Simulations of shear yielding of glassy solids: Effects of Age, Rate and Temperature

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KITP workshop on
Friction, Fracture and Earthquake Physics
(August 2005)

Shear and flow of glassy matter

- “Hard glasses”: polymers (PS, PC), bulk metallic glasses (BMG)
- “Soft glasses”: colloids, pastes, emulsions, foams

Some fundamental questions:

- What is the elementary mechanism?
  Shear transformation zone (amorph)  Dislocation (crystal)

- What leads to shear localization (bands)?

- Is "jamming" a common feature of these materials?
  What is the nature of the jammed state? Can we "unjam" by applying stress?

Nonequilibrium phase diagram?

A.J.Liu/S.R.Nagel,
Origin of engineering interest in glassy materials

- yield stress of glassy metals can be twice that of steel
- elastic range is much higher
- very promising materials for structural applications

Nonequilibrium molecular dynamics

Bead spring model for polymers:  Binary (80% r₁ - 20% r₂) LJ mixture:

- Lennard-Jones (LJ) potential \( V_{LJ} \) → van der Waals interaction, energy \( u_0 \sim \text{meV} \), length \( d \sim \text{nm} \), time \( \sim \text{ps} \), max force \( f_{LJ} \)
- Covalent bonds for polymers
→ computer glass transition and amorphous glassy state below \( T_g \sim 0.3 \ u_0 / k_B \)

- Molecular dynamics: \( \ddot{r}_i = \sum F_{ij} / m_i \)
  integrate classical equations of motion of many-particle system
- Follow particle motion, measure local or integrated response of system
Deformation of glasses: simulation and experiment

~ 30000 particles

Maximum or overshoot:
yield stress $\tau^y$

unrecoverable strain $\varepsilon_r$

Bulk Metallic Glass
($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$)

Polymer glass (PMMA)

Quinson et al., J. Mat. Sci. 32, 1371 (1997)


Microscopic plastic events during shear

- divide solid into small volume elements
- calculate shear stress and nonaffine disp. $\Sigma_i(r_i - \varepsilon_i r_i)^2$ within each bin
- record number of jumps in a small strain interval as a function of strain
- # and size of stress jumps rises rapidly (exponentially) as peak stress is approached, but present at small strains $\rightarrow$ irreversibility before macroscopic yield point

$\rightarrow$ no single energy barrier, time between jumps strain-dependent!

When does a glassy solid yield?

- Many amorphous materials obey a pressure-modified von Mises criterion:
  \[
  \tau^y_{\text{dev}} = \tau_0 + \alpha p = \frac{1}{3} [ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 ]^{1/2} - (\sigma_1 + \sigma_2 + \sigma_3)/3
  \]

- Assumes isotropic solid

![Loading with general stress states](image)

- when shear localization on a plane occurs, other criteria are suggested:
  - pressure-modified Tresca criterion:
    \[
    \tau_{\text{max}} = \frac{1}{2} |\sigma_1 - \sigma_2|_{\text{max}} = \frac{3}{\sqrt{2}} (\tau_0 + \alpha p)
    \]
  - Mohr-Coulomb criterion:
    \[
    \tau_y = \tau_0 - \sigma_n \tan \Phi
    \]

Obeyed by model glasses, but pbc prevent localization

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Strain rate/temperature dependence of \( \tau^y \)

- polymer and binary mixture: logarithmic rate dependence
  \[
  \tau^y_{\text{dev}} = \tau_0 + s \ln(\dot{\varepsilon})
  \]
  or power law
  \[
  \tau^y_{\text{dev}} = \tau_0 + \dot{\varepsilon}^n
  \]

- Offset \( \tau_0 \) varies linearly with \( T \)
- Prefactor/exponent independent of \( T \), but slightly larger for polymer glass

- Note: all states prepared through rapid quench and very short "waiting time" \( t_w = 750 \tau_{\text{LJ}} \) before straining

Aging in structural glasses

- below $T_g$, glasses are not stationary, but continue to evolve configurational degrees of freedom (aging)

\[ T = 0.2 \frac{u_0}{k_B} \]

\[ T_g \approx 0.3 \frac{u_0}{k_B} \]

- Time-translation invariance broken, quantities depend on $t$ and $t_w$
- Glass compactifies \textit{logarithmically} in absence of deformation when maintaining zero hydrostatic pressure
- strongly temperature dependent, no change at $T=0.01 \frac{u_0}{k_B}$
  \[ \rightarrow \text{aging disappears at lower T!} \]

Effect of aging on shear yield stress

- yield stress also increases \textit{logarithmically} with waiting time
  (see also Varnik/Bocquet/Barrat, J. Chem. Phys. (2004))
- slope independent of shear rate
- qualitatively consistent with $S$(oft) $G$(lassy) $R$(heology) model
Temperature and Aging

- logarithmic behavior at all T
- slope variation with T broadly consistent with linear behavior
- importance of thermodynamic temperature for aging

Combined rate/age effects at $T=0.2 \ u_0/k_B$

- $t_w=750,000 \ \tau_{LJ}$: weak logarithmic behavior at smaller rates
- stresses and rate sensitivity strongly increase with age
- ideal logarithmic behavior at $t_w=750,000 \ \tau_{LJ}$
A phenomenological model

- assume response depends on state variable $\theta(t)$ as in friction models
  \[ \tau^y = \tau_0 + s_0 \ln(\theta) + s_1 \ln(\dot{\epsilon}) \]

- specify evolution of $\theta(t)$: here $\dot{\theta} = f(\varepsilon_{zz}, T)$ and integrate to yield
  \[ \tau^y = \tau_0 + s_0 \ln(t_w + \alpha / \dot{\epsilon}) + s_1 \ln(\dot{\epsilon}) \]

- Note:  
  - if $f$ independent of strain: $\alpha = \varepsilon^y$ (strain at yield)
  - if rejuvenation before yield: $\alpha < \varepsilon^y$
  - if strain accelerates aging: $\alpha > \varepsilon^y$

- Predicts "universal" plot in $\dot{\epsilon}_{tw}$

\[ \tau^y + (s_1 - s_0) \ln(t_w / t_w^0) = \tau_0 + s_0 \ln(\dot{\epsilon}_{tw} + \alpha) + (s_1 - s_0) \ln(\dot{\epsilon}_{tw}) \]

- Note: description does not invoke simple relations between "relaxation time" and waiting time.

Universal behavior

- data collapses onto single curve when rate is rescaled with $t_w$ AND shifted by waiting time dependent constant

- regime I: $t_w$ irrelevant, only aging during straining. $\tau^y \propto (s_1 - s_0) \ln(\dot{\epsilon}_{tw})$

- regime II: no intrinsic dynamics before yielding. $\tau^y \propto s_1 \ln(\dot{\epsilon}_{tw})$

- crossover when $t_w = \alpha / \dot{\epsilon}$

(JR and M. O. Robbins, condmat/0506586)
Peak stress vs. steady shear flow stress

- in steady shear, system is constantly stirred ("rejuvenated"); never older than $1/\dot{\varepsilon}$

![Graph showing peak stress vs. steady shear flow stress for different temperatures](image)

(JR and M. O. Robbins, PR E (2003))

- in regime I, the (transient) peak stress should start to behave like steady state flow stress. Slopes are indeed comparable.

- slope indep. of $T$: role of effective temperature in driven glass?

Conclusions

- simple molecular models for polymers and binary glasses capture phenomenology of elastoplastic deformation

- pressure-modified von Mises shear yield criterion $\tau_y = \tau_0 + \alpha p$ holds for general triaxial loading conditions and homogeneous deformation

- rate and temperature dependence exhibits complex interplay with the intrinsic "aging" dynamics of the glass

- in general logarithmic rate dependence, but slope depends on age and changes when age $\sim$ time to yield.

- rate-state model based on internal state variable provides unifying description of age/rate/temperature effects

$\rightarrow$ Future work: better connection between coarse-grained models and molecular level processes