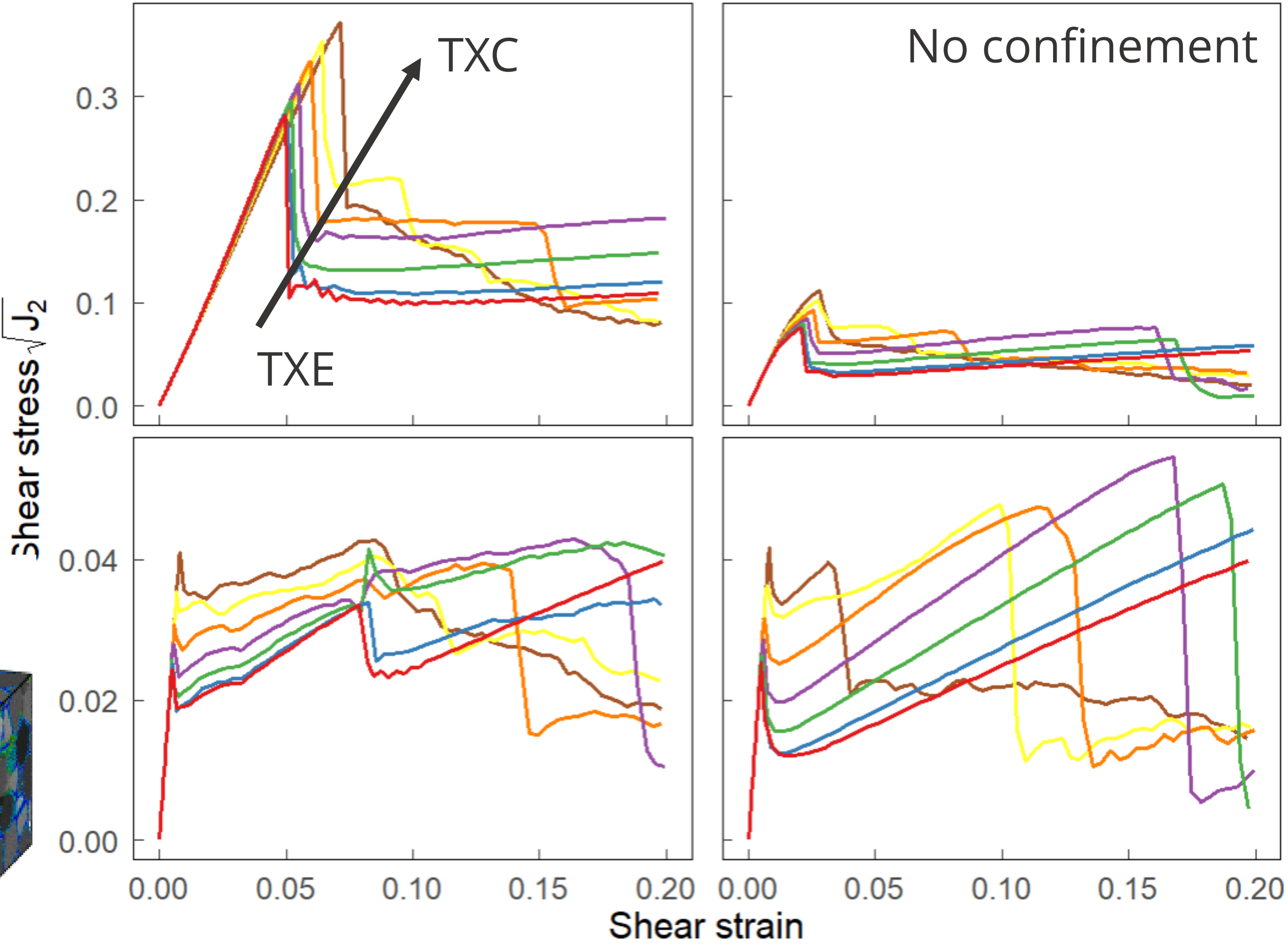

Lode angle $\theta = \frac{1}{3}\text{asin}\left(\frac{J_3}{2}\left(\frac{3}{J_2}\right)^{3/2}\right)$

# Current focus: yield/failure surface

Using Voronoi cell grain structure, see marked dependence on Lode angle

Stronger in compression than extension as expected, but also yields at different strains and has changing softening/hardening regimes



# Focusing on the initial peak stress – failure

Consider a single slice, or a $\pi$-plot

Fixed mean pressure $P = 0.0$

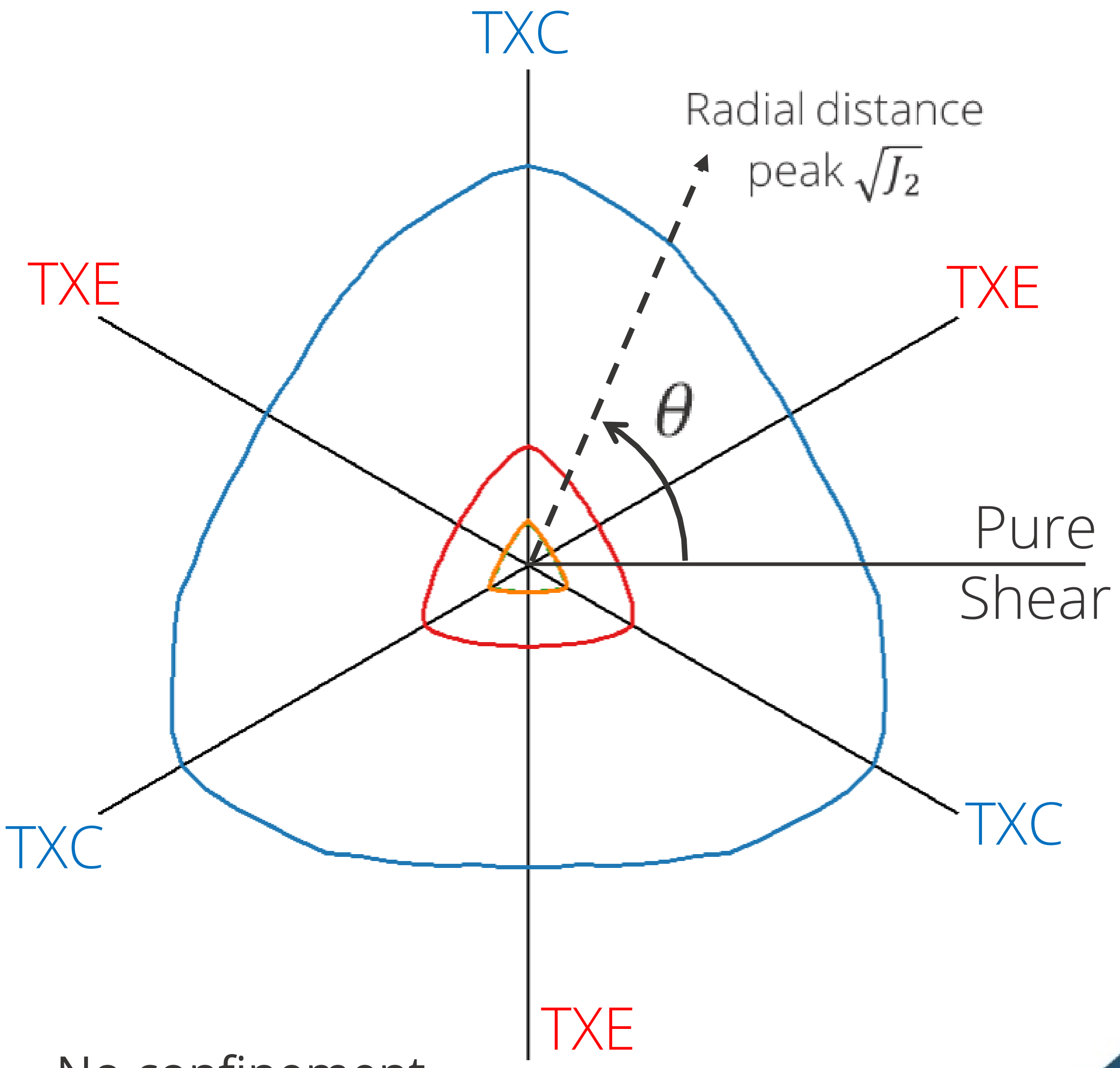
Elastic binder, $T_{glass} < T$, with strong adhesion is the strongest case

With weak adhesion, no difference seen in high vs low $T_{glass}$

Very angular, Mohr-Coulomb-like, with pronounced tensile-compressive asymmetry

(Drucker Prager would be a circle)

Elastic binder + Strong adhesion
Elastic binder + Weak adhesion
Plastic binder + Strong adhesion
Plastic binder + Weak adhesion




No confinement

# Focusing on the initial peak stress – failure

Adding compression, mean pressure $P = 0.3$ of binder bulk modulus, see dramatic change

Elastic binder + Strong adhesion:

No asymmetry, weak pure shear

Elastic binder + Weak adhesion:

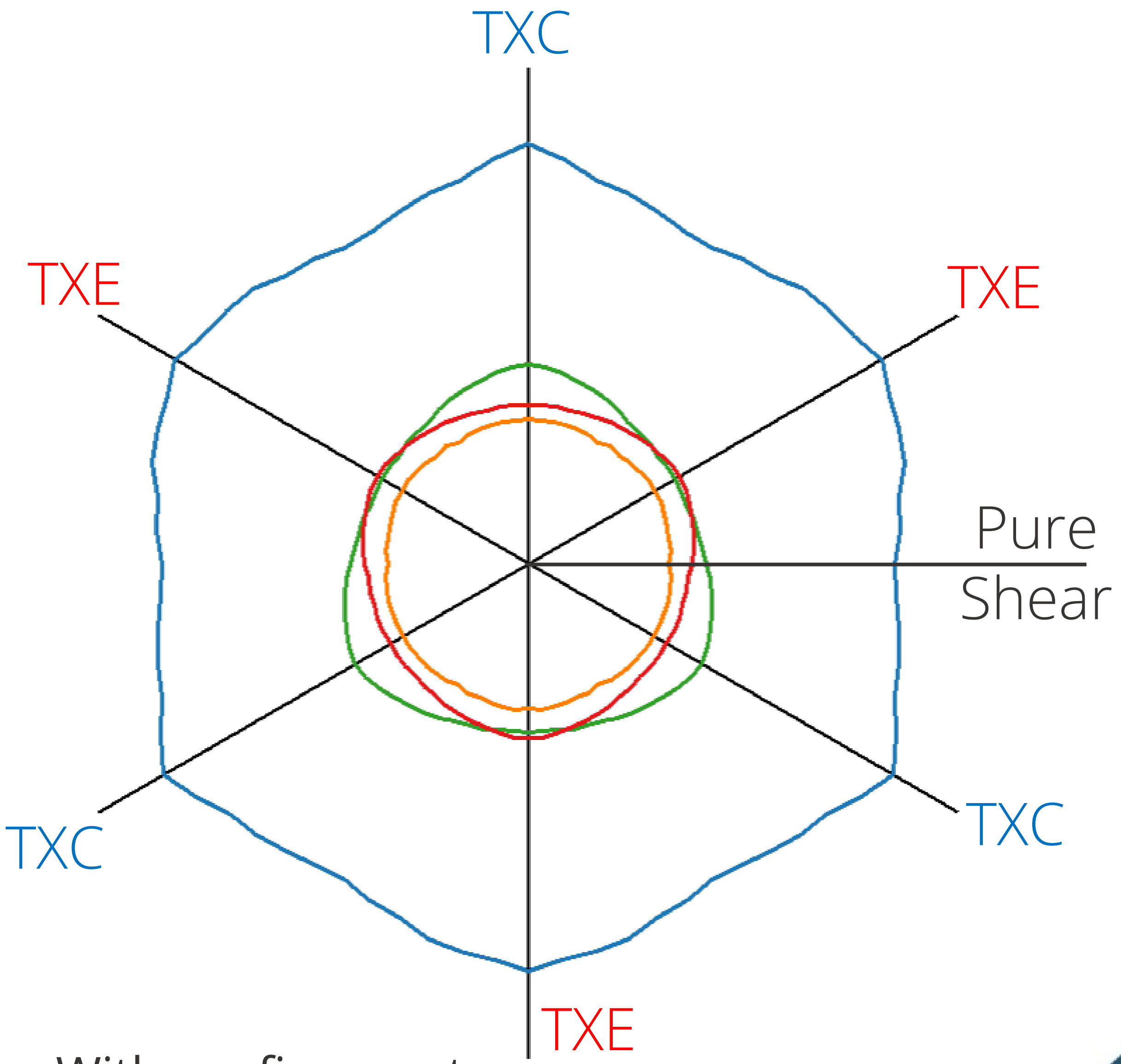
Rounding of angles, but ~same shape

Plastic binder + Strong adhesion:

Inverted tensile-compressive asymmetry

Plastic binder + Weak adhesion:

Drucker-Prager-like, no $\theta$–dependence




With confinement

# Summary

There is a need for flexible, efficient modeling of mesoscale dynamics of polymer-bound granular composites

Simple bonded particle models can fulfill this need
Reproduce key pressure-dependent experimental trends in PBX formulations with low- and high- $T_{glass}$ binders

Provides insight into how the complex macroscopic response is dictated by evolution of microscopic activation of inelastic mechanisms

Identify new nontrivial Lode angle dependence

Can rapidly extend to test key assumptions of continuum constitutive modeling, hope to inform future development