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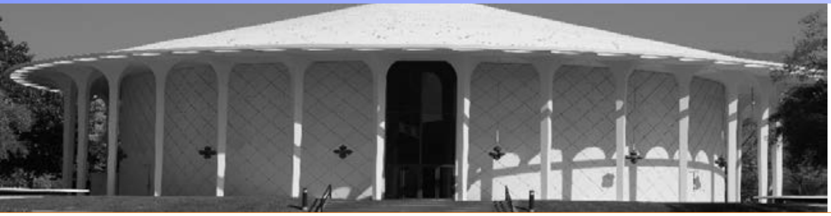


universitätbonn

The Anomalous Elastic and Yield Behavior of Fused Silica Glass: A Variational and Multiscale Perspective

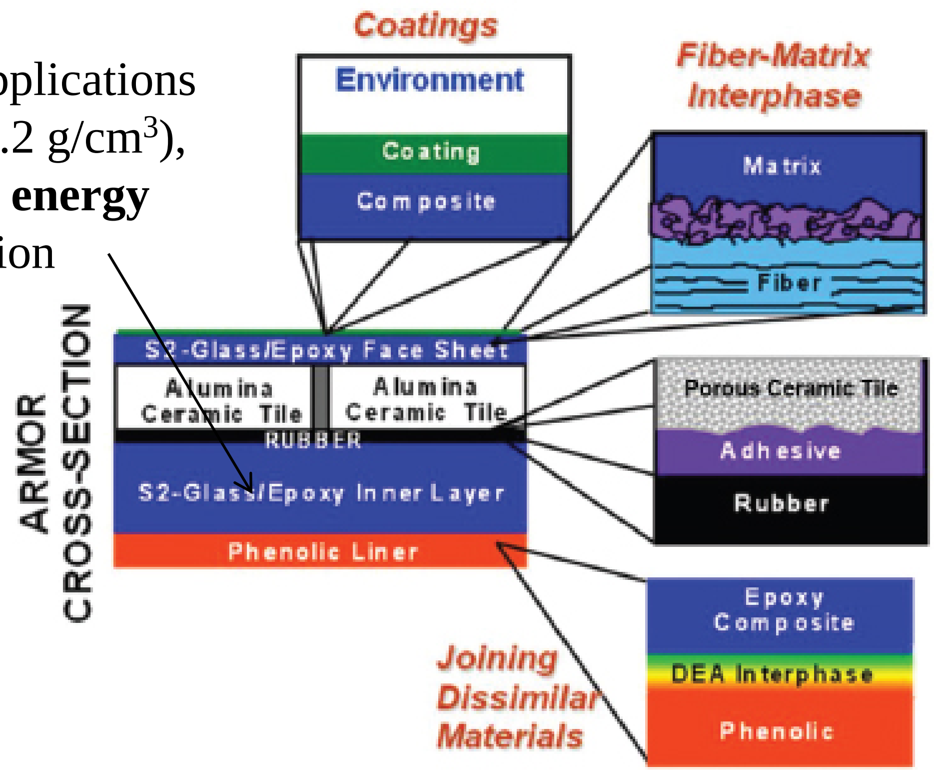
Michael Ortiz
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

with: S. Heyden, J.P. Mendez & W. Schill (Caltech), S. Conti and S. Müller (uni-Bonn), L. Stainier (Nantes)

EUROMECH Colloquium on Damage and Failure of Engineering Materials under Extreme Loading Conditions, Madrid, Spain, May 21–24, 2019

Glass as protection material

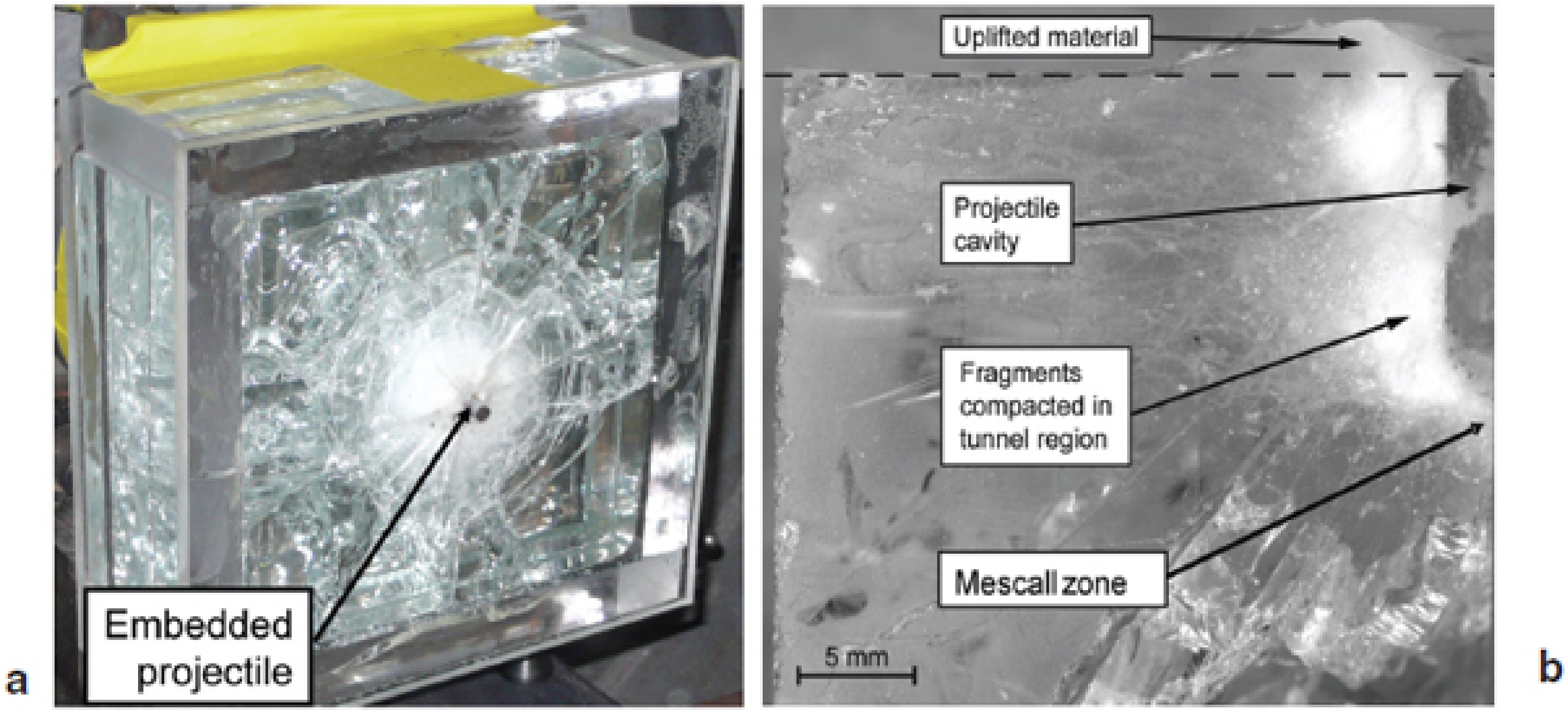
- Glass is attractive in many applications because of its **low density** (2.2 g/cm^3), **high strength** (5-6 GPa) and **energy dissipation** due to densification



Cross section of armor tile typically used in armored vehicles showing complexity of armor architecture.

J.W. McCauley, in: *Opportunities in Protection Materials Science and Technology for Future Army Applications*, US National Research Council, 2011.

Glass as protection material

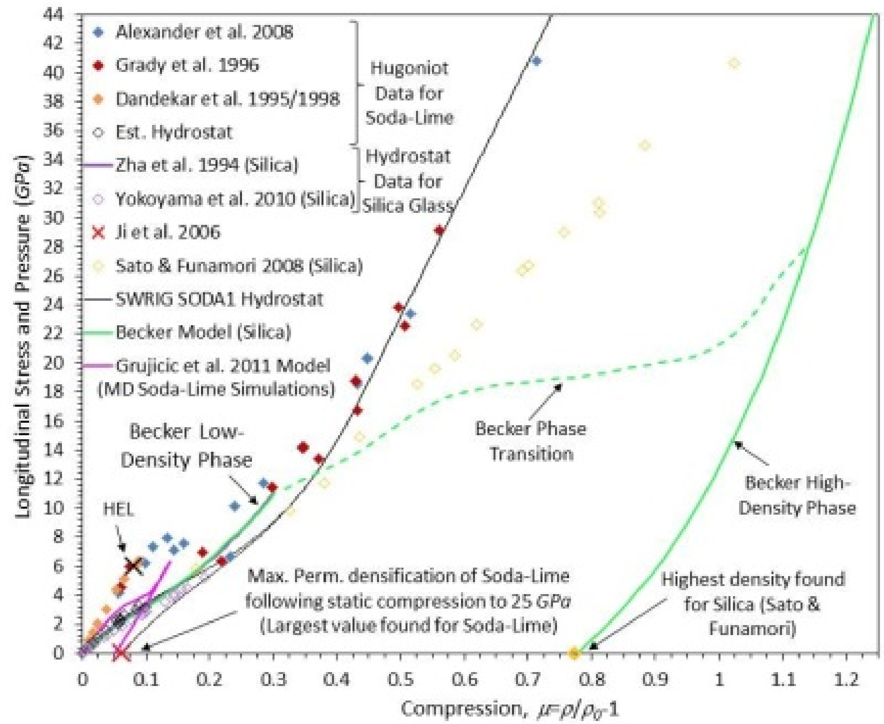


A soda lime glass target impacted by steel rod at 300 m/s[1].

[1]Shockey, D., Simons, J. and Curran D.,
Int. J. Appl. Ceramic Tech., **7**(5):566-573, 2010.

Fused silica glass: Densification

- The equation of state of glass in compression exhibits a **densification** phase transition at a pressure of 20 Gpa
- For a glass starting in its low-density phase, upon the attainment of the transition pressure the glass begins to undergo a **permanent reduction in volume**
- Reductions of up to 77% at pressures of 55 GPa have been reported
- The transformation is **irreversible**, and unloading takes place along a densified equation of state resulting in permanent volumetric deformation



Compilation of equation-of-state data for glass (soda lime and fused silica)[1].

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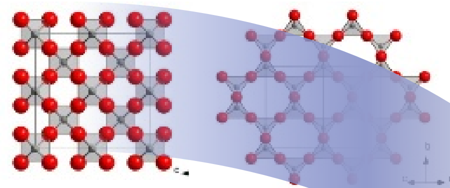
[1]R. Becker, *ARL Ballistics Protection Technology Workshop*, 2010.

Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

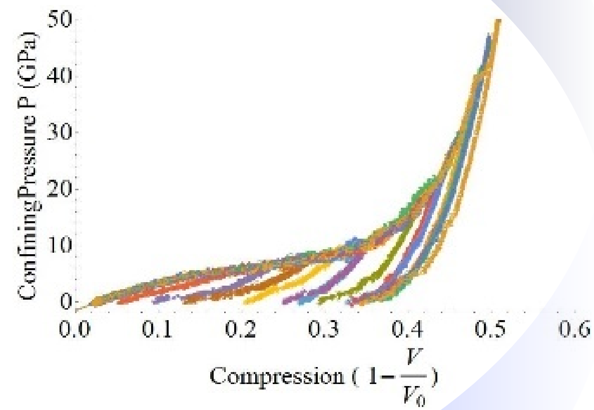


Data Mining

Mesoscopic modeling:

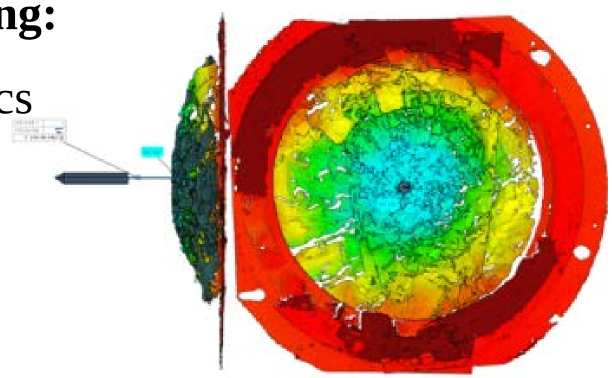
- Critical-state plasticity
- Relaxation
- Shear banding

Continuum Models



Macroscopic modeling:

- Terminal ballistics



(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications

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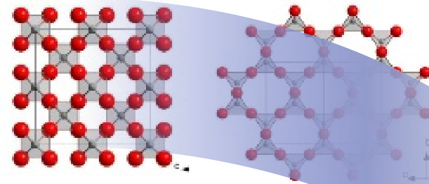

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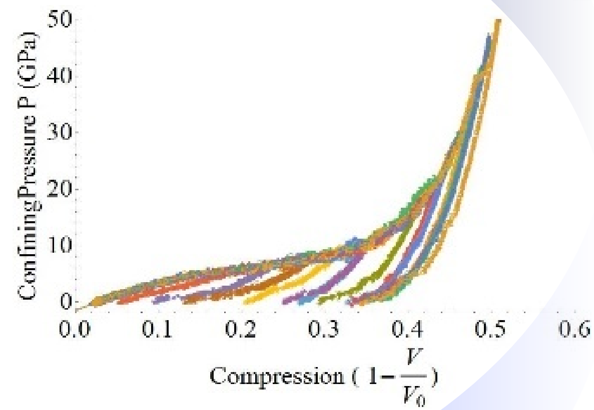

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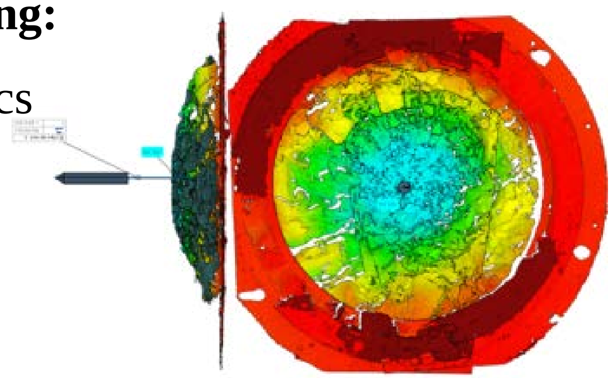

Applications

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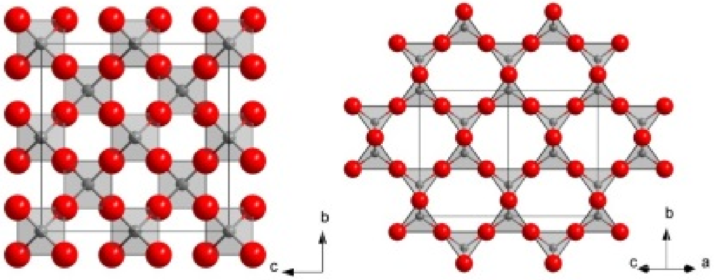
Computational model – MD

Molecular Dynamics Calculations: **SNL LAMMPS**[1]

Starting structure: β-cristobalite

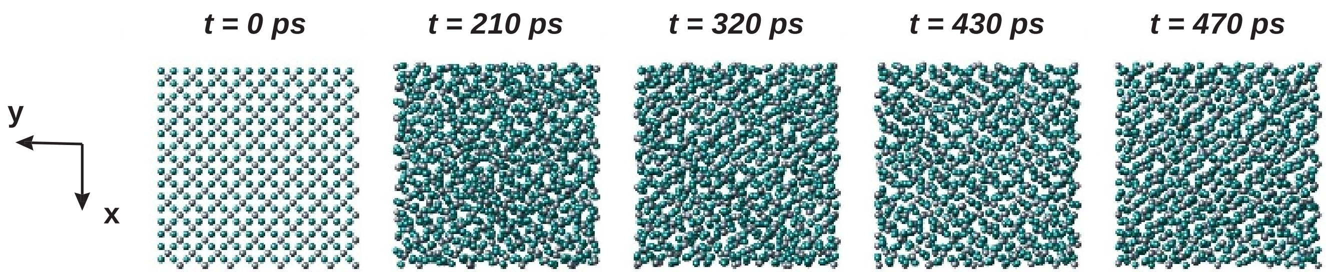
β-cristobalite: Polymorph characterized by **corner-bonded SiO_4 tetrahedra**



Ideal structure of β-cristobalite (adapted from https://en.wikipedia.org/wiki/Cristobalite)

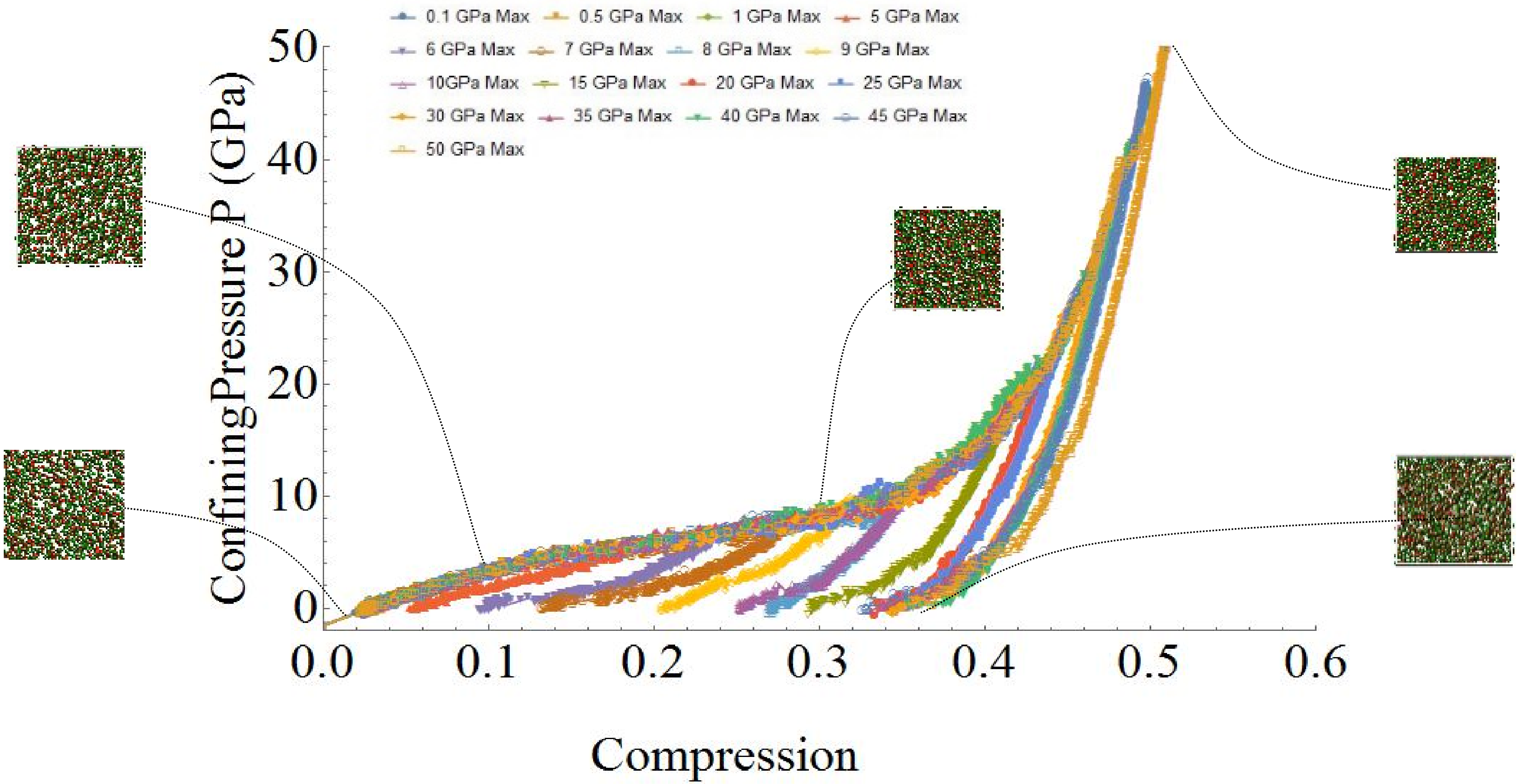
Amorphous structure of fused silica: Obtained through the **fast quenching** of a melt

- Uniform temperature decrease from 5000 K to 300 K, decreasing the temperature with steps of 500 K
- Total cooling time: 470 ps



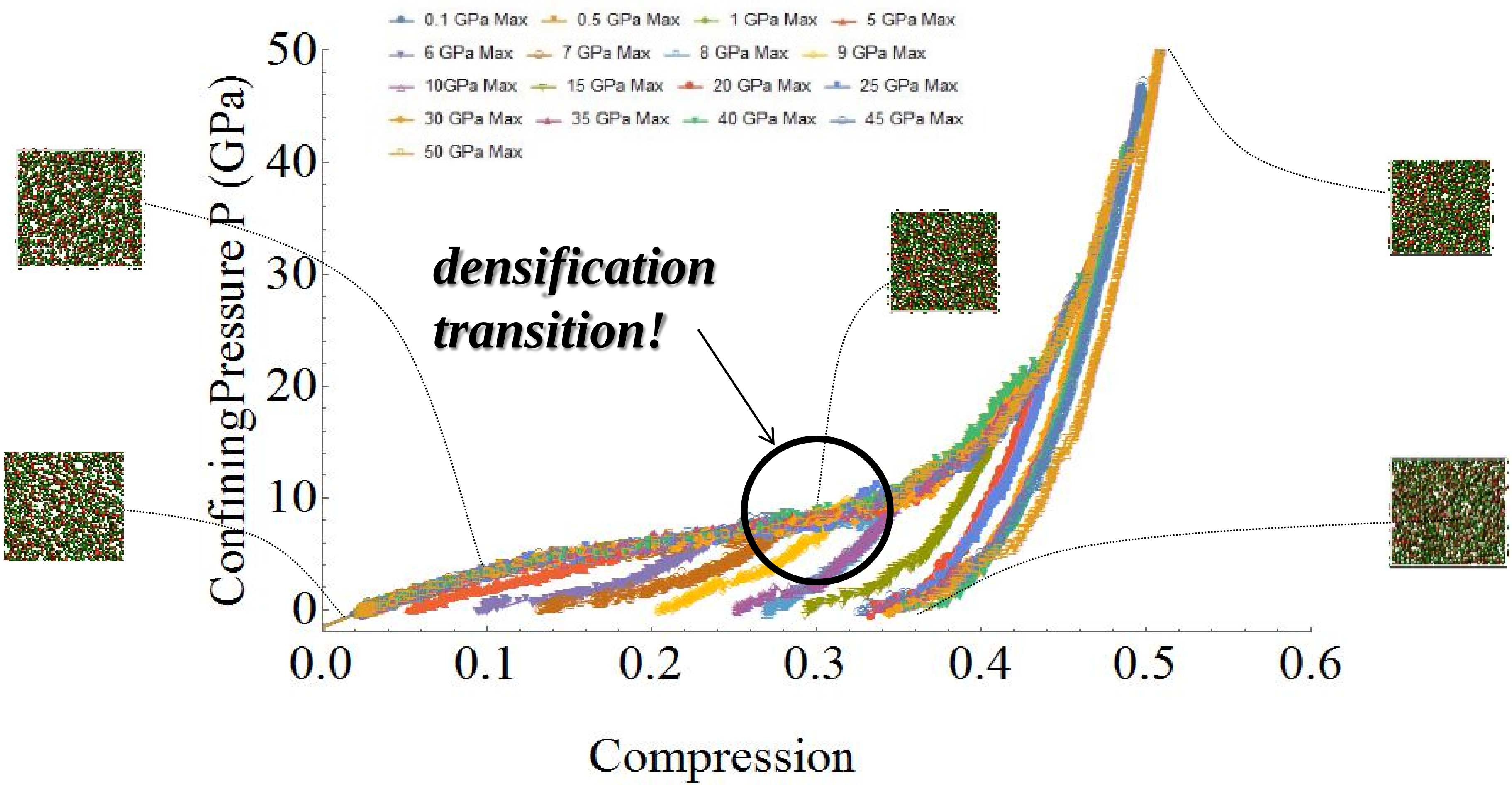
Plimpton S, *J Comp Phys*, **117** (1995) 1-19.

Results – Volumetric compression



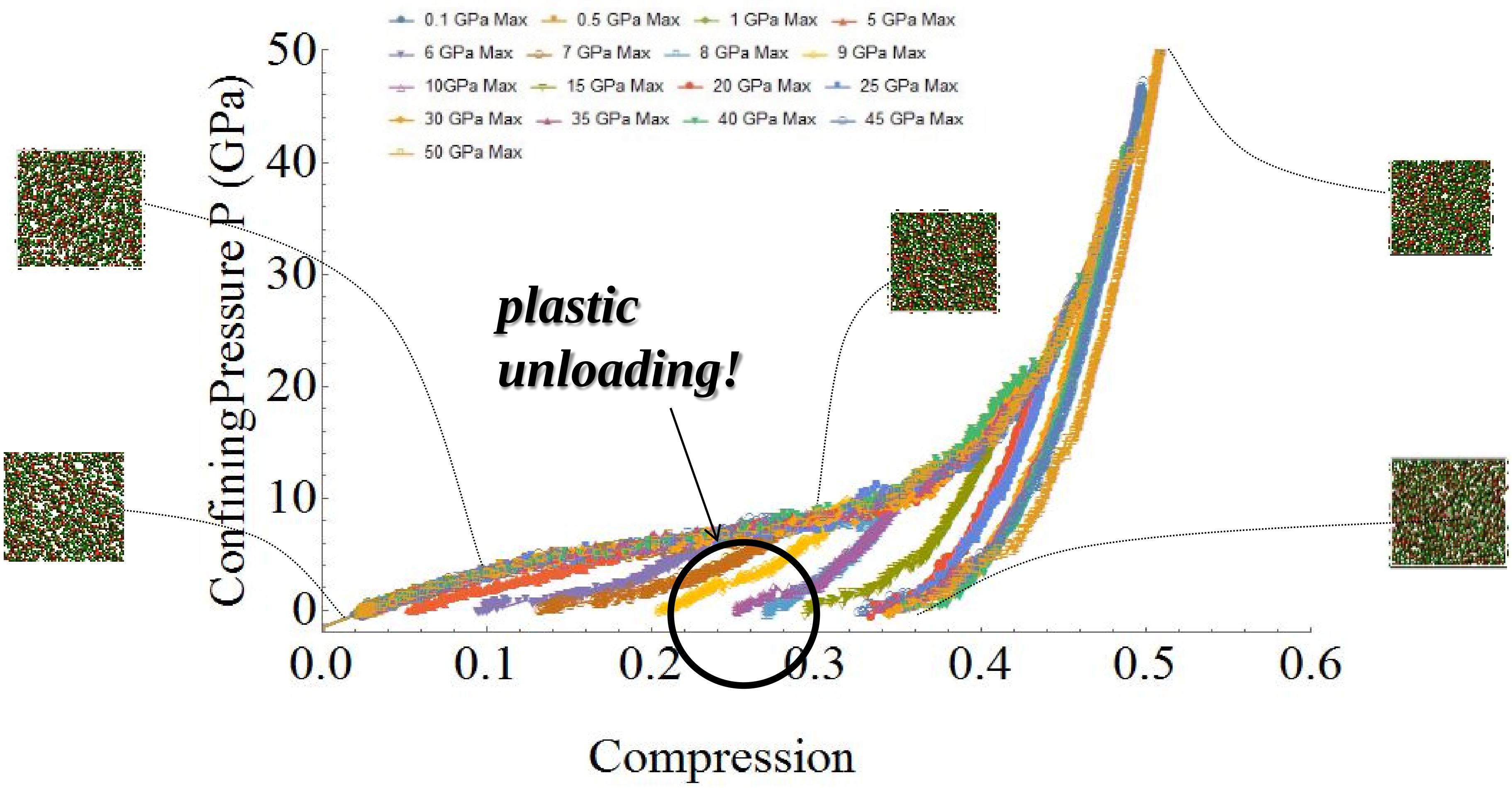
Schill, W., Hayden, S., Conti, S. and Ortiz, M., *JMPS*, **113** (2018) 105-125.

Results – Volumetric compression



Schill, W., Hayden, S., Conti, S. and Ortiz, M., *JMPS*, **113** (2018) 105-125.

Results – Volumetric compression

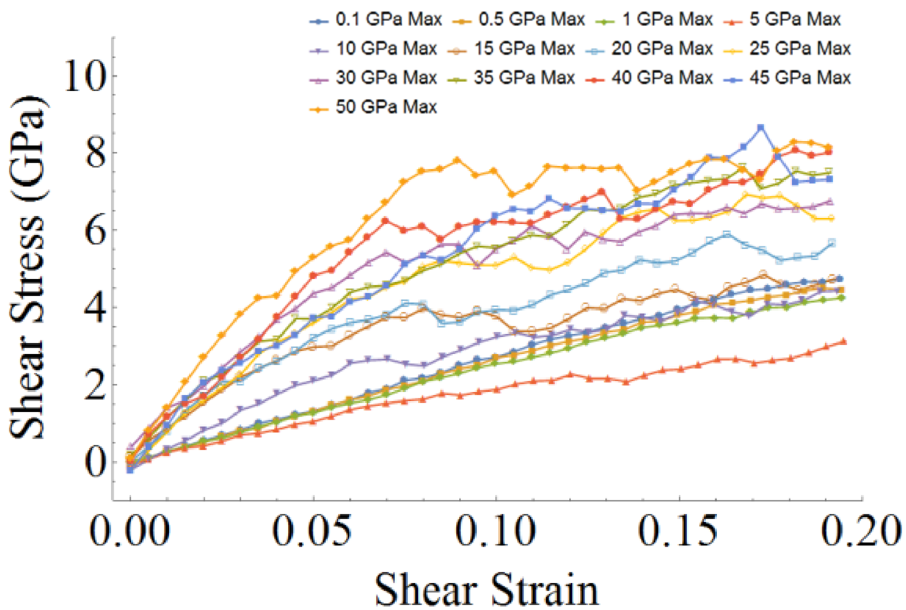


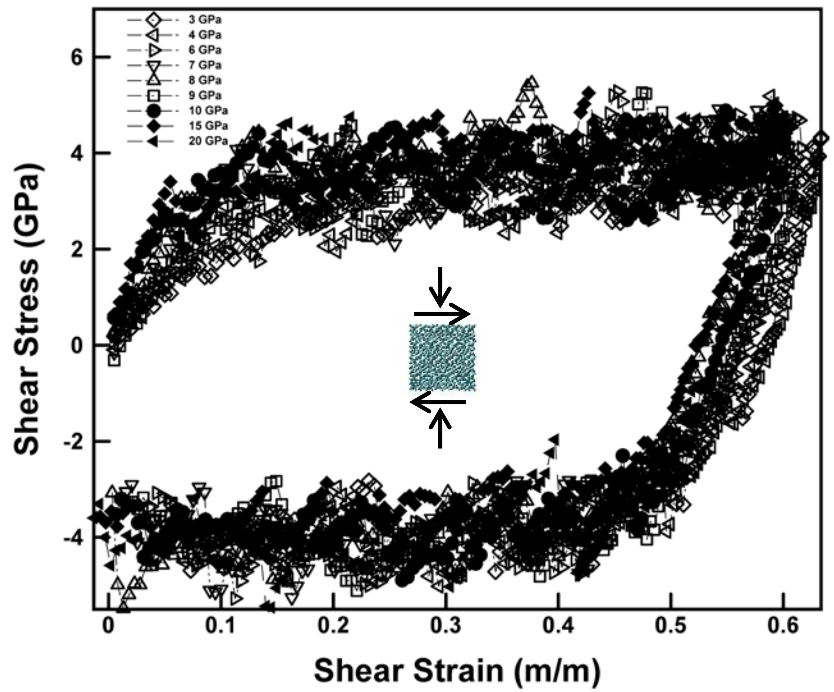
Schill, W., Hayden, S., Conti, S. and Ortiz, M., *JMPS*, **113** (2018) 105-125.

Pressure-shear coupling

Simple shear of amorphous silica at constant hydrostatic pressure:

- Hydrostatic compression is performed followed by simple shear
- The pressure-dependent shear response is computed





Shear deformation is irreversible upon unloading!

(permanent or plastic shear deformation, pressure-dependent plasticity)

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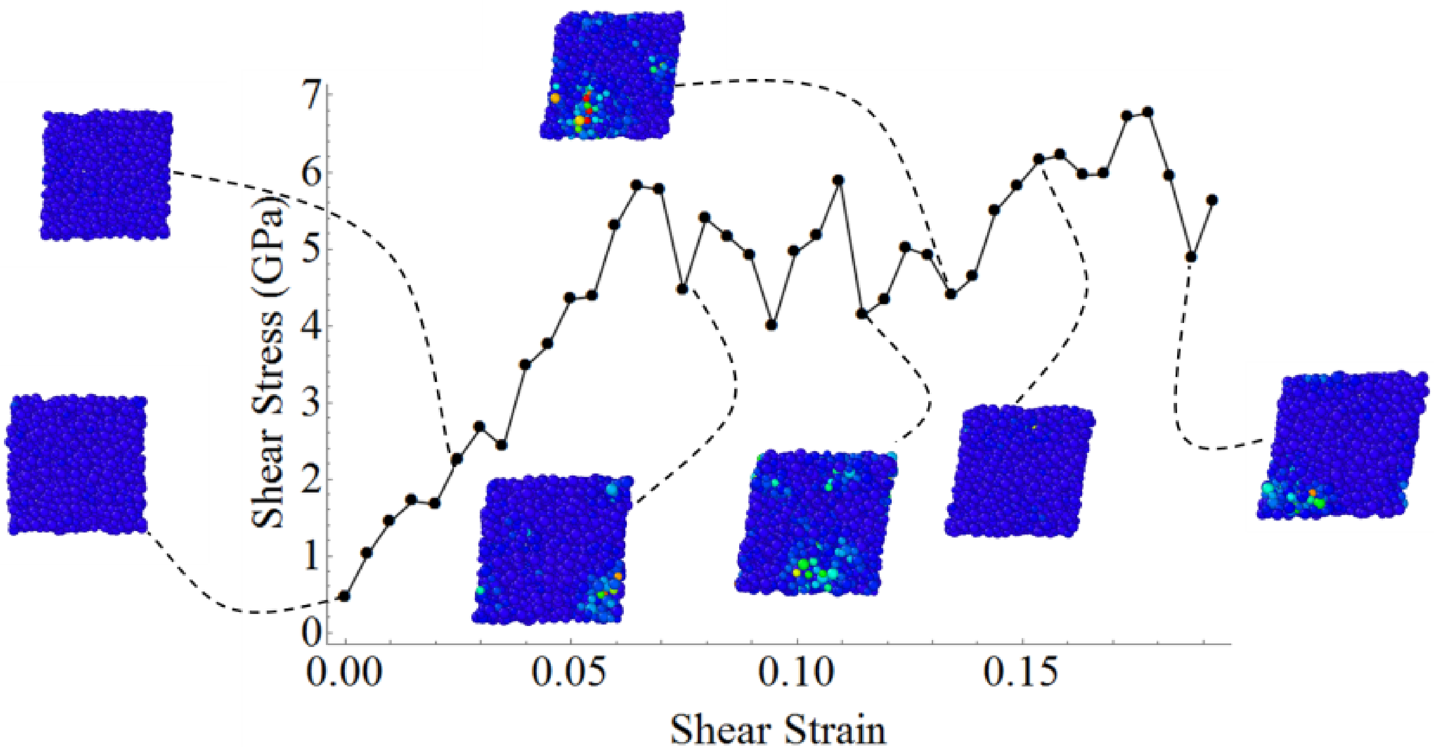
Molecular basis of glass plasticity

Shear Transformation Zones:

- Local microstructural rearrangements accommodate shear deformation
- Colored regions indicate large deviation from affine deformation from the previous step



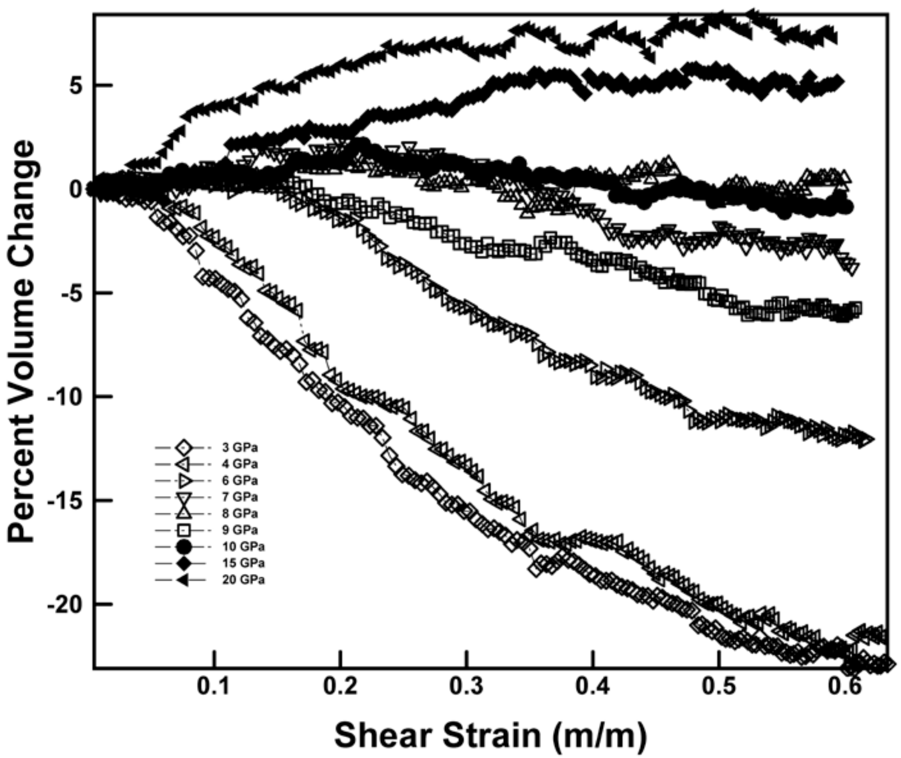
Local avalanches controlled by free-volume kinetics!

(shear deformation proceeds inhomogeneously through local bursts)

Volume evolution

Volume vs. shear and degree of pre-consolidation:

- Volume attains constant value after sufficient shear deformation (critical state)
- Volume decreases (increases) in under- (over-) consolidated samples



Evidence of critical state behavior!

(in analogy to granular media)

Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

Mesoscopic modeling:

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- Relaxation
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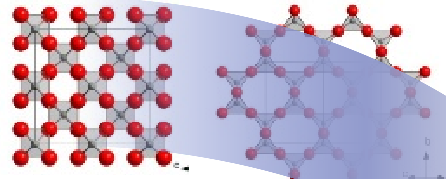
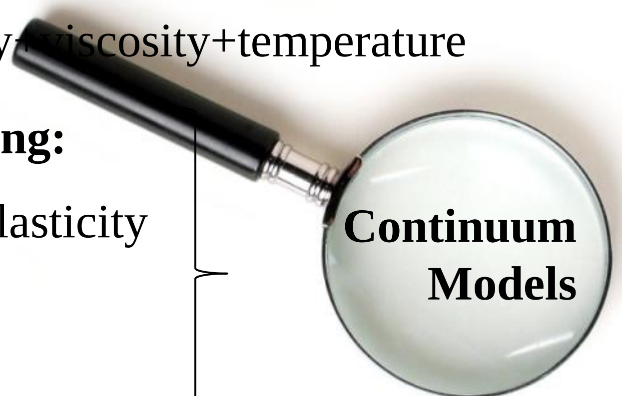
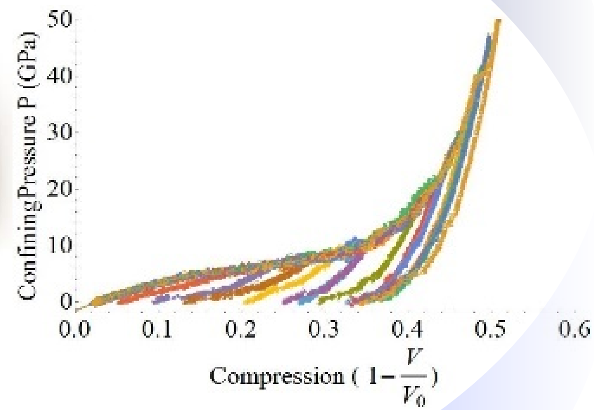
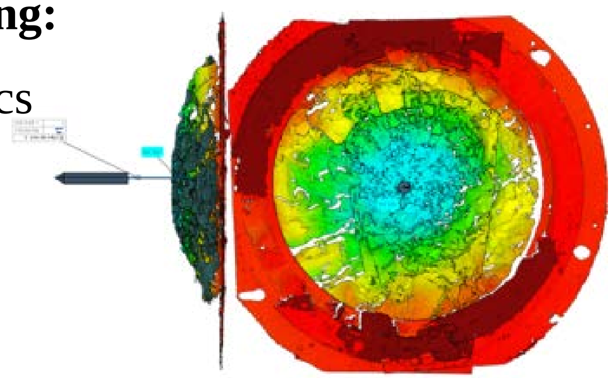
- Terminal ballistics



Data Mining







(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications

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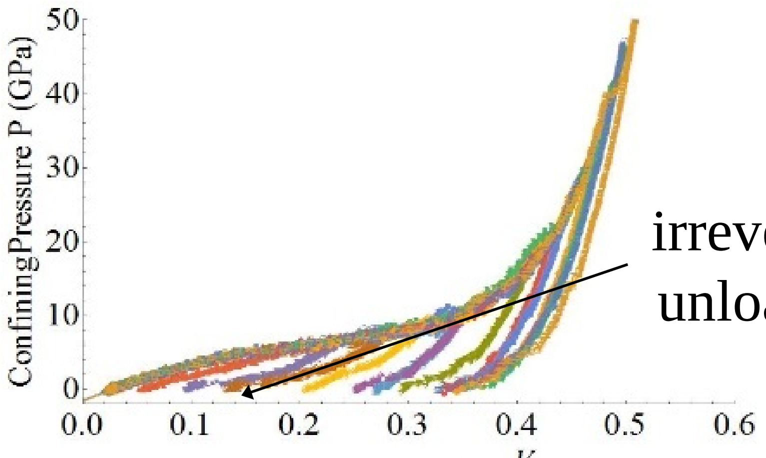
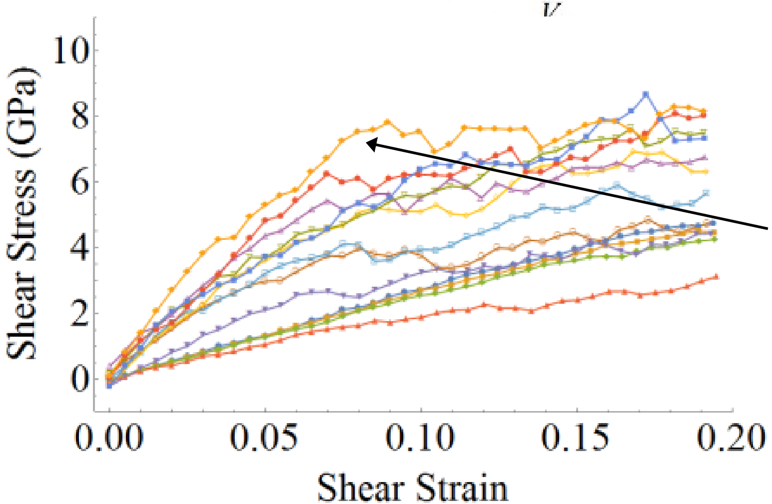
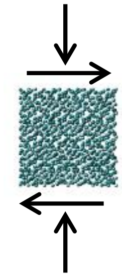
Critical-state plasticity model

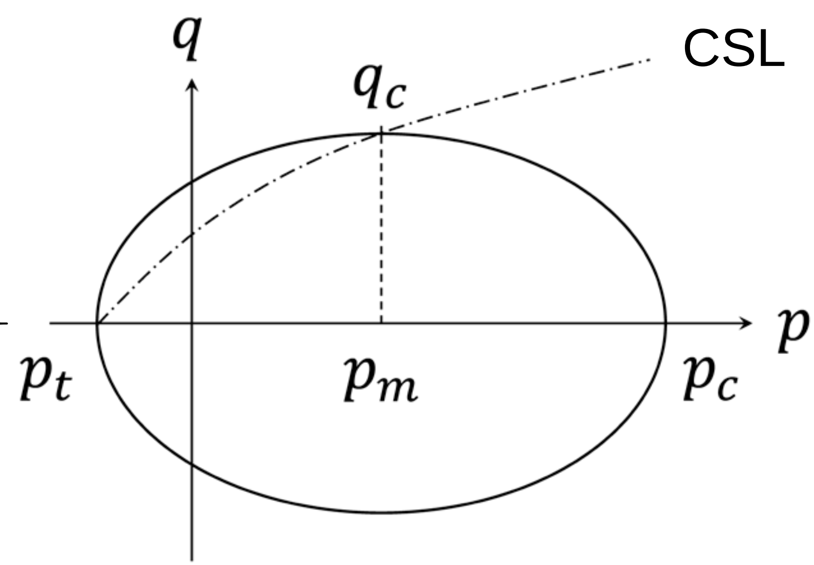
Modeling approach:

- Critical-state theory of plasticity (Cam-Clay)







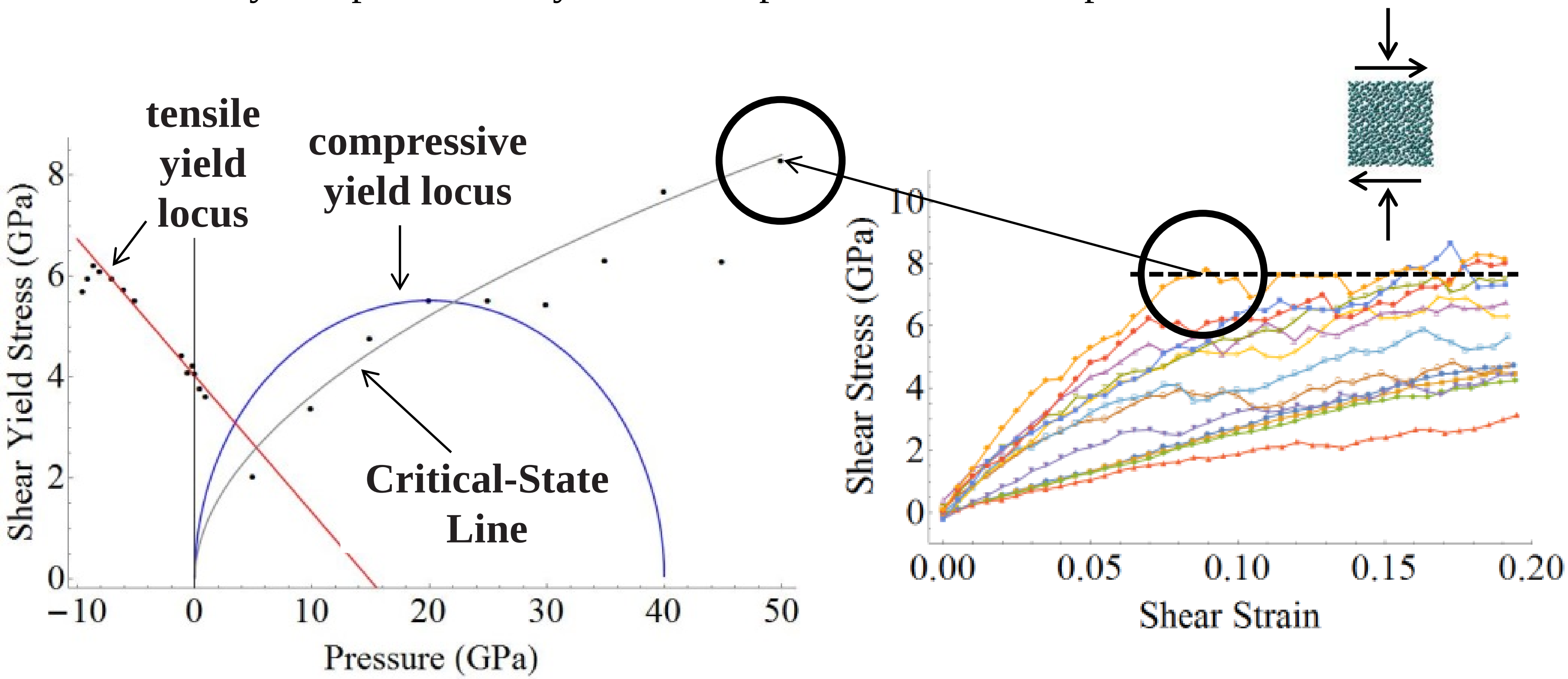


Assumed yield locus in pressure (p) Mises shear stress (q) plane and critical-state line (CSL)

Critical-state plasticity model

Yield Surface:

- Identify computed shear yield stress–pressure relationship as Critical Line



Anomalous pressure dependence of shear yield stress!
Non-convex critical-state line!

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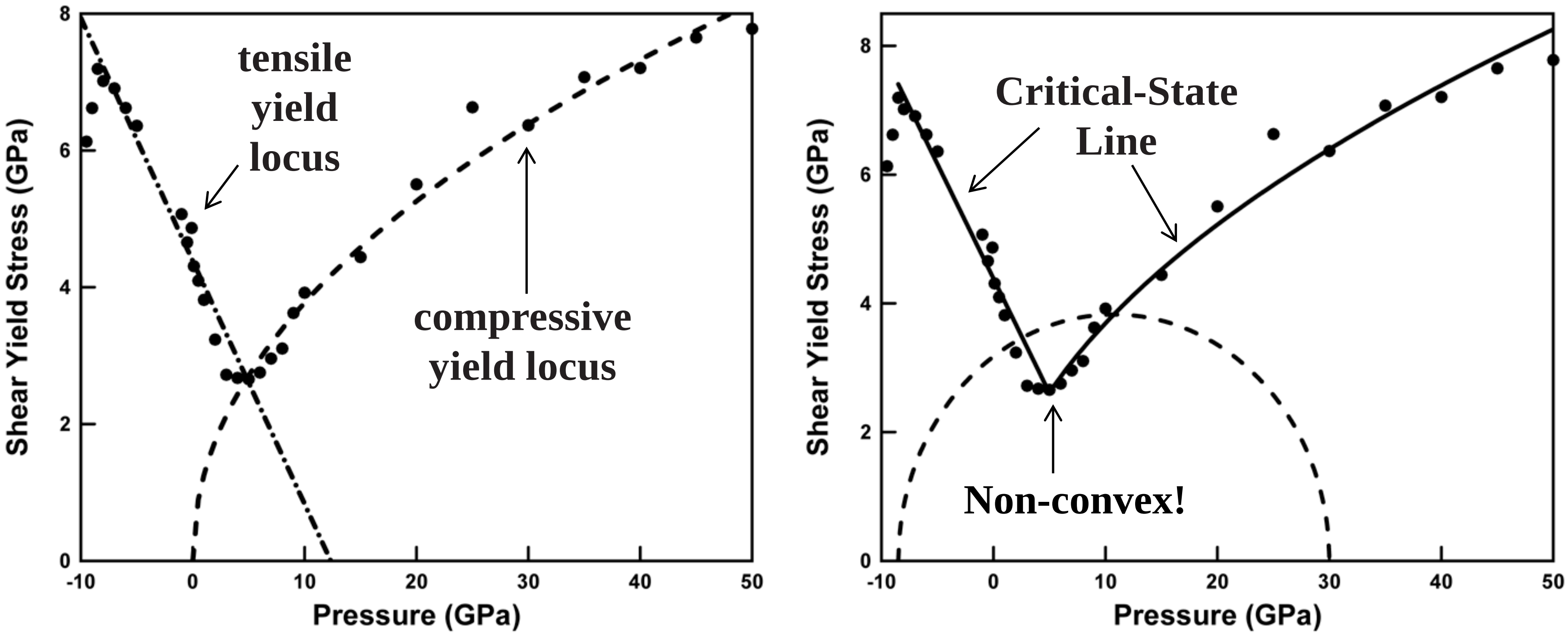
Critical-state plasticity model

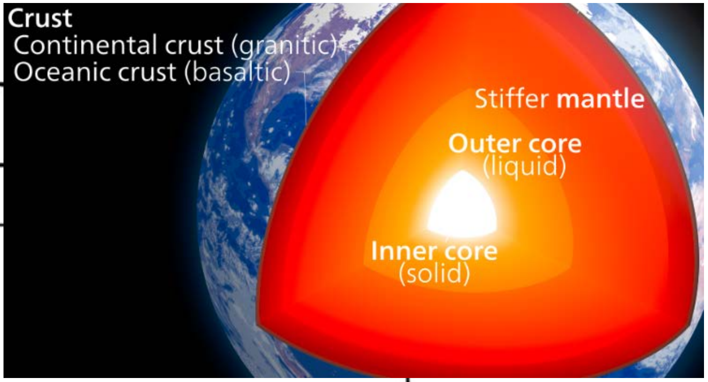


Anomalous pressure dependence of shear yield stress!
Non-convex critical-state line !

Anomalous plasticity of fused silica

Effect of a Coordination Change on the Strength of Amorphous SiO_2

CHARLES MEADE AND RAYMOND JEANLOZ



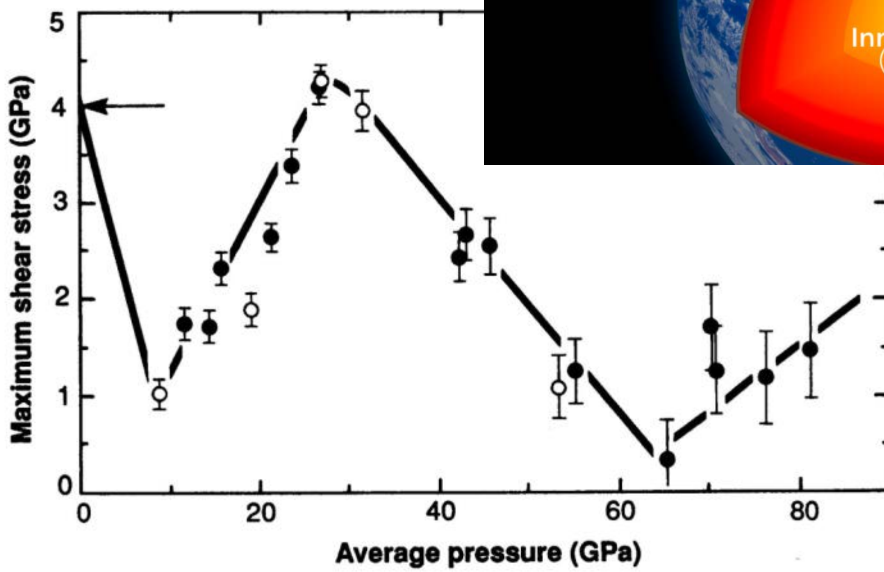


Fig. 1. Maximum shear stress in silica glass at room temperature and average pressures ($\bar{P}$) between 8.6 and 81 GPa. Each point corresponds to a separate sample, and the heavy line shows the general trend of the data. The shear stress is determined from Eq. 1, and it is a measure of the yield strength of the sample at high pressures. The error bars represent the combined uncertainties from the measurements of h and $\partial P/\partial r$. The open circles show the strength of samples that were initially compressed to 50 GPa, unloaded, and then recompressed. The arrow marks the zero pressure strength of silica glass (*19*).

SCIENCE, VOL. 241

Anomalous shear yield stress documented in geophysics literature!

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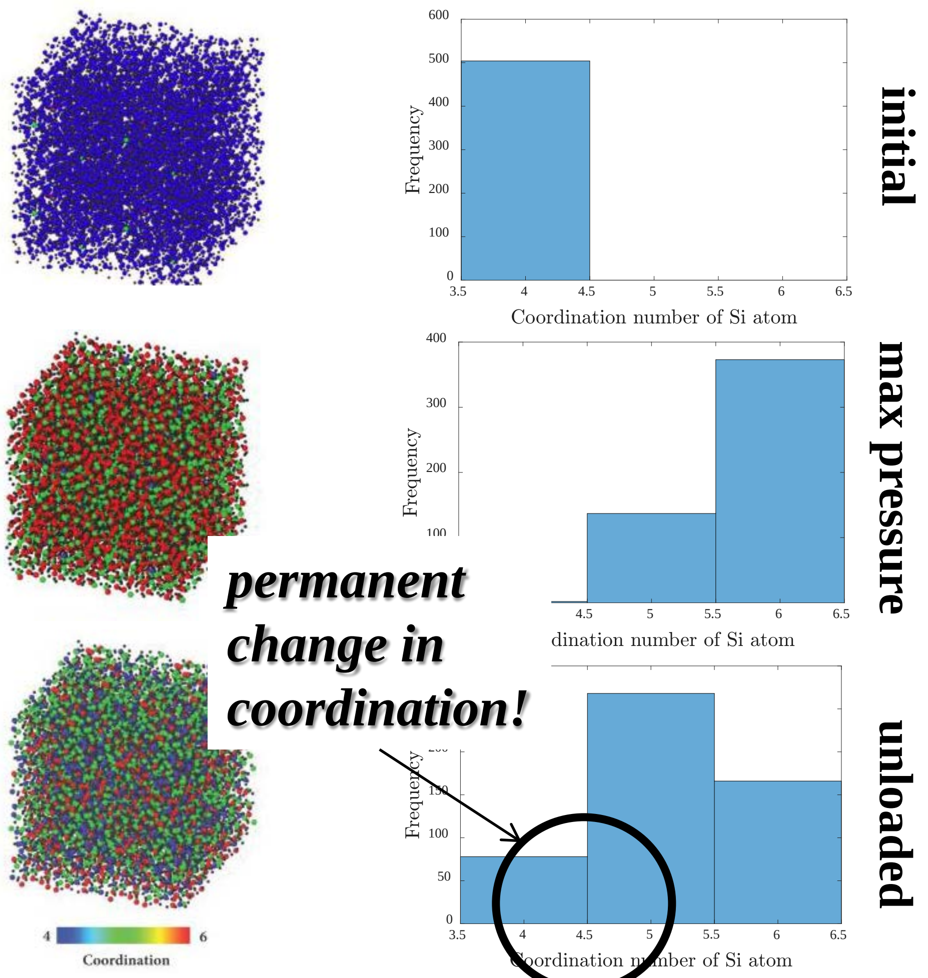
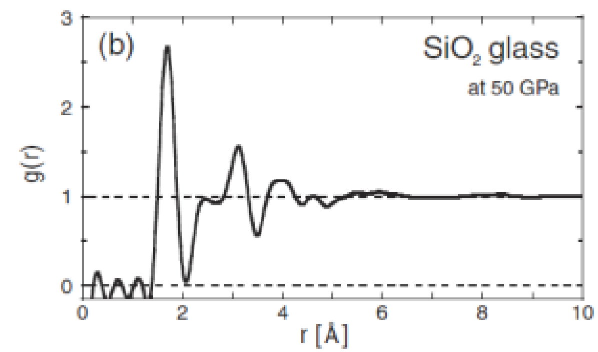
Molecular basis of anomalous plasticity

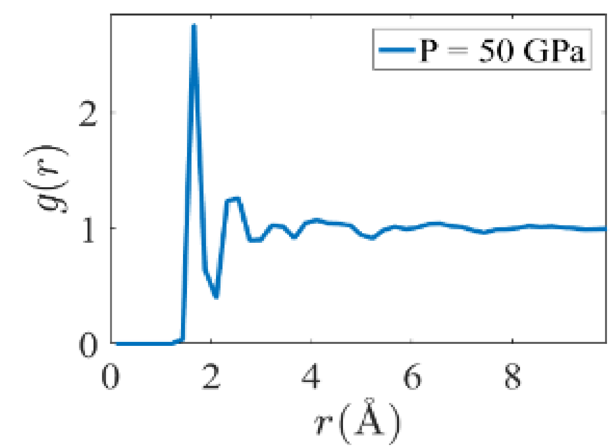
Hydrostatic compression/ decompression of amorphous silica:

- Molecular dynamics results exhibit irreversible densification at 14-20 GPa
- Molecular dynamics generated rdf are in good overall agreement with data





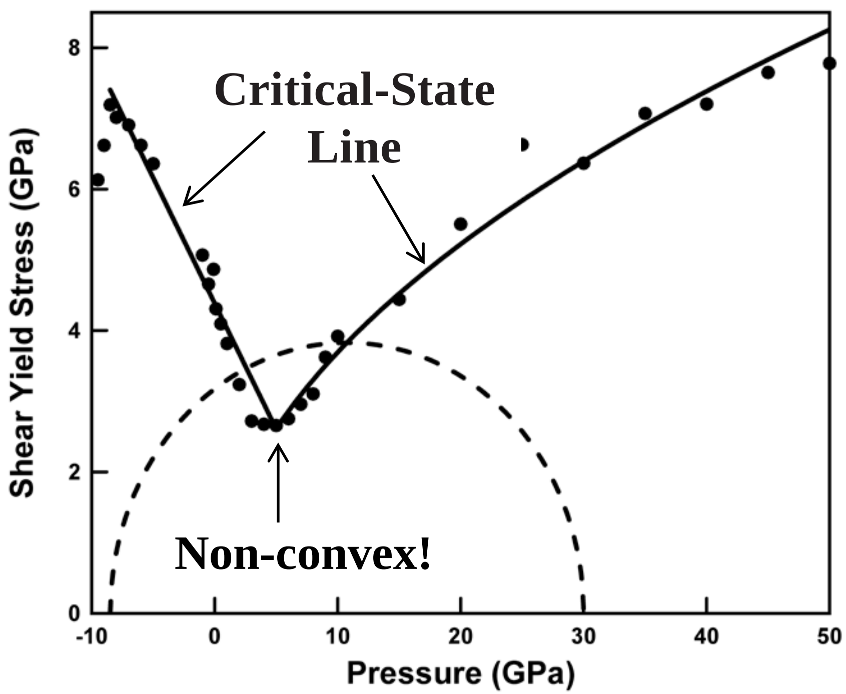
(Sato and Funamori, 2010)

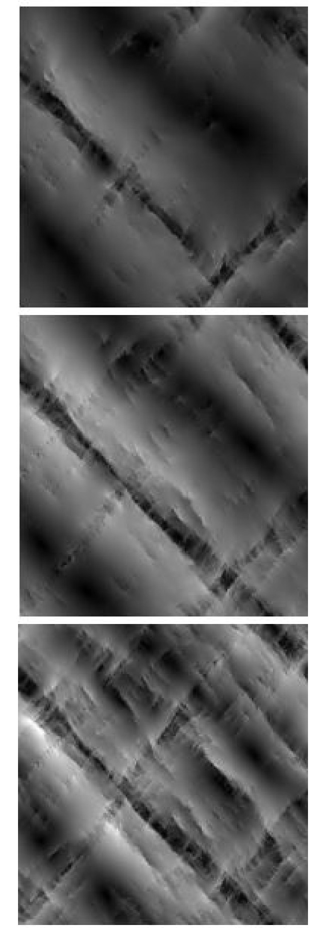


Non-convex plasticity – Relaxation

Relaxation:

- Strong non-convexity (material instability) is exploited by the material to maximize dissipation (**relaxation**, per calculus of variations)
- Relaxation occurs through the formation of fine **microstructure**[1] (finely patterned stress and deformation fields at the microscale) →





[1]C.E. Maloney and M.O. Robbins, *J. Phys.: Cond. Matter*, 20(24):244128, 2008.
Schill, W., Hayden, S., Conti, S. and Ortiz, M., *JMPS*, **113** (2018) 105-125.

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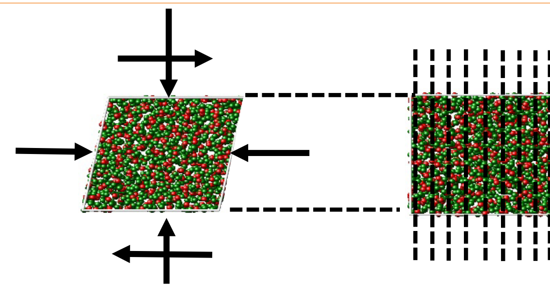
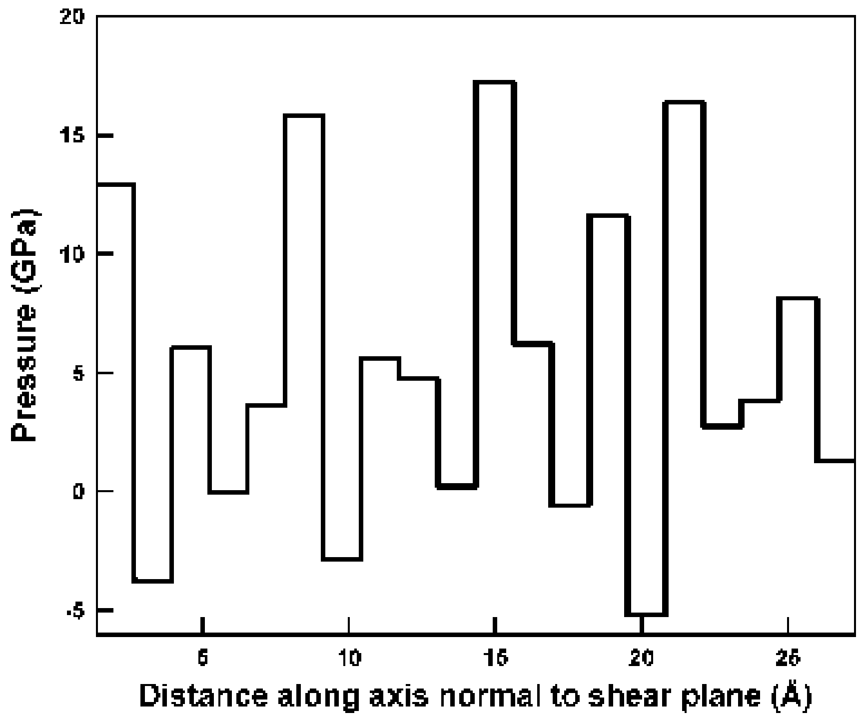
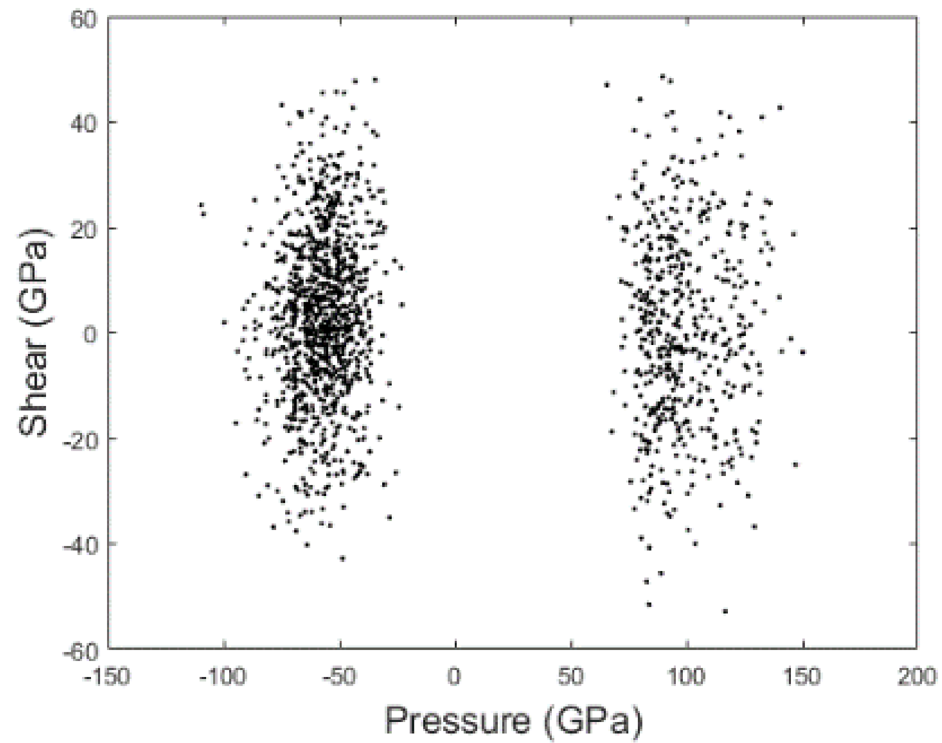




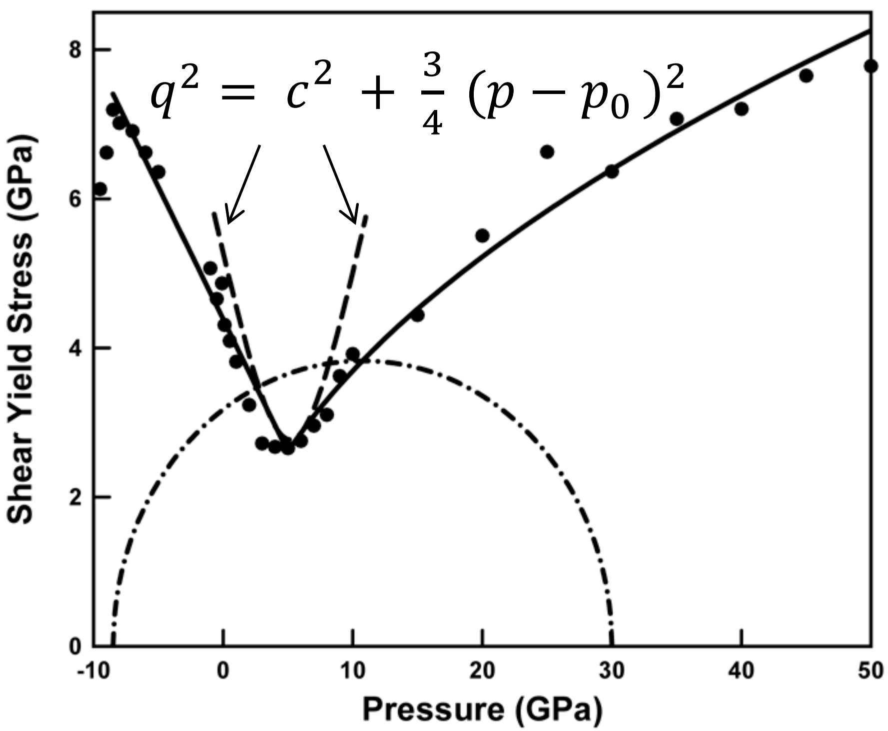


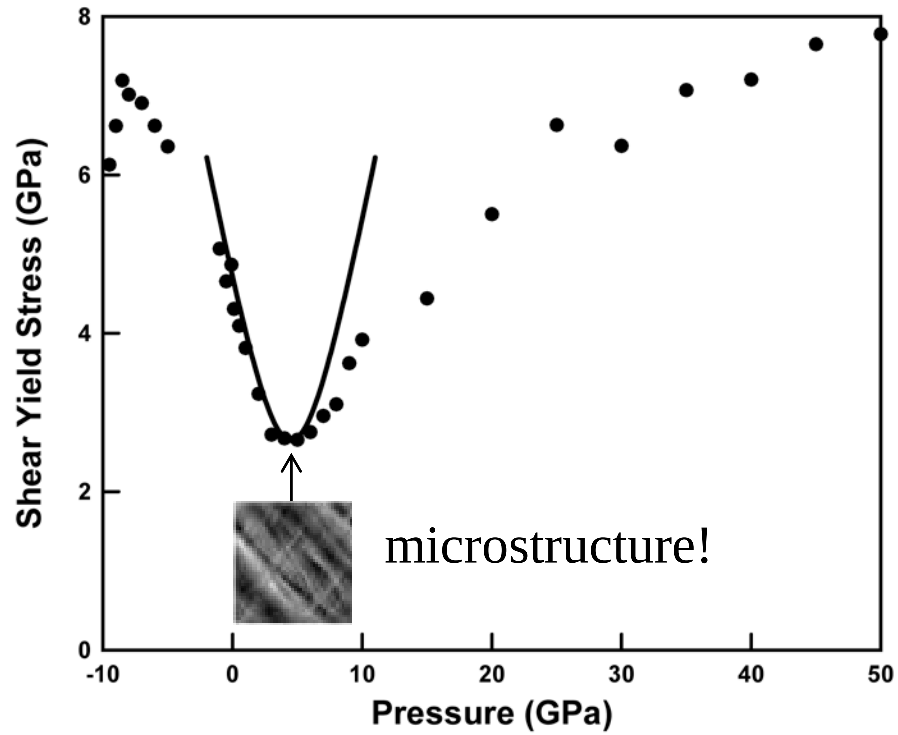
Micro-stress patterning to accommodate non-convex yield!

Non-convex plasticity – Relaxation

Div-quasiconvex envelop of glass elastic domain:

- **Theorem** (Tartar'85). *The function* $f(\sigma) = 2|\sigma|^2 - \mathrm{tr}(\sigma)^2$ *is div-quasiconvex.*
- **Theorem**. *The set* $\{\sigma : \; q^2 \le c^2 + \frac{3}{4}(p - p_0)^2\}$ *is div-quasiconvex.*
- **Theorem** (CMO'17) *The div-quasiconvex envelop of K is:*





L. Tartar "Estimations nes des coefficients homogeneises". In Ennio De Giorgi colloquium (Paris, 1983), vol. 125 of Res. Notes in Math., pp. 168-187, Pitman, Boston, MA, 1985.

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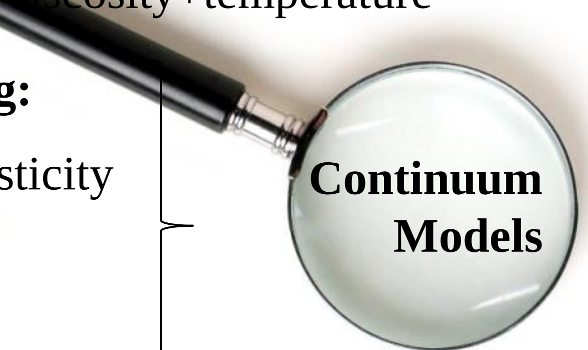
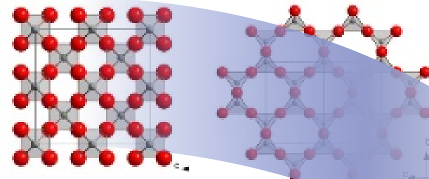
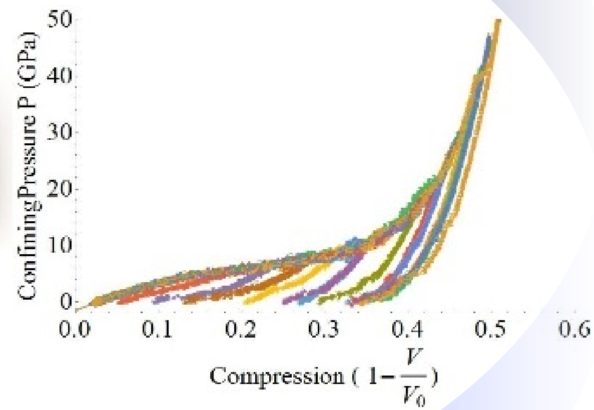


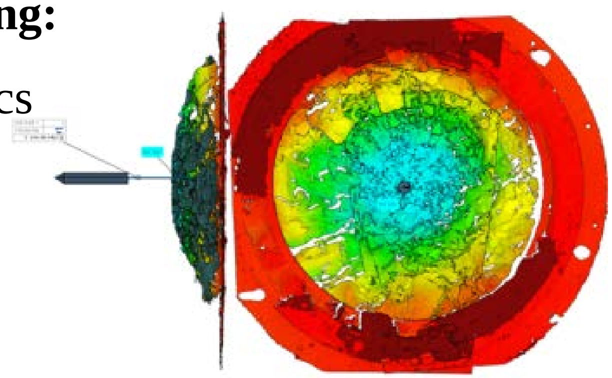
Macroscopic modeling:

- Terminal ballistics



Data Mining





(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications

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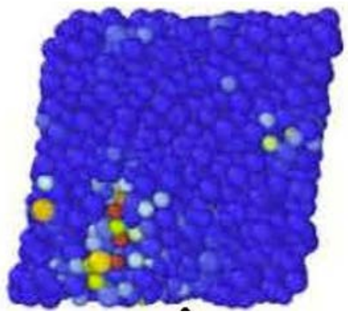
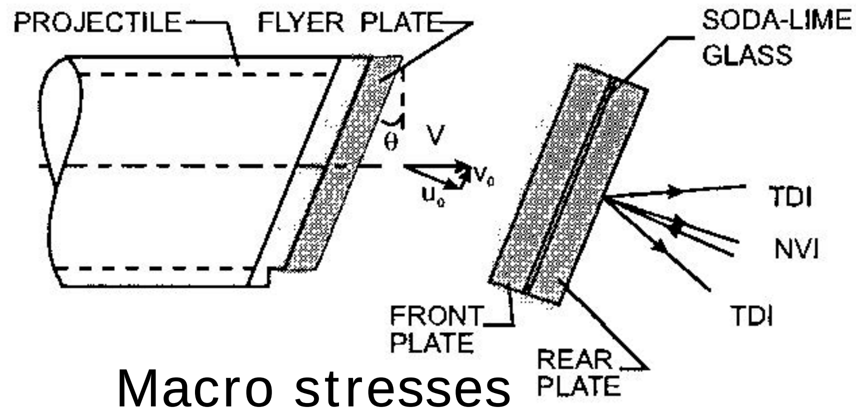
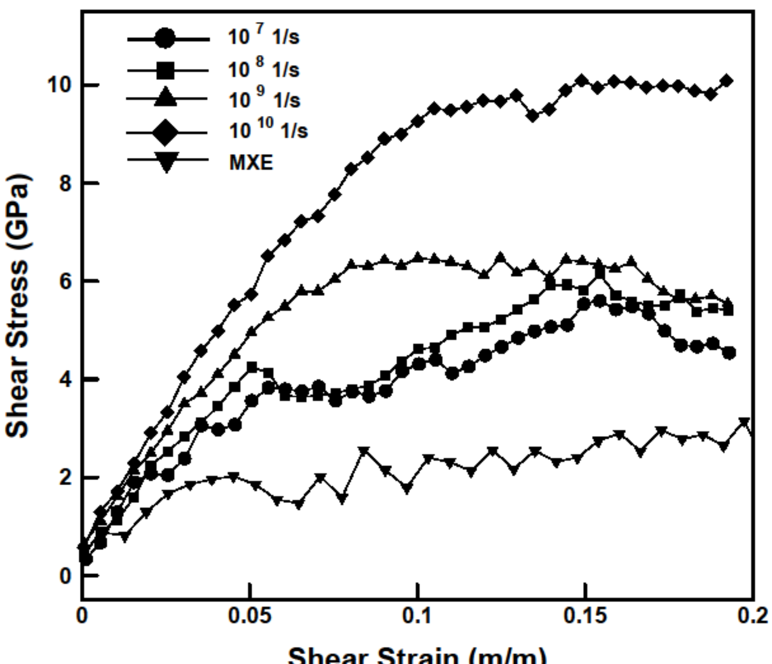
The micro-macro gap…

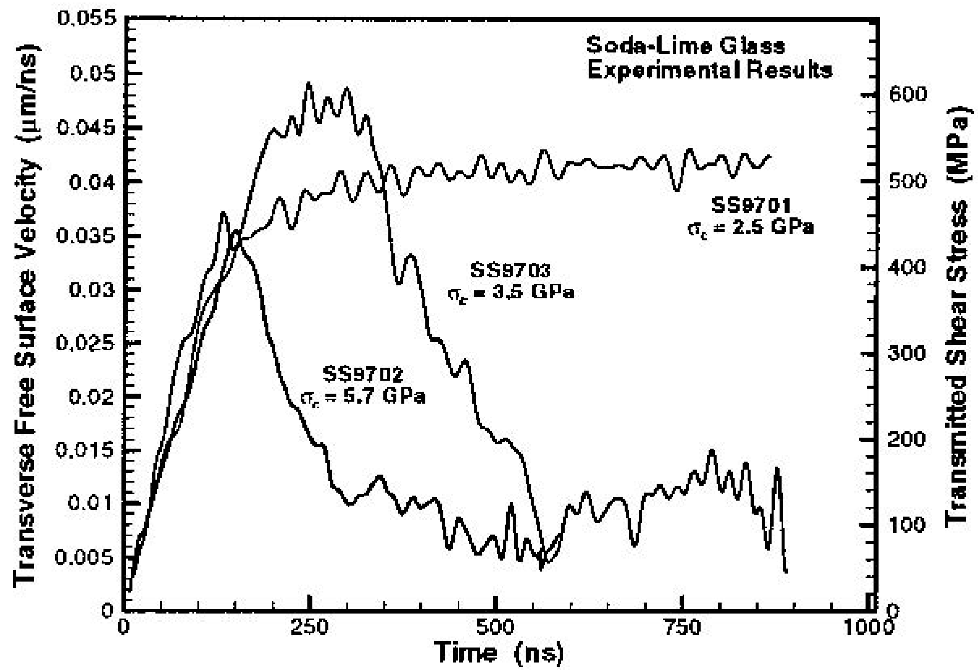


Micro stresses



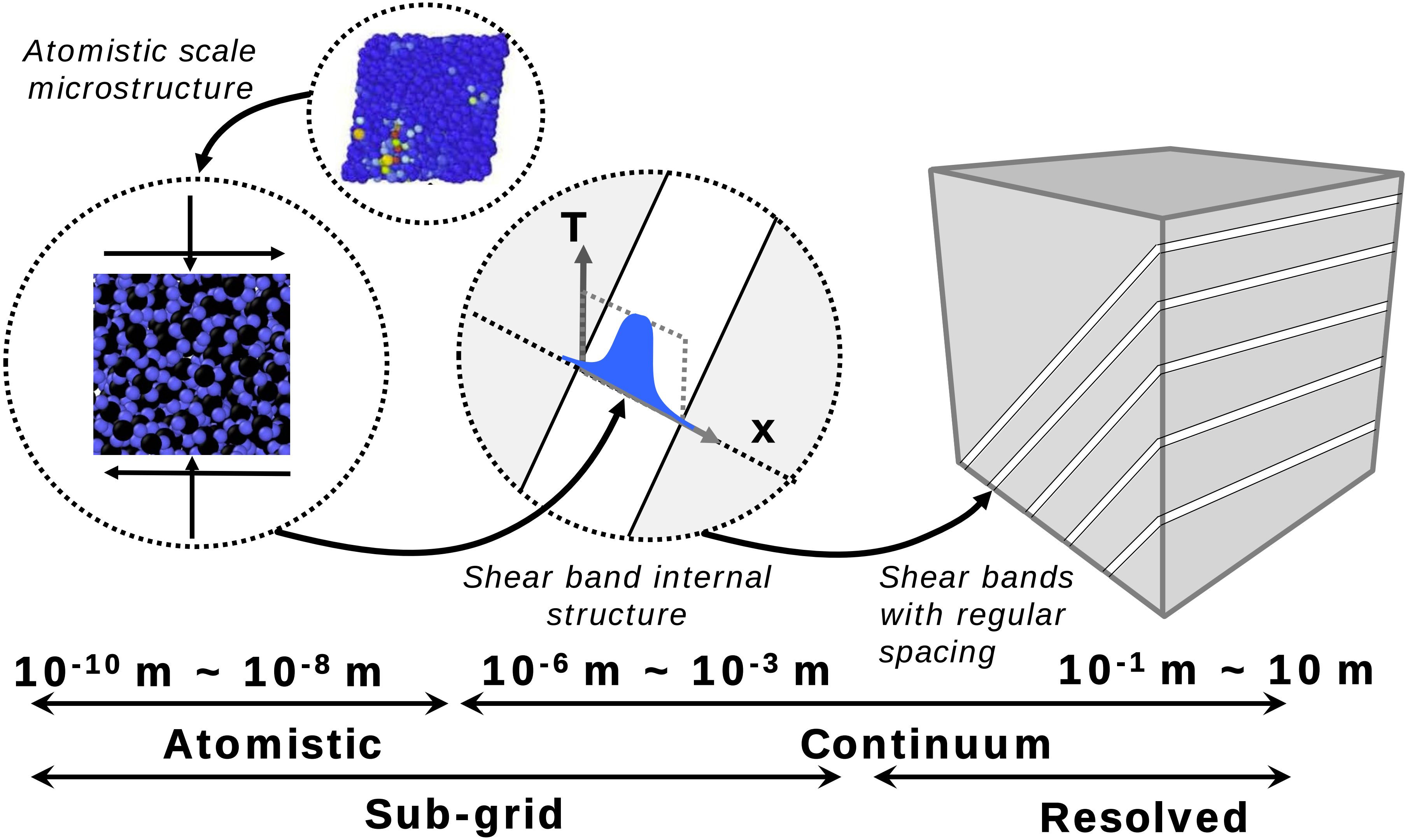
Macro stresses





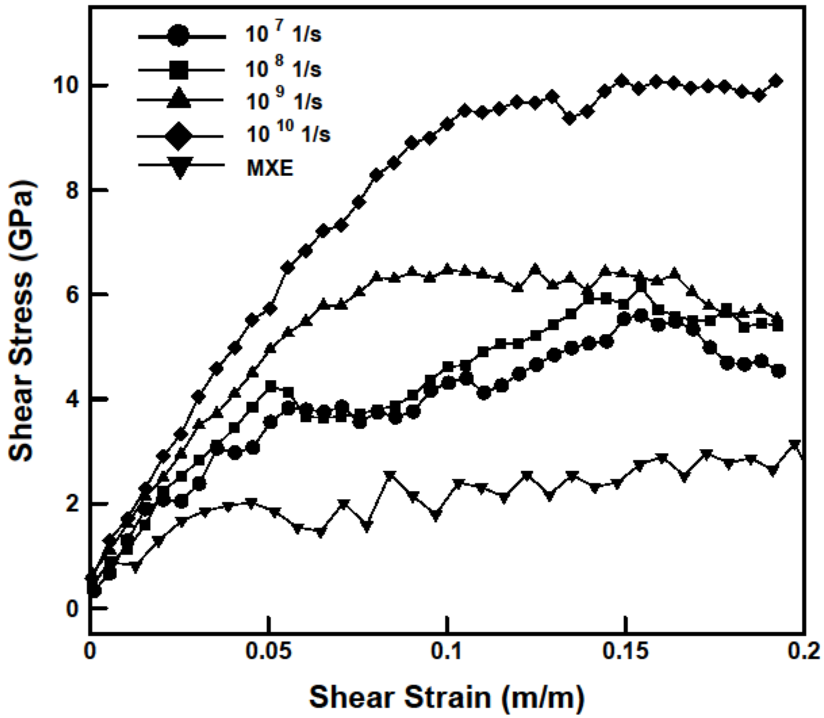
S. Sundaram and R. J. Clifton, *Amer. IoP Conf. Series*, **429** (1998) 517.

Shear-banding analysis

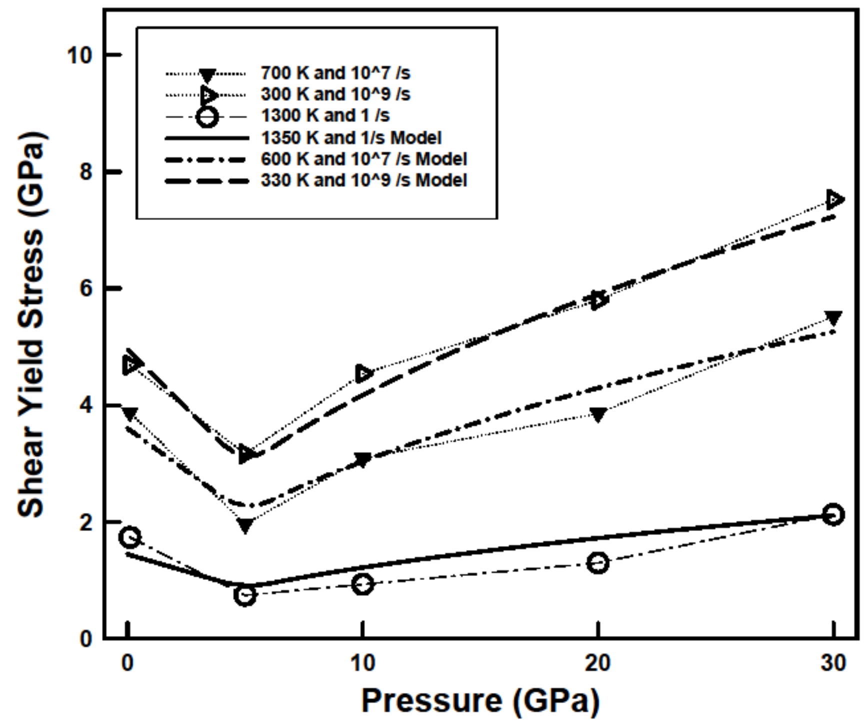


Extension to temperature and rate

Strain rate



Temperature



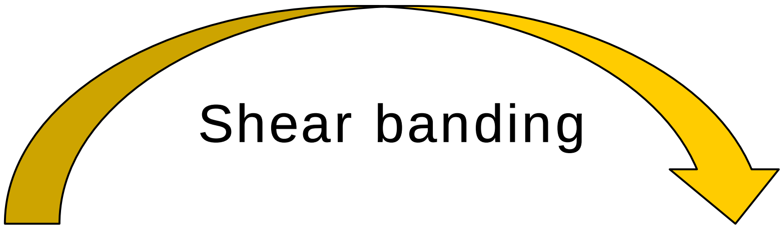
Fitted exponents

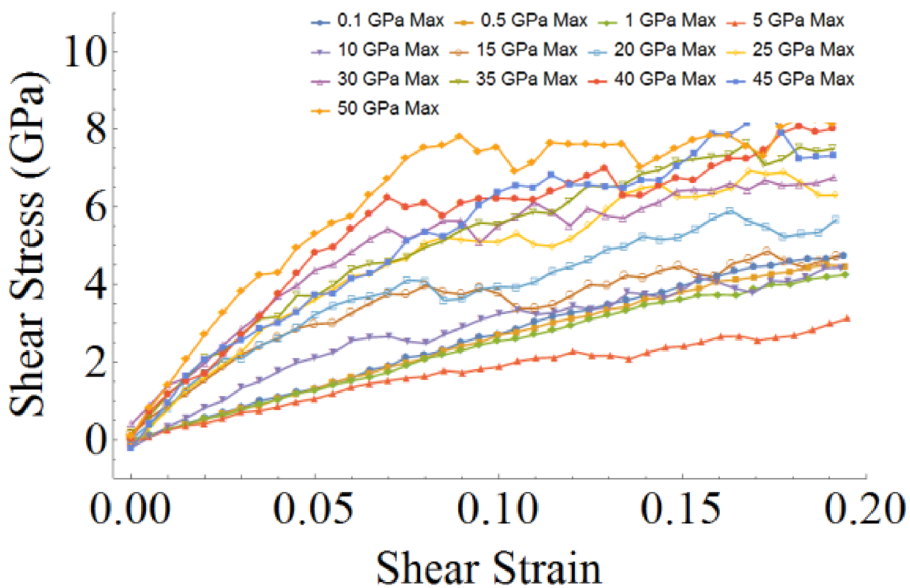
ν	m
-0.268517	0.0176988

$\Longrightarrow$ $m + \nu < 0$ $\Longrightarrow$ Localization!

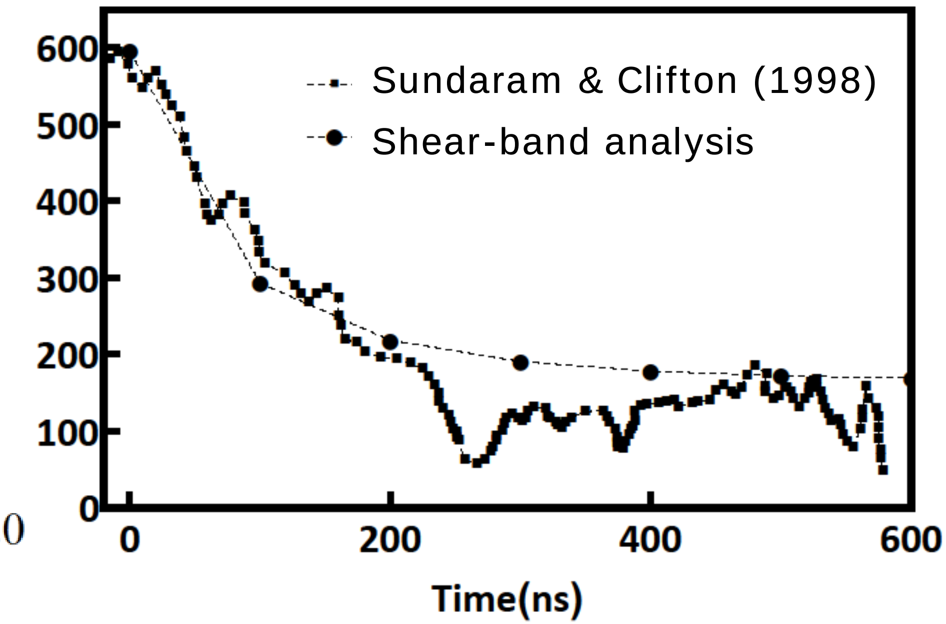
A. Molinari and R. J. Clifton, *JAM ASME*, **54**(4) (1987) 806-812

Shear-banding analysis





Micro stresses



Macro stresses

Stress knock-down factor ~ 10!

S. Sundaram and R. J. Clifton, *Amer. IoP Conf. Series*, **429** (1998) 517.

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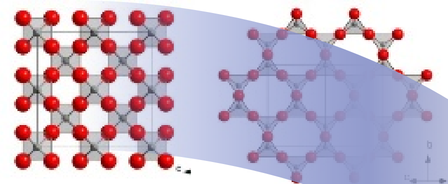
Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

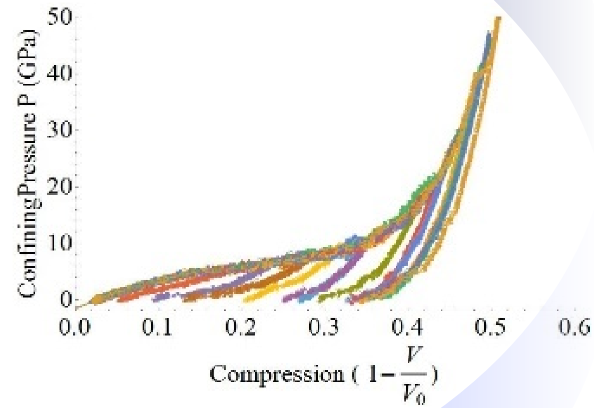


Data Mining

Mesoscopic modeling:

- Critical-state plasticity
- Relaxation
- Shear banding

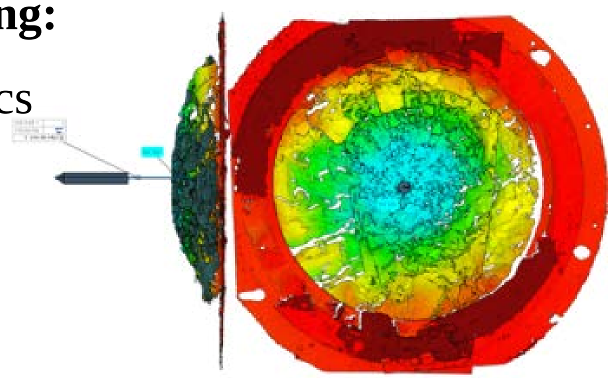
Continuum Models



Macroscopic modeling:

- Terminal ballistics

(OTM ballistic simulation of brittle target , Courtesy B. Li)



Applications

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Take-home thoughts…

- Some natural materials (e.g., fused silica glass) are characterized by elastic domains that are *non-convex* (but not too much...)
- Convexity is not a requirement for the *well-posedness* of the elastic-plastic BVP (existence requires *div-quasiconvexity* only...)
- Direct relevance of atomic-level calculations to macroscopic/engineering properties/applications is often exaggerated
- In most cases, there are several *intervening length/time scales*, relaxation mechanism, between the atomistic and device scales...

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