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

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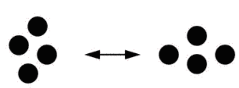
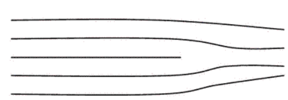
Shear and flow of glassy matter

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

Some fundamental questions:

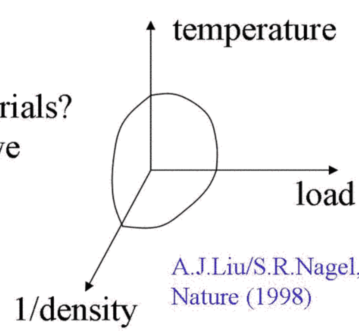
- What is the elementary mechanism?
  Shear transformation zone (amorph) Dislocation (crystal)





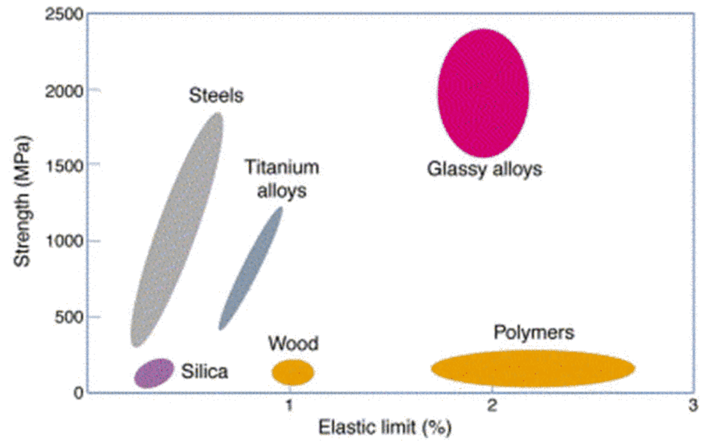
- What leads to shear localization (bands)?
- Is "jamming" a common feature of these materials? What is the nature of the jammed state? Can we "unjam" by applying stress?

Nonequilibrium phase diagram?



A.J.Liu/S.R.Nagel, Nature (1998)

Origin of engineering interest in glassy materials

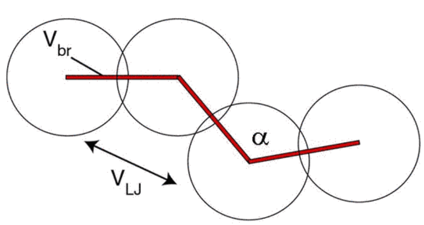


Materials Today, March 2004

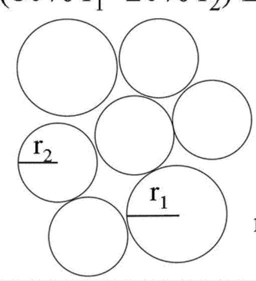
- yield stress of glassy metals can be twice that of steel
- elastic range is much higher
- very promising materials for structural applications

Nonequilibrium molecular dynamics

Bead spring model for polymers:



Binary (80% r_1 - 20% r_2) LJ mixture:



$r_2/r_1 = 0.88$

- Lennard-Jones (LJ) potential $V_{LJ} \rightarrow$ van der Waals interaction, energy $u_0 \sim$ meV, length d ~ nm, time ~ ps, max force f_{LJ}
- Covalent bonds for polymers

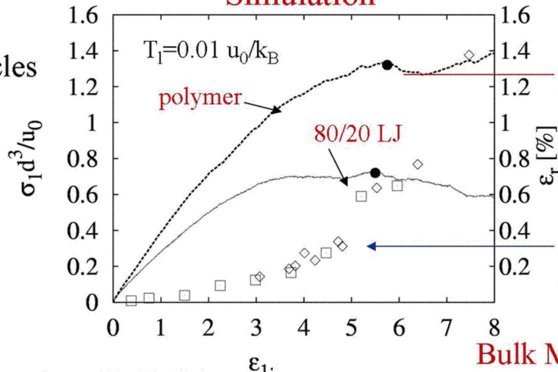
$\rightarrow$ computer glass transition and amorphous glassy state below $T_g \sim 0.3\ u_0/k_B$

- Molecular dynamics: $\ddot{\mathbf{r}}_i = \sum_{i,j} \mathbf{F}_{i,j} / m_i$
  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

Simulation

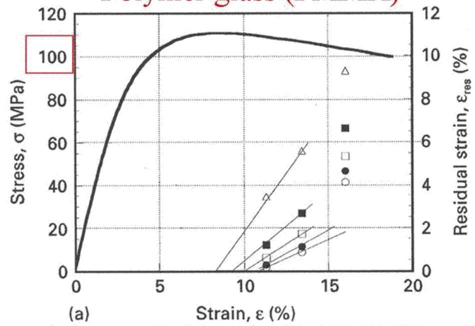
~ 30000 particles



Maximum or overshoot: yield stress τ^y

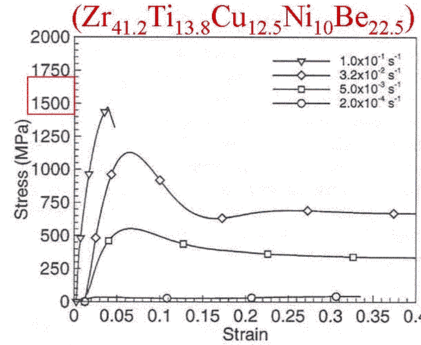
unrecoverable strain ε_r

Polymer glass (PMMA)



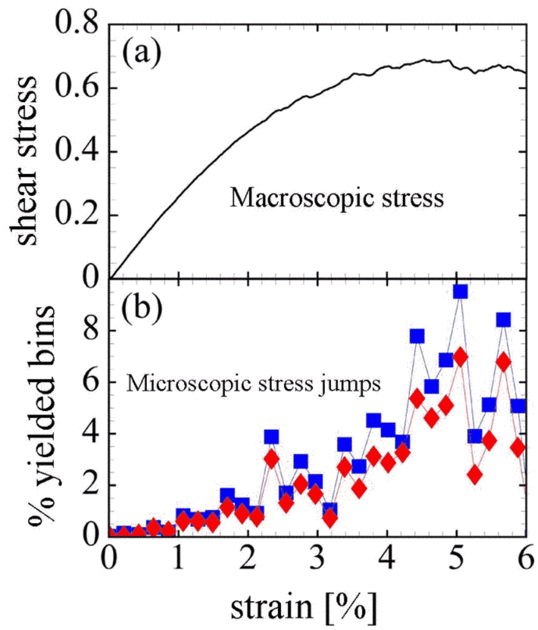
Quinson et al., J. Mat. Sci. **32**, 1371 (1997)

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



Lu et al., Acta Mat., **51, 3429** (2003)

Microscopic plastic events during shear



- divide solid into small volume elements
- calculate shear stress and nonaffine disp. $\Sigma_i(r_i-\varepsilon_{ij}r_j)^2$ 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 → irreversibility before macroscopic yield point

→ no single energy barrier, time between jumps strain-dependent!

JR, M. O. Robbins, Comp. Phys. Comm. (2005)

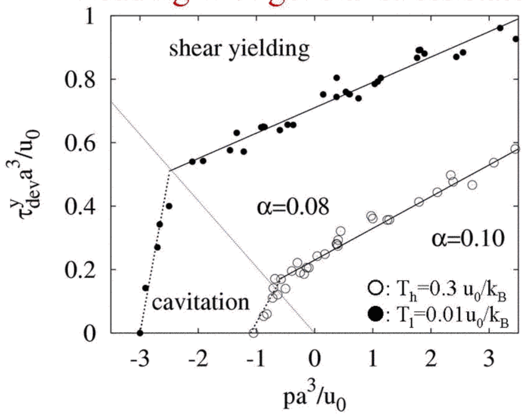
When does a glassy solid yield?

- Many amorphous materials obey a pressure-modified von Mises criterion:

$$\tau^y_{dev} = \tau_0 + \alpha p \qquad \tau_{dev} = \frac{1}{3}\left[(\sigma_1-\sigma_2)^2 + (\sigma_2-\sigma_3)^2 + (\sigma_3-\sigma_1)^2\right]^{1/2} \quad p = -(\sigma_1+\sigma_2+\sigma_3)/3$$

- Assumes isotropic solid

Loading with general stress states



Obeyed by model glasses, but pbc prevent localization

- when shear localization on a plane occurs, other criteria are suggested:

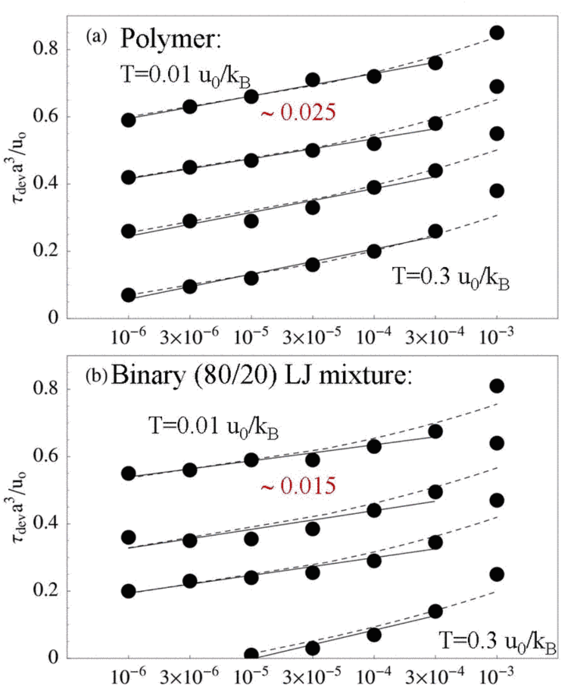
pressure-modified Tresca criterion:

$$\tau_{max} = \frac{1}{2}|\sigma_i - \sigma_j|_{max} = \frac{3}{\sqrt{2}}(\tau_0 + \alpha p)$$

Mohr-Coulomb criterion:

$$\tau_y = \tau_0 - \sigma_n \tan\Phi$$

Strain rate/temperature dependence of τ^y



- polymer and binary mixture: logarithmic rate dependence

$$\tau^y_{dev} = \tau_0 + s\ln(\dot{\varepsilon})$$

or power law

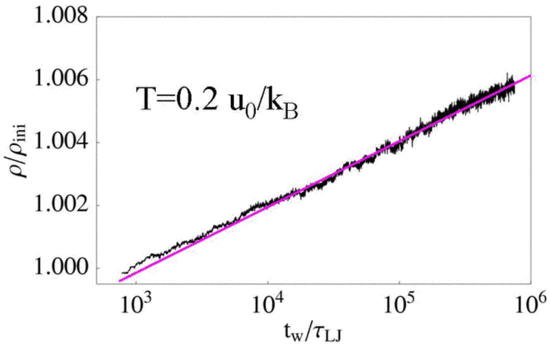
$$\tau^y_{dev} = \tau_0 + \dot{\varepsilon}^n$$

- offset τ_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 τ_{LJ} before straining

JR and M. O. Robbins, Phys. Rev. E **68**, 011507 (2003)

Aging in structural glasses

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

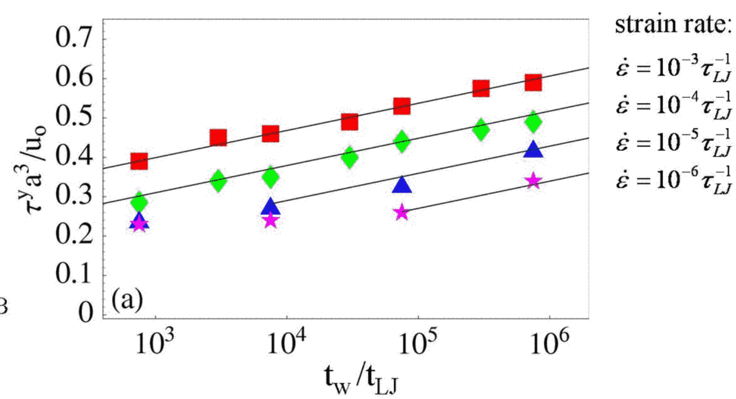


$T_g \sim 0.3\ u_0/k_B$

- Time-translation invariance broken, quantities depend on t and t_w
- Glass compactifies logarithmically in absence of deformation when maintaining zero hydrostatic pressure
- strongly temperature dependent, no change at T=0.01 u_0/k_B
  → aging disappears at lower T!

Effect of aging on shear yield stress

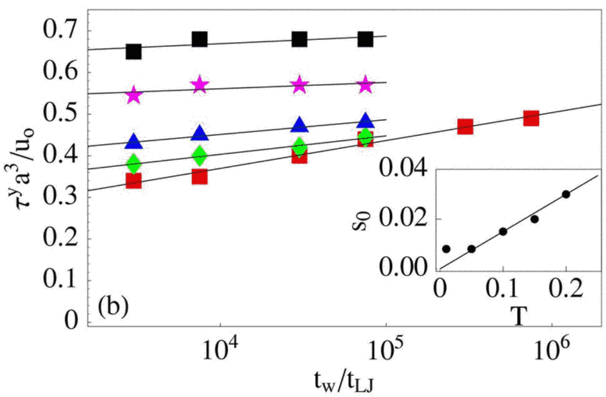
one fixed
T=0.2 u_0/k_B



- yield stress also increases 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

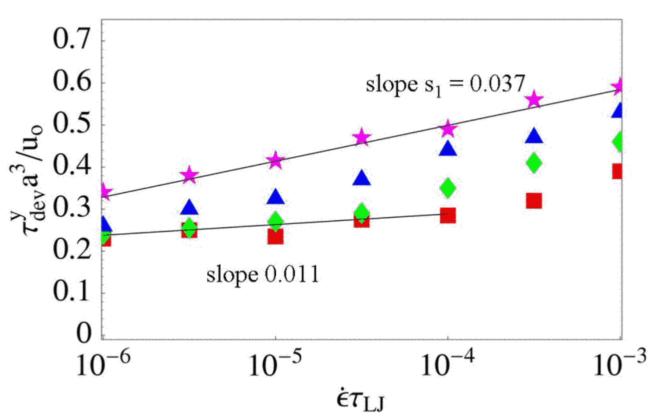
T=0.01 u_0/k_B
T=0.05 u_0/k_B
T=0.1 u_0/k_B
T=0.15 u_0/k_B
T=0.2 u_0/k_B



one fixed
$\dot{\varepsilon} = 10^{-4}\tau_{LJ}^{-1}$

- 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 τ_{LJ}
t_w=75,000 τ_{LJ}
t_w=7,500 τ_{LJ}
t_w=750 τ_{LJ}

- t_w=750 τ_{LJ}: weak logarithmic behavior at smaller rates
- stresses and rate sensitivity strongly increase with age
- ideal logarithmic behavior at t_w=750,000 τ_{LJ}

A phenomenological model

- assume response depends on state variable θ(t) as in friction models

$$\rightarrow \ \tau^y = \tau_0 + s_0 \ln(\theta) + s_1 \ln(\dot{\varepsilon})$$

- specify evolution of θ(t): here $\dot{\theta} = f(\varepsilon_{zz}, T)$ and integrate to yield

$$\tau^y = \tau_0 + s_0 \ln(t_w + \alpha / \dot{\varepsilon}) + s_1 \ln(\dot{\varepsilon})$$

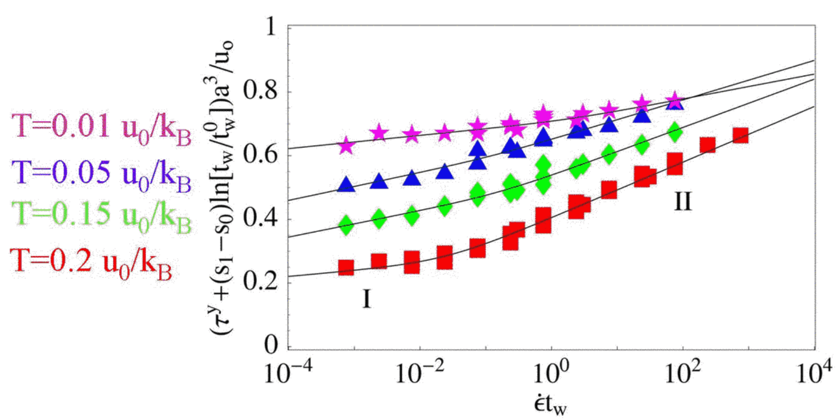
- Note:
  - if *f* independent of strain: $\alpha = \varepsilon^y$ (strain at yield)
  - if rejuvenation before yield: $\alpha < \varepsilon^y$
  - if strain accelerates aging: $\alpha > \varepsilon^y$

- Predicts "universal" plot in $\dot{\varepsilon} t_w$

$$\tau^y + (s_1 - s_0)\ln(t_w / t_w^0) = \tau_0 + s_0 \ln(\dot{\varepsilon} t_w + \alpha) + (s_1 - s_0)\ln(\dot{\varepsilon} t_w)$$

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

Universal behavior



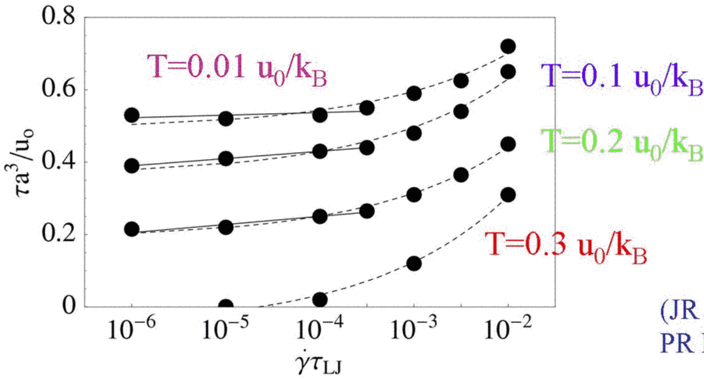
For ALL temperatures!

- 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, $\tau^y \propto (s_1 - s_0)\ln(\dot{\varepsilon} t_w)$
- regime II: no intrinsic dynamics before yielding, $\tau^y \propto s_1 \ln(\dot{\varepsilon} t_w)$
- crossover when $t_w = \alpha / \dot{\varepsilon}$

(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 $1/\dot{\varepsilon}$



(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 ~ time to yield.
- rate-state model based on internal state variable provides unifying description of age/rate/temperature effects

→ Future work: better connection btwn coarse grained models and molecular level processes