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

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Glass as protection material

- Glass is attractive in many applications because of its **low density** (2.2 g/cm³), **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.

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)\(^1\).

Fused silica glass: Pressure-shear

Measured elastic moduli showing anomalous dependence on pressure\(^1\)

\[\text{Maximum shear stress (GPa)}\]

\[\text{Average pressure (GPa)}\]

\[0 \rightarrow 80\]

Measured shear yield stress vs. pressure showing non-convex dependence on pressure\(^2\)


Fused silica glass: Pressure-shear

Molecular Dynamics (MD) simulation of amorphous solid showing patterning of deformation field

Multiscale modeling approach

Atomistic modeling of fused silica:
- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity + viscosity + temperature

Mesoscopic modeling:
- Critical-state plasticity

Macroscopic modeling:
- Relaxation

(Data Mining)

Applications

(OVM ballistic simulation of brittle target, Courtesy B. Li)
Multiscale modeling approach

Atomistic modeling of fused silica:
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Computational model – MD

Molecular Dynamics Calculations:

Long-Range Coulombic Interactions:
- Summation is performed in K-space using Ewald summation

Short-Range Interactions:
- BKS Interatomic potential
  \[ E(r_{ij}) = A \exp(-r_{ij}/\rho) - C/r_{ij}^6 + D/r_{ij}^{12} \]

Other computational details:
- Stresses computed through virial theorem
- Strain rate ~ 1x10^7 1/s
- NVE ensemble: temperatures computed from kinetic energy
- NVT ensemble: Thermostating

RVE setup – Quenching

Starting structure: $\beta$-cristobalite

$\beta$-cristobalite: Polymorph characterized by corner-bonded $\text{SiO}_4$ tetrahedra

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

Steps taken during quenching process$^1$:

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

Rapid cooling of a $\beta$-cristobalite melt: Generation of an amorphous structure

Quenching procedure for the generation of amorphous silica. $T=5000K$ at $t=0ps$ and $T=300K$ at $t=470ps$. 
Volumetric compression

Hydrostatic compression/ decompression of amorphous silica:

- Molecular dynamics results exhibit irreversible densification at 14-20 GPa

MD calculations


Molecular basis of densification

Hydrostatic compression/decompression of amorphous silica:

- Irreversible 4-fold to 6-fold coordination transition
- Intermediate 5-fold coordinated dense silica polymorph

\[ \text{(Sato and Funamori, 2010)} \]

Shear modulus vs. pressure

Shear modulus of amorphous silica at constant pressure:

- Shear modulus decreases (increases) at low (high) pressure
- Anomalous shear modulus shows agreement with experiment

Initial shear modulus *versus* pressure

*Anomalous pressure dependence of shear modulus!*

(shear modulus initially decreases with increasing pressure)
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)
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

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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)

Irreversible unloading!

Yield!

Elastic pressure-shear response

Neo-Hookean elastic response fitted to:

- Volumetric compression data (elastic unloading)
- Pressure-shear data (elastic regime)

\[ W^e(C_e) = \frac{\mu(J_c^e)}{2} \left( J_c^{e-2/3} \text{tr}(C_e^e) - 3 \right) + f(J_c^e) \]

Critical-state plasticity model

Densification:

- Pressure-volume response of fuse silica interpreted as consolidation curve in critical state plasticity

\[
\rho_c = -\frac{K_b}{k_b} \left[ (J_p)^{-k_b} - 1 \right] + \Gamma
\]

<table>
<thead>
<tr>
<th>Table 1: Hardening Rule Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_B$</td>
</tr>
<tr>
<td>8.48613 GPa</td>
</tr>
</tbody>
</table>
Critical-state plasticity model

Pressure-shear plasticity:

- Critical states (yielding at constant volume) define Critical State Line

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 SiO₂

CHARLES MEADE AND RAYMOND JEANLOZ

Fig. 1. Maximum shear stress in silica glass at room temperature and average pressures ($P$) 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 $dP/dh$. 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).

Anomalous shear yield stress documented in geophysics literature!
Multiscale modeling approach

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Data Mining

Applications

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Non-convex limit analysis – 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)

Non-convex limit analysis – Relaxation

**Relaxation:**

- Classical limit analysis, kinematic and static problems:
  \[ \inf_v \sup_{\sigma} \left\{ \int_\Omega \sigma \cdot \nabla v \, dx : \sigma(x) \in K, \ v(x) = g(x) \text{ on } \partial \Omega \right\} \]

- Reformulation for non-convex elastic domain \( K \):
  \[ \sup_{\sigma} \inf_v \left\{ \int_\Omega \sigma \cdot \nabla v \, dx : \sigma(x) \in K, \ v(x) = g(x) \text{ on } \partial \Omega \right\} \]

- Reduced static problem:
  \[ \sup_{\sigma} \left\{ \int_{\partial \Omega} \sigma \nu \cdot g \, d\mathcal{H}^2 : \sigma(x) \in K, \ \text{div} \sigma(x) = 0 \text{ in } \Omega \right\} \]

- Supremum non-attained for strongly non-convex \( K \)!

- Div-quasiconvex envelop of \( K \):
  \[ \bar{K} = \{ \sigma : \xi_h \rightarrow \sigma, \ \xi_h(x) \in K, \ \text{div} \xi_h(x) = 0 \text{ in } \Omega \} \]

- Relaxed static problem (attained):
  \[ \sup_{\sigma} \left\{ \int_{\partial \Omega} \sigma \nu \cdot g \, d\mathcal{H}^2 : \sigma(x) \in \bar{K}, \ \text{div} \sigma(x) = 0 \text{ in } \Omega \right\} \]

Non-convex limit analysis – Relaxation

Div-quasiconvex envelop of glass elastic domain:

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

\[
q^2 = c^2 + \frac{3}{4}(p - p_0)^2
\]

Critical-state plasticity – Relaxation

Equilibrium stress field

Pressure oscillations

macrostate
\((\bar{p}, \bar{q})\)

microstates

locus of macrostates

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Applications: Solvers!

Data Mining

Continuum Models

(OTM ballistic simulation of brittle target, Courtesy B. Li)
Recall: Glass as protection material

A soda lime glass target impacted by steel rod at 300 m/s\(^1\).

Optimal transportation problems

• Mass + linear-momentum transport (Eulerian):
  \[
  \begin{align*}
  \partial_t \rho + \nabla \cdot (\rho v) &= 0, \quad \text{in } [0, T] \times \Omega_t, \\
  \partial_t (\rho v) + \nabla \cdot (\rho v \otimes v) &= \nabla \cdot \sigma, \quad \text{in } [0, T] \times \Omega_t, \\
  \sigma &= \sigma(\text{deformation history}), \quad \text{in } [0, T] \times \Omega_t.
  \end{align*}
  \]

• Lagrangian reformulation:
  \[
  \begin{align*}
  \partial_t \varphi &= v \circ \varphi, \\
  \rho \circ \varphi &= \rho_0 / \det(\nabla \varphi).
  \end{align*}
  \]

Geometrically exact!
Optimal transportation — Time-discrete

- Semidiscrete action: \( A_d(\varphi_1, \ldots, \varphi_{N-1}) = \)

\[
\sum_{k=0}^{N-1} \left\{ \frac{1}{2} \frac{d_W^2(\rho_k, \rho_{k+1})}{(t_{k+1} - t_k)^2} - \frac{1}{2} [U(\varphi_k) + U(\varphi_{k+1})] \right\} (t_{k+1} - t_k)
\]

inertia  
potential energy

- Discrete Euler-Lagrange equations: \( \delta A_d = 0 \Rightarrow \)

\[
\frac{2\rho_k}{t_{k+1} - t_{k-1}} \left( \frac{\varphi_{k\rightarrow k+1} - x}{t_{k+1} - t_k} + \frac{\varphi_{k\rightarrow k-1} - x}{t_k - t_{k-1}} \right) = \nabla \cdot \sigma_k + \rho_k b_k
\]

\[
\rho_{k+1} \circ \varphi_{k\rightarrow k+1} = \rho_k / \det (\nabla \varphi_{k\rightarrow k+1})
\]

Geometrically exact!

Optimal Transportation Meshfree (OTM)

nodal points: $x_{a,k}$

material points: $x_{p,k}$

- Material points
- Nodal points

$\varphi_{k\rightarrow k+1}$

$t_k \rightarrow t_{k+1}$

Max-ent interpolation

Max-ent shape functions, $\gamma = \beta h^2$

(i) Explicit nodal coordinate update:

\[ x_{k+1} = x_k + (t_{k+1} - t_k)(v_k + \frac{t_{k+1} - t_k - 1}{2} M_{k-1} f_k) \]

(ii) Material point update:

- position: \( x_{p, k+1} = \varphi_{k\rightarrow k+1}(x_{p, k}) \)
- deformation: \( F_{p, k+1} = \nabla \varphi_{k\rightarrow k+1}(x_{p, k}) F_{p, k} \)
- volume: \( V_{p, k+1} = \det \nabla \varphi_{k\rightarrow k+1}(x_{p, k}) V_{p, k} \)
- density: \( \rho_{p, k+1} = m_p / V_{p, k+1} \)

(iii) Constitutive update at material points

(iv) Reconnect nodal and material points (range searches), recompute max-ext shape functions

Fracture Solver – Material-point erosion

- $\epsilon$-neighborhood construction:
  Choose $h \ll \epsilon \ll L$

- Erode material point $p$ if
  \[ G_{p,h,\epsilon} \approx \frac{E_p h \epsilon}{|K_{\epsilon}|} \geq G_C \]

- Proof of convergence to Griffith fracture:
Fracture of SiO$_2$

Tensile test, brittle fracture, specific fracture energy:
- Common reported values (experimental and MD): $G = 1-10$ J/m$^2$

\[ \gamma = \frac{(E_{\text{final}} - E_{\text{initial}})}{A} \]

\[ G = 2\gamma = 3.1969 \text{ J/m}^2 \]
Fracture of SiO$_2$

Tensile test, brittle fracture, specific fracture energy:
- Variability with respect of initial conditions, area, width

\[ G = 2\gamma = 2.9387 \frac{J}{m^2} \]

\[ G = 2\gamma = 3.03192 \frac{J}{m^2} \]

\[ G = 2\gamma = 3.1969 \frac{J}{m^2} \]
Failure wave in pyrex rod at 210 m/s.

OTM Solver – Failure wave in glass rod

Comparison to Experiment:

- After impact, the failure wave propagates in close agreement with experiment

- \[ V_{\text{failure}}(\text{sim}) = 4.7 \text{ mm/\mu s} \]
- \[ V_{\text{failure}}(\text{exp}) = 4.5 \text{ mm/\mu s} \]

Close Agreement!
OTM Solver – Failure wave in glass rod

A faster impact speed: \( V = 336 \text{ m/s} \)

- Again, the failure wave propagates in close agreement with experiment

\[
V_{\text{failure (sim)}} = 5.4 \text{ mm/\mu s}
\]

\[
V_{\text{failure (exp)}} = 5.2 \text{ mm/\mu s}
\]

Close Agreement!
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Concluding remarks

- Fused silica glass (amorphous) lends itself ideally to multiscale modeling, atoms to solvers.
- Elasticity and yielding of fused silica glass are anomalous:
  - *Shear modulus decreases with increasing pressure*
  - *Critical state line (limit elastic domain) non-convex!*
- Non-convexity of yielding can be relaxed (explicitly and in closed form) by allowing for stress patterning (under equilibrium constraint) at the microscale.
- Particle solvers are powerful for applications involving complex fracture, fragmentation.
- Unmodeled: Thermal EoS, thermal softening, nonlinear viscosity, shear banding...
Thank you