Deformation Mechanisms and Rates in Glasses

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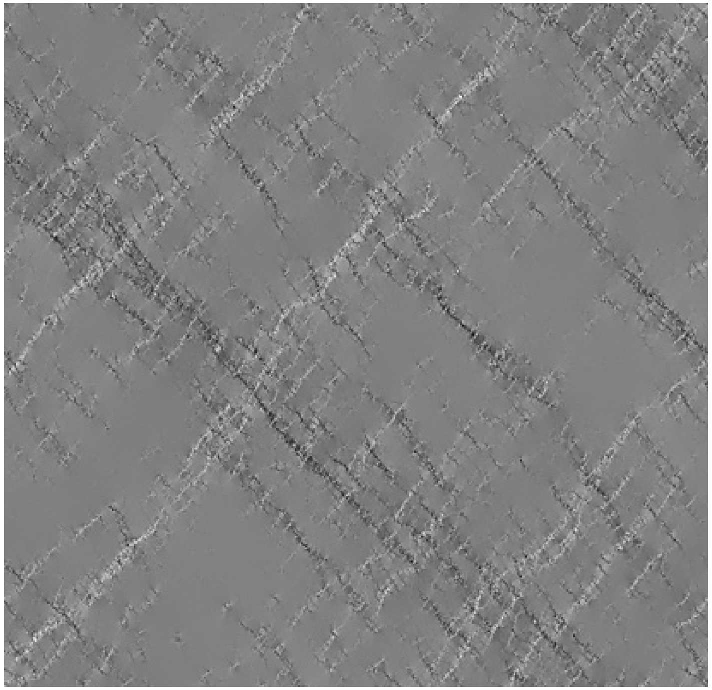
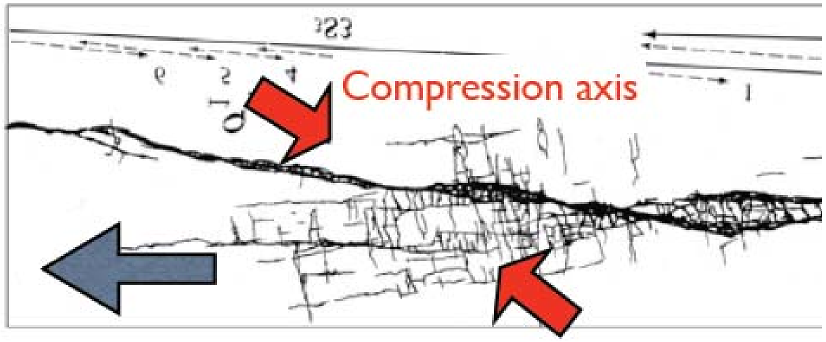
KITP, June 15, 2010





What values of stress tensor σ_{ij} cause yield?

Isotropic $\Rightarrow$ Construct scalars from eigenvalues of σ_{ij}

$$p = -(\sigma_1 + \sigma_2 + \sigma_3)/3$$

$$\tau_{dev} = \frac{1}{3}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]^{1/2} \qquad \tau_{\max} = \frac{1}{2}\left|\sigma_i - \sigma_j\right|_{\max}$$

Classic yield criteria for atomic and granular solids:

von Mises → yield when shear energy large $U \propto \tau^2_{dev}$

Glasses harder to shear when under pressure

$\Rightarrow$ Pressure-modified von Mises: $\tau^y_{dev} = \tau_0 + \alpha p$

Influence of all σ_i $\Rightarrow$rotating region not sliding on plane

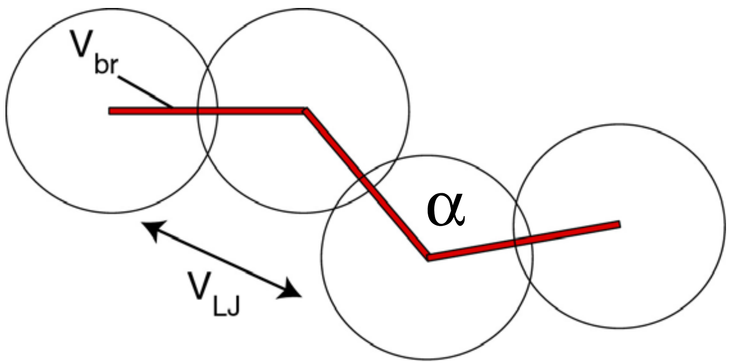
Pressure-modified Tresca (PMT): $\tau^y_{\max} = \frac{3}{\sqrt{2}}(\tau_0 + \alpha p)$

Mohr-Coulomb (MC) → friction motivated, anisotropic

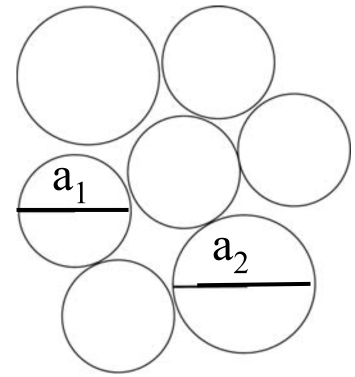
Yield if (shear stress)/(normal stress) > μ on some plane

Potentials and Shear Geometries

Bead spring model for polymers:

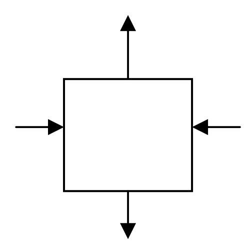


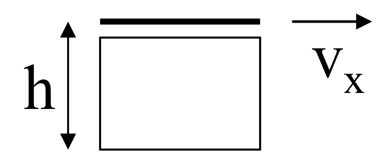
Binary mixture: LJ or harmonic



Kobb-Andersen model

- Lennard-Jones potential $V_{LJ}(r) = 4u_0[(a/r)^{12} - (a/r)^6] \rightarrow$ van der Waals
  energy $u_0 \sim$ meV, length $a \sim$ nm, time $\tau_{LJ} \sim$ ps, max force f_{LJ}
- Covalent bonds $V_{br} \rightarrow$ FENE potential form linear chains of N spheres
  bond-angle potential straightens chains $\rightarrow$ change entanglement length N_e
- Competing lengths $\Rightarrow$Frustration $\rightarrow$ amorphous glass below $T_g \sim 0.35u_0/k_B$





Vary T from 0.0 to $0.3u_0/k_B \sim T_g$

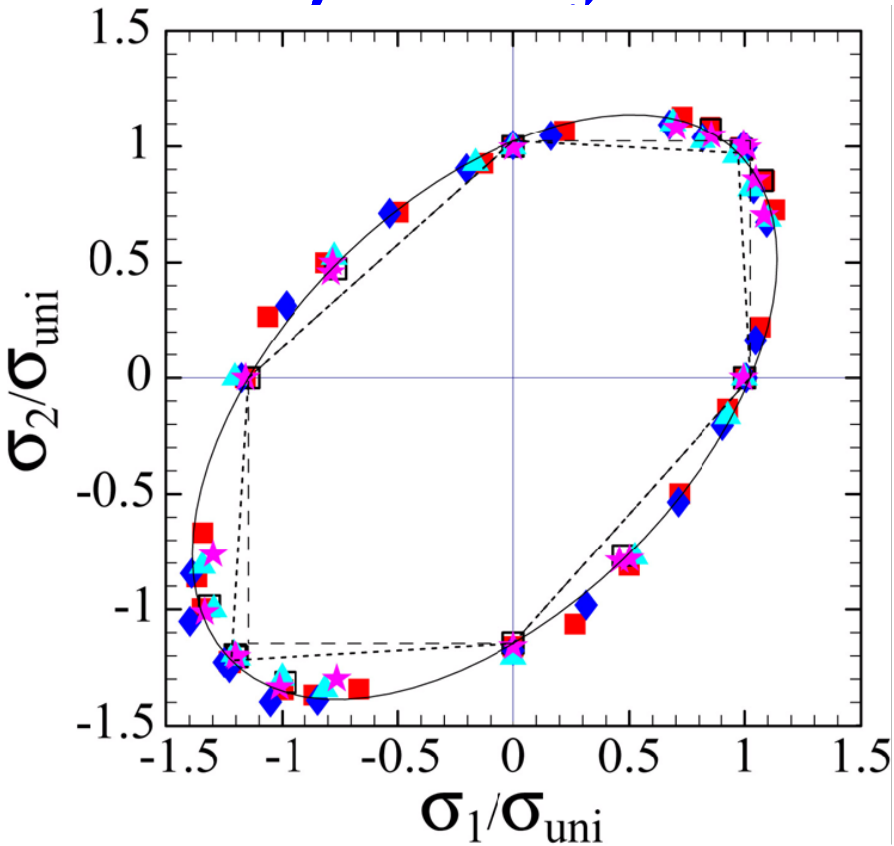
Apply strain in two ways:

Strain periodic cell by changing L_x, L_y, L_z at fixed $\dot{\varepsilon}_z = L_z^{-1}\, dL_z/dt$

Confine binary mixture between moving walls$\rightarrow$ mean $\dot{\gamma} = v_x/h$

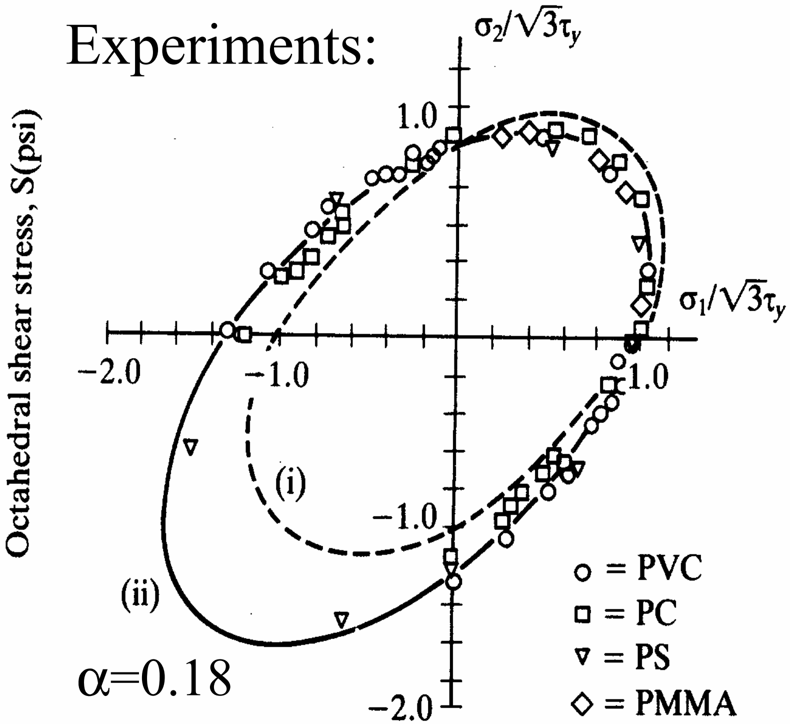
At least 32,768 beads in system unless noted

Test of shear yield criteria for biaxial loading



T=0.01-0.3~T_g, binary LJ,
short & long chains, flex & semiflex

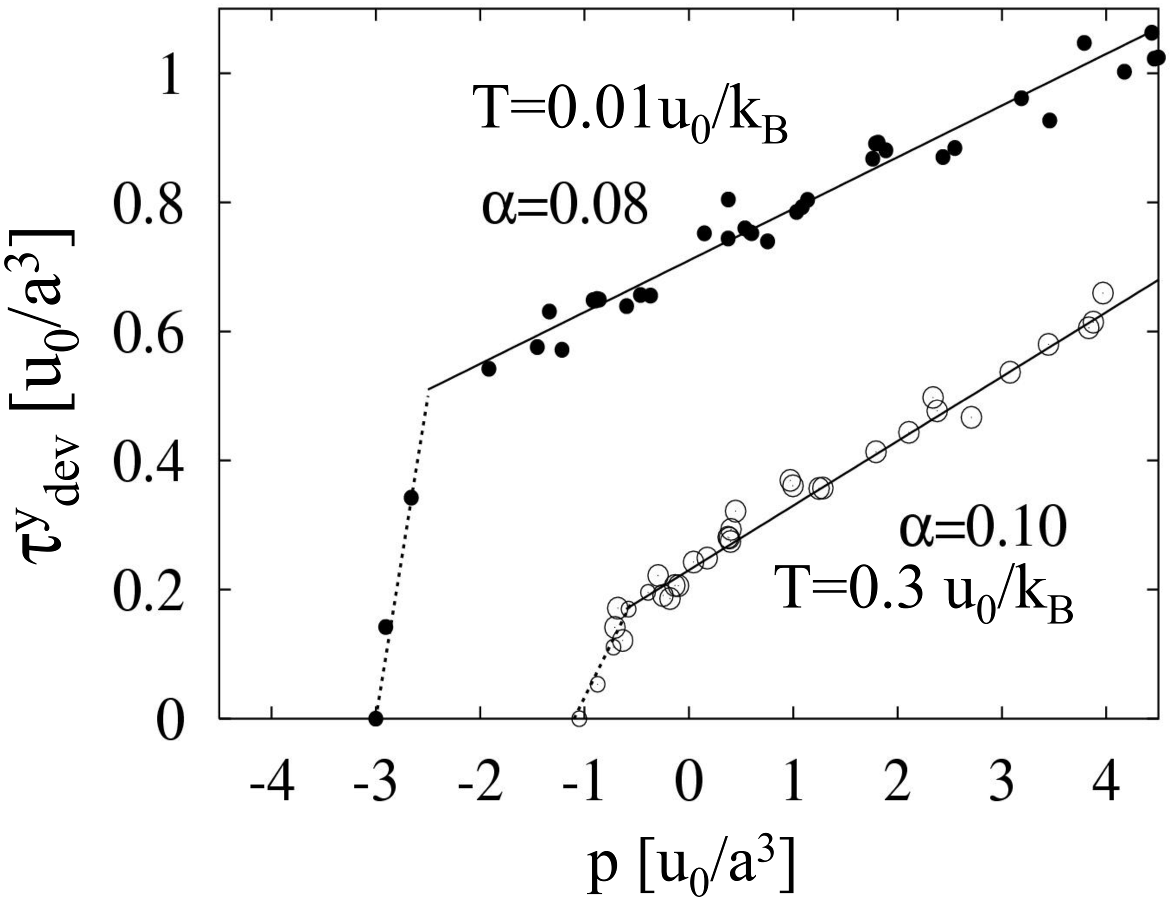
Phys. Rev. E 64, 051801 (2001)



From: T.H.Courtney, Mechanical Behavior of Materials

- Define yield by peak in stress-strain curve. 0.2% yield gives same behavior
- Pressure modified Von Mises → elliptical yield surface fits data for different chain lengths, bond-angle forces, system sizes, adhesion
- Tresca (dotted) and Mohr-Coulomb (dashed) → polygonal yield surface, poor fit

Pressure-modified Von Mises collapses multiaxial results



Equally good collapse for binary mixture, flexible & semiflexible polymers

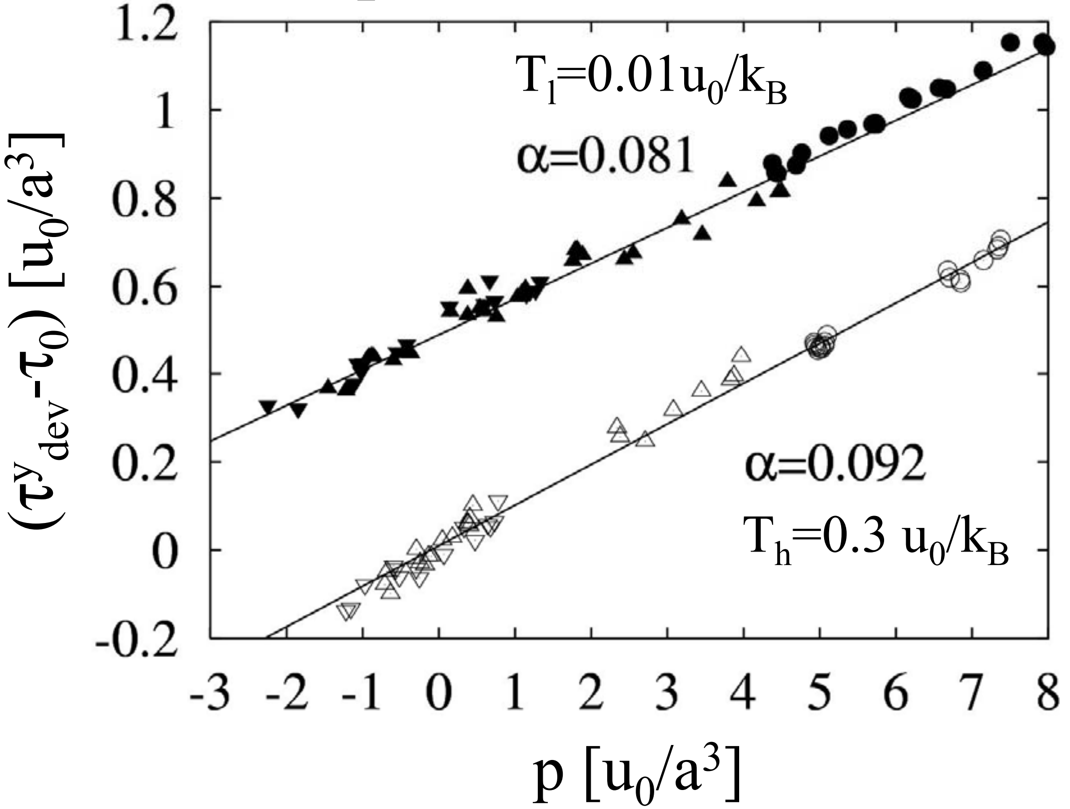
(JR and MOR, Phys. Rev. E 64, 051801 (2001))

⇒Von Mises criterion $\tau^{y}_{dev} = \tau_0 + \alpha p$ describes yield by shear under multiaxial loading (solid lines)

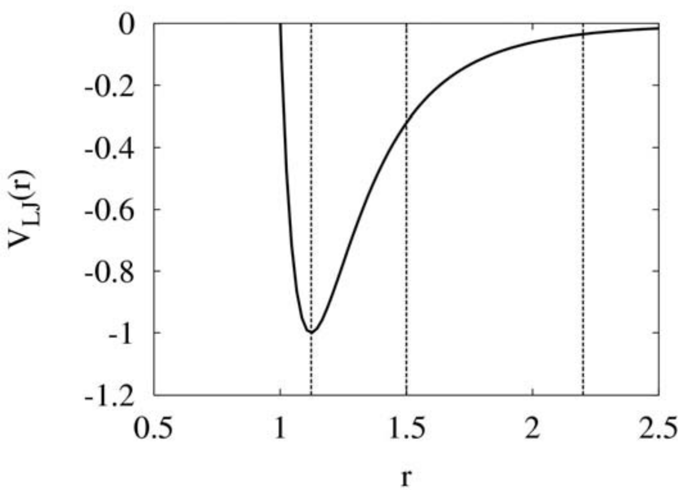
⇒ Fails when system cavitates → craze forms if $N \geq 2N_e$
New criteria for cavitation $p^c = p_0 + \beta\tau_{dev}$ (dashed lines)

What determines τ_0 and α?

Data collapse for 3 different amounts of adhesion → r_c



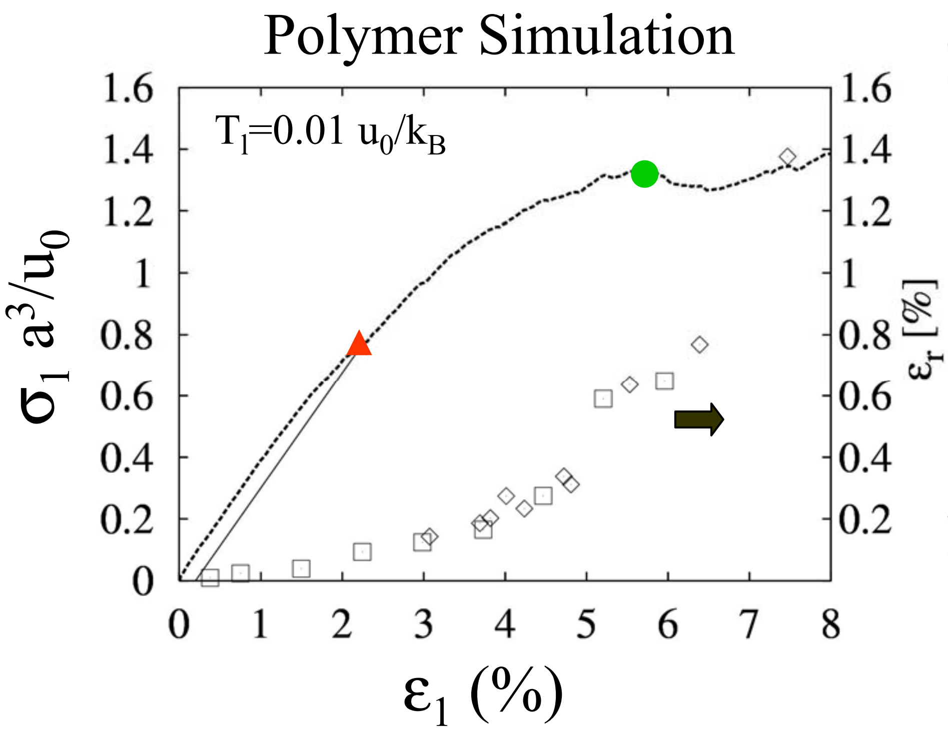
3 cutoff ranges r_c

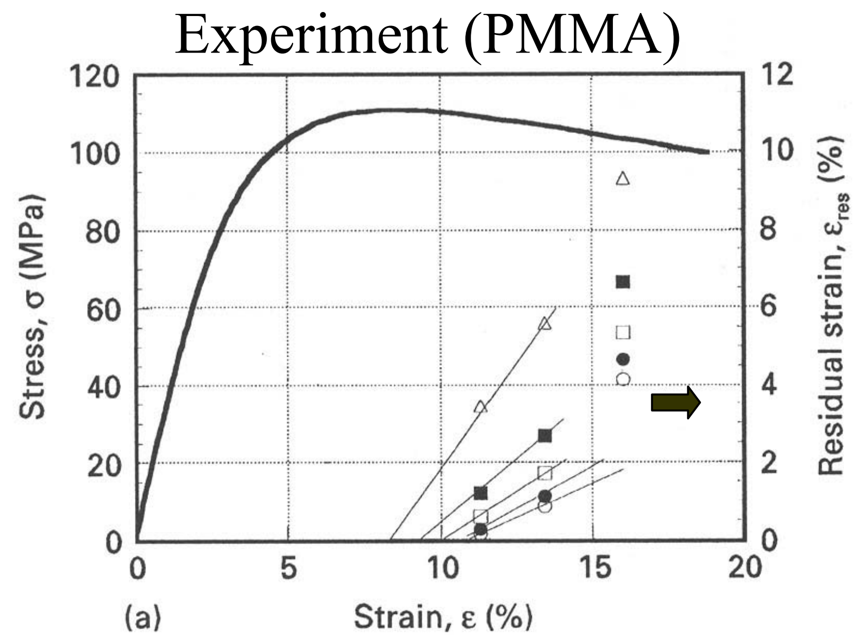


$$\tau^y_{dev} = \tau_0 + \alpha p$$

- τ_0 set by adhesive interaction (cutoff range r_c)
- α independent of r_c, set by bead geometry, as in solid friction
- No dependence on chain length N, only local structure important
- Difficulty of rotating region increases with pressure confining it

Residual Strain After Stress Cycle → No Elastic Region





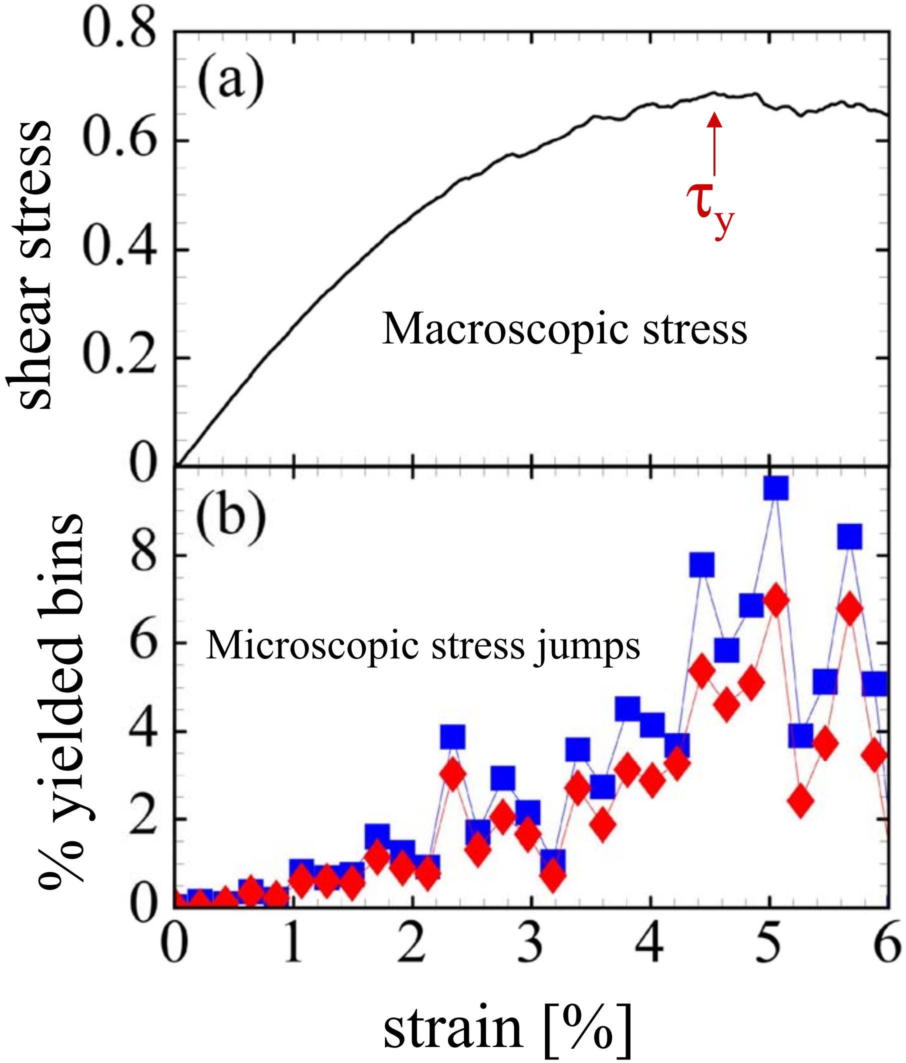
Quinson et al., J. Mat. Sci. **32**, 1371 (1997)

- Simulation and experiment show similar stress curves
- Simulations indicate any nonzero strain gives ε_r>0 in thermodynamic limit!
- As increase system size → first event at smaller strain
  → decrease structure on σ_1 from individual plastic events
- Common to define yield at maximum stress ●, 0.2% yield stress ▲

MR4

Microscopic plastic events during shear

J. Rottler and M. O. Robbins, Comp. Phys. Comm. (2005)

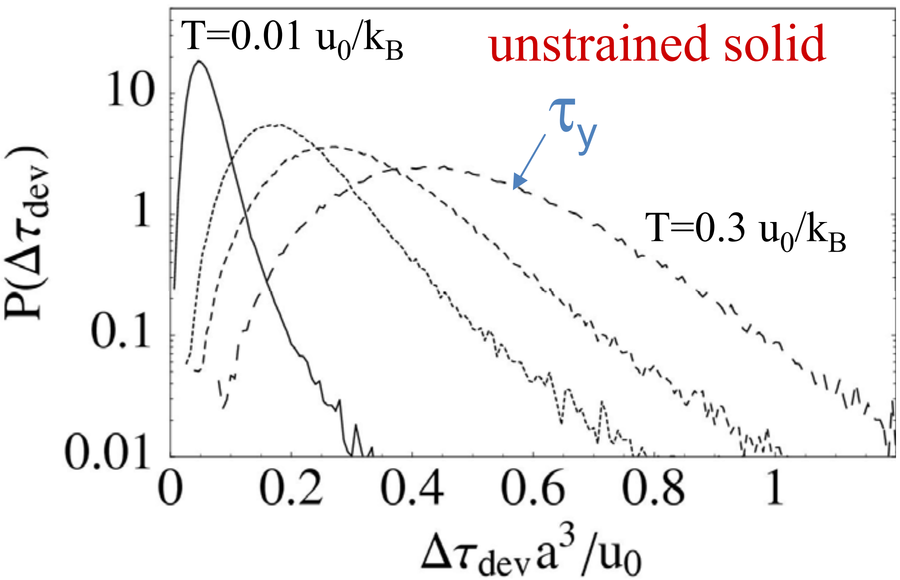


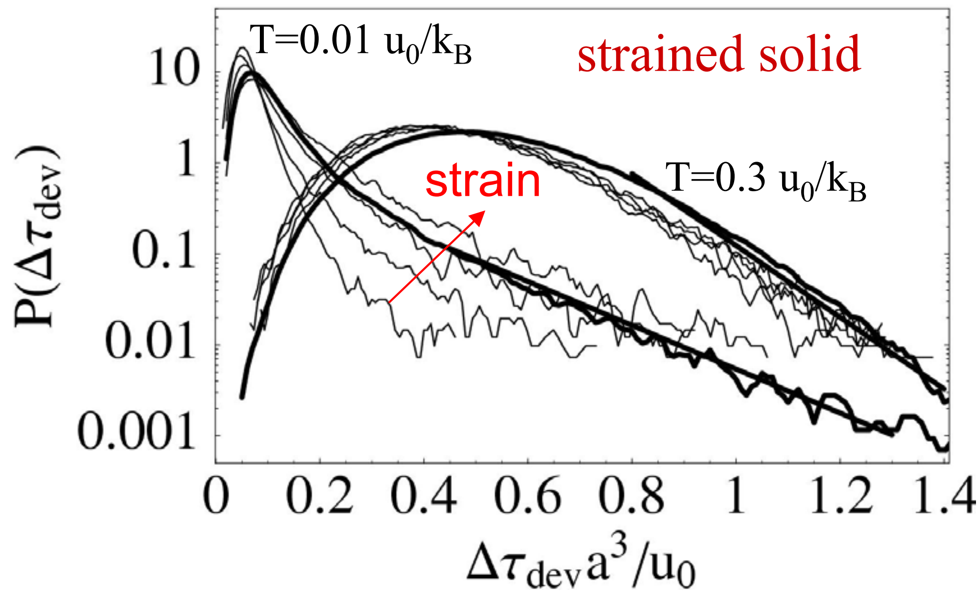
- Divide solid into small volumes: $8a^3$
- Calculate shear stress and nonaffine disp. $\Sigma_i(r_i-\varepsilon_{ij}r_j)^2$ in each
- Record number of jumps in a small strain interval as a function of strain
- # and size of stress jumps rises rapidly as peak stress is approached, but present at arbitrarily small strains
  → no clear point where yield starts
  → Identify yield stress with initial peak in octahedral stress
- At low T, strain increases event rate
- Near Tg the rate of events is nearly independent of strain

MR4 What can one say about relation between rate of plastic deformation and deviation from linear elasticity? Is it a tautology that the acoustic emission tracks the anelastic behavior, or does one need to lookat work and energy to figure this out?

Mark Robbins, 2/4/2007

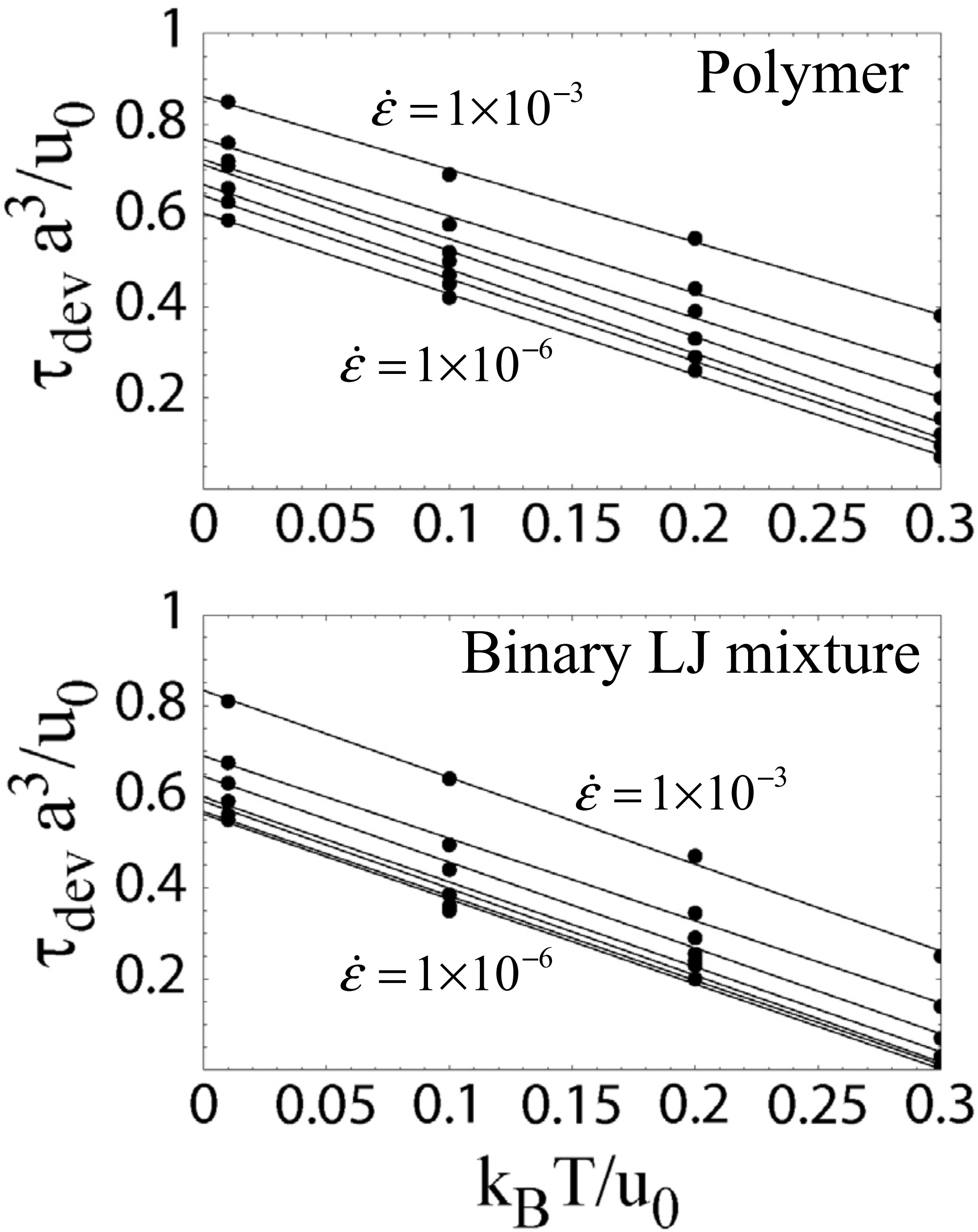
Microscopic Stress Dynamics





- $\Delta\tau_{dev}$ - change in local stress tensor over $7.5\tau_{LJ}$ in small volume elements containing 7-8 particles
- close to T_g=0.35, $P(\Delta\tau_{dev})$ ~ independent of shear strain
- low T, tail grows with increasing strain
- tail can be fitted to exponential,
  similar slope near peak stress as for steady shear – dark lines
  ⇒ microscopic evidence for noise temperature "x"?

Temperature dependence of τ^{y}_{dev}



- Both models show linear decrease in τ^{y}_{dev} as T rises (fix p=0 not density)
- Slope independent of strain rate, offset varies with rate
- Yield stress vanishes above rate-dependent "T_g"

MR5

Thermal and Energetic Stresses

Total stress: $\sigma_{tot}=-(\partial w/\partial\lambda) =(\partial u/\partial\lambda)-(\partial q/\partial\lambda)=\sigma_U+\sigma_Q$

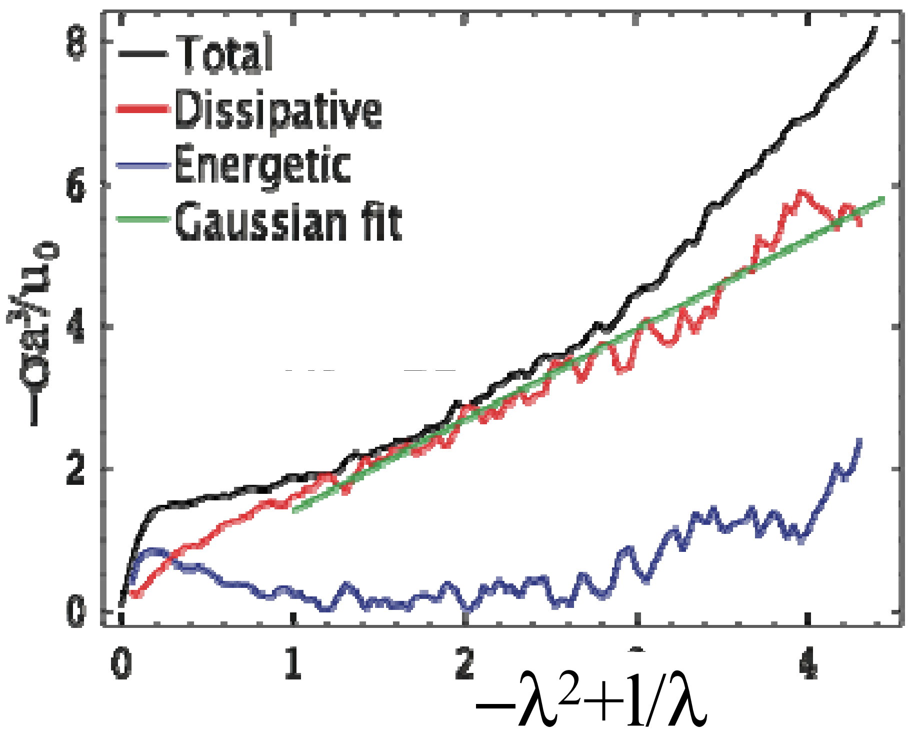
Find energetic stress strongly dependent on initial conditions

Thermal stress σ_Q strongly correlated with dissipated energy

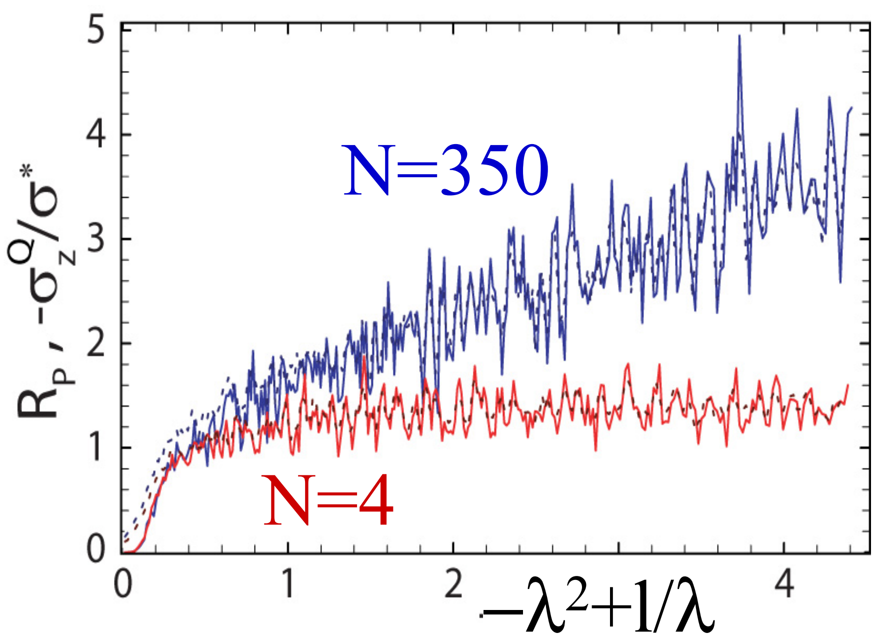
T=0 direct relation to rate of plasticity $R_P \equiv f/\delta\varepsilon$

Fraction f of bonds (r<1.5a) that "break" ($|\Delta r|$>20%)

over small strain interval $\delta\varepsilon$=0.005



Uniaxial: $\lambda=L_z/L_{z0}$



MR5 Mention experiment

Mark Robbins, 3/7/2007

Main Conclusions

1. Yield criterion provides information about deformation mode
   Find pressure-modified von-Mises in experiment and theory
   Implies all eigenvalues of pressure-stress tensor matter, not just smallest and largest that define shear plane.
   Suggests complex domains with boundaries in all directions move past each other, not simple plane of slip

2. Plastic rearrangements occur at arbitrarily small strains in the thermodynamic limit.
   Observe as bond-breaking, large changes in stress or non-affine displacements, unrecoverable strain after unloading
   Rate of plasticity rises rapidly as approach peak stress (yield) then saturates in steady state

Main Conclusions (cont.)

3. Common view is that stress plays a key role in reducing barriers for plastic flow and enhancing thermal activation
   Direct measure of rate and magnitude of local changes shows large stress effect at low temperatures – $T_g/30$
   However, near T_g stress has little affect on rate of plasticity
   Consistent with observation that yield stress has dropped significantly from intrinsic value set by density and scale of interactions $\Rightarrow$ fluctuations overwhelm T=0 barriers
   Yield stress drops nearly linearly at each strain rate hitting zero at something like strain-rate dependent T_g

4. Dissipative stress = rate of work – rate of pot. energy rise scales directly with rate of bond breaking events

References

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