Plastic Deformation in Amorphous Solids: Effective Temperature and Shear Localization

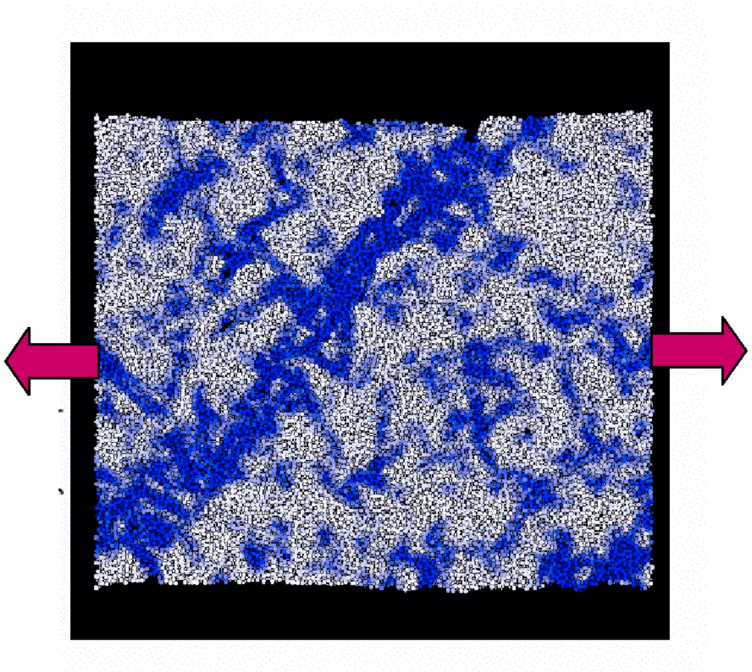
J.S. Langer, UCSB
KITP Granular Materials Seminar
April 21, 2005

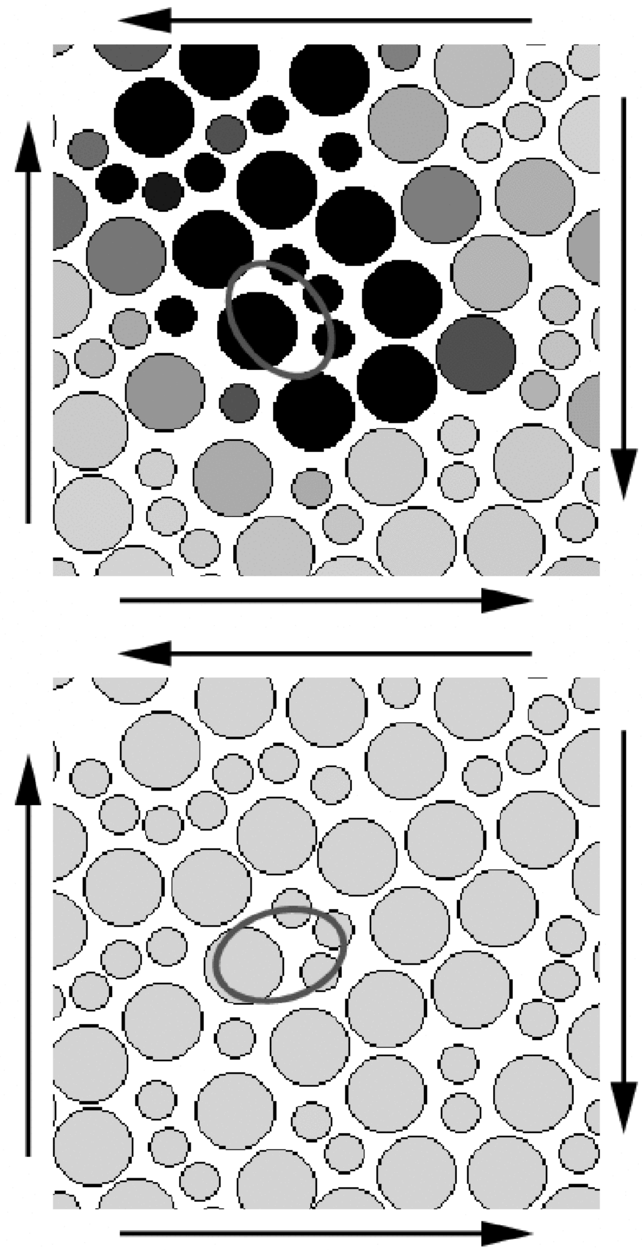
Fundamental Puzzles in Solid Mechanics

- How can we understand brittle and ductile behaviors – especially in noncrystalline solids?
- What is the origin of memory effects in simple noncrystalline solids?
- What is the origin of dynamic instabilities in brittle fracture?

M. Falk, MD Simulation of Tensile Deformation

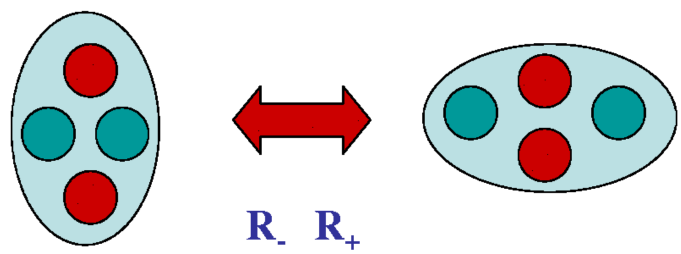
STZ Activity





Low-Temperature STZ Theory

Simple Two-State Version



R_- R_+

Plastic strain rate $= \dot{\varepsilon}^{pl} \propto R_+(s)\,n_+ - R_-(s)\,n_-$

$s =$ deviatoric (shear) stress

$$\dot{n}_\pm = R_\pm n_\pm - R_\mp n_\mp + \Gamma(s,\ldots)\left(\frac{n_\infty}{2} - n_\pm\right)$$

STZ Order Parameters
(Internal State Variables)

$\Lambda = \dfrac{n_+ + n_-}{n_\infty} =$ scaled, scalar density of STZ's

$\Delta = \dfrac{n_- - n_+}{n_\infty} =$ orientational bias of STZ's (becomes traceless, symmetric tensor)

$n_\infty =$ low-temperature, steady-state density of STZ's

Dissipation (Production) Rate

Energy balance: $2\dot{\varepsilon}^{pl} s = \frac{d}{dt}\Psi(\Lambda,\Delta) + Q$

$2\dot{\varepsilon}^{pl} s =$ rate at which work is done

$\Psi =$ recoverable energy

$Q =$ dissipation rate > 0 (second law)

Pechenik's conjecture: $Q \propto \Lambda\,\Gamma(s,\Lambda,\Delta)$

Use equations of motion and second law to solve for Γ and Ψ

$$\Gamma = \frac{4\Lambda(\Lambda s - \Delta)^2}{(1+\Lambda)(\Lambda^2 - \Delta^2)}; \quad \Psi = \frac{\Lambda}{2}\left(1 + \frac{\Delta^2}{\Lambda^2}\right)$$

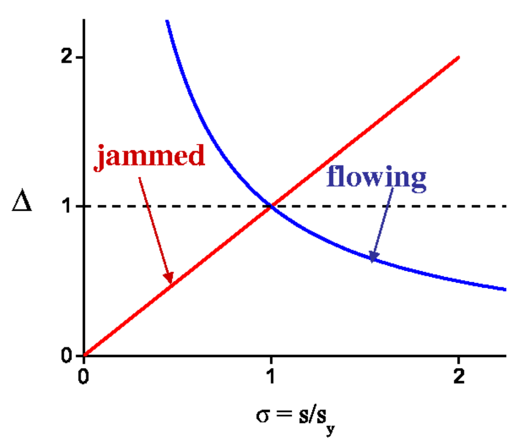
Quasilinear (Approximate) Equations of Motion

$\Lambda \to 1; \quad s/s_{yield} \to \sigma$

$\dot{\varepsilon}^{pl} \propto \sigma - \Delta$ (effective stress)

$\Gamma \propto \frac{(\sigma-\Delta)^2}{1-\Delta^2}$ (dissipation rate)

$\dot{\Delta} \propto \frac{(\sigma-\Delta)(1-\sigma\Delta)}{1-\Delta^2}$

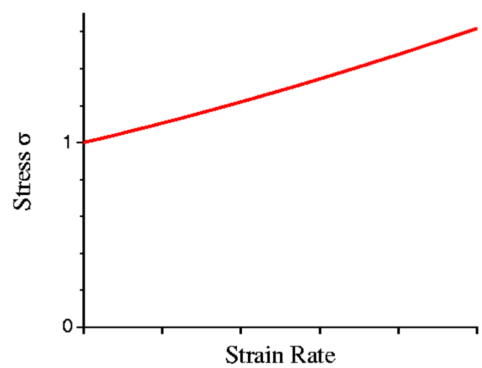


Exchange of stability at σ=Δ=1, between jammed states (Δ= σ) and flowing states (Δ =1/σ)

Steady-State Solutions

Low-temperature limit, quasilinear approximation

$$\dot{\varepsilon}^{pl} \propto \begin{cases} \sigma - \dfrac{1}{\sigma} & \text{for } \sigma > 1; \\ 0 & \text{for } 0 < \sigma < 1. \end{cases}$$



Available online at www.sciencedirect.com
SCIENCE @ DIRECT®
Pergamon
Acta Materialia 51 (2003) 3429–3443
Acta MATERIALIA
www.actamat-journals.com

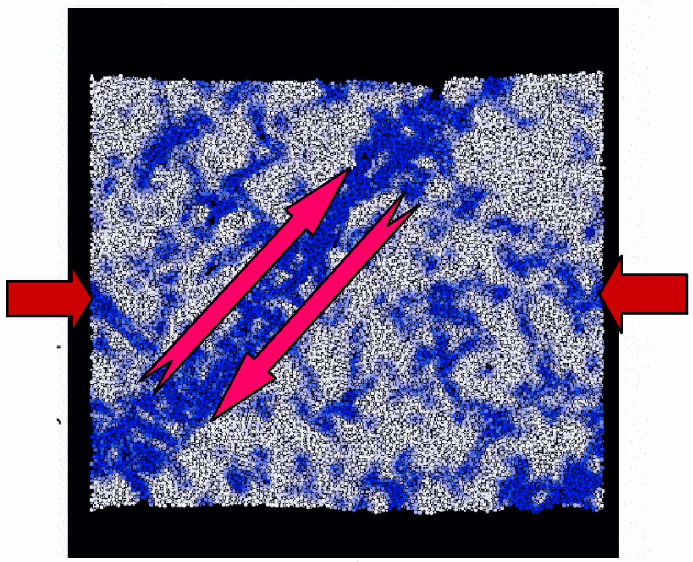
Deformation behavior of the $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ bulk metallic glass over a wide range of strain-rates and temperatures

J. Lu [a], G. Ravichandran [a,*], W.L. Johnson [b]

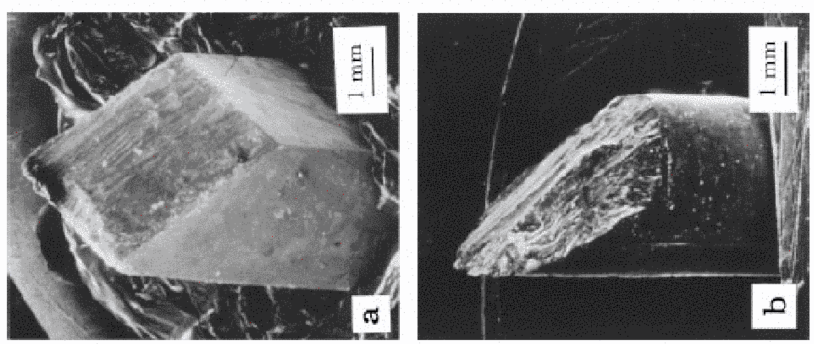
[a] *Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, CA 91125, USA*
[b] *W.M. Keck Laboratory of Engineering Materials, California Institute of Technology, Pasadena, CA 91125, USA*

Received 15 November 2002; received in revised form 9 March 2003; accepted 12 March 2003

Earlier paper: Kato, Kawamura, Inoue and Chen, "Newtonian to non-Newtonian master flow curves of a bulk glass alloy Pd Ni Cu P," Applied Physics Letters 73, 3665 (1998)

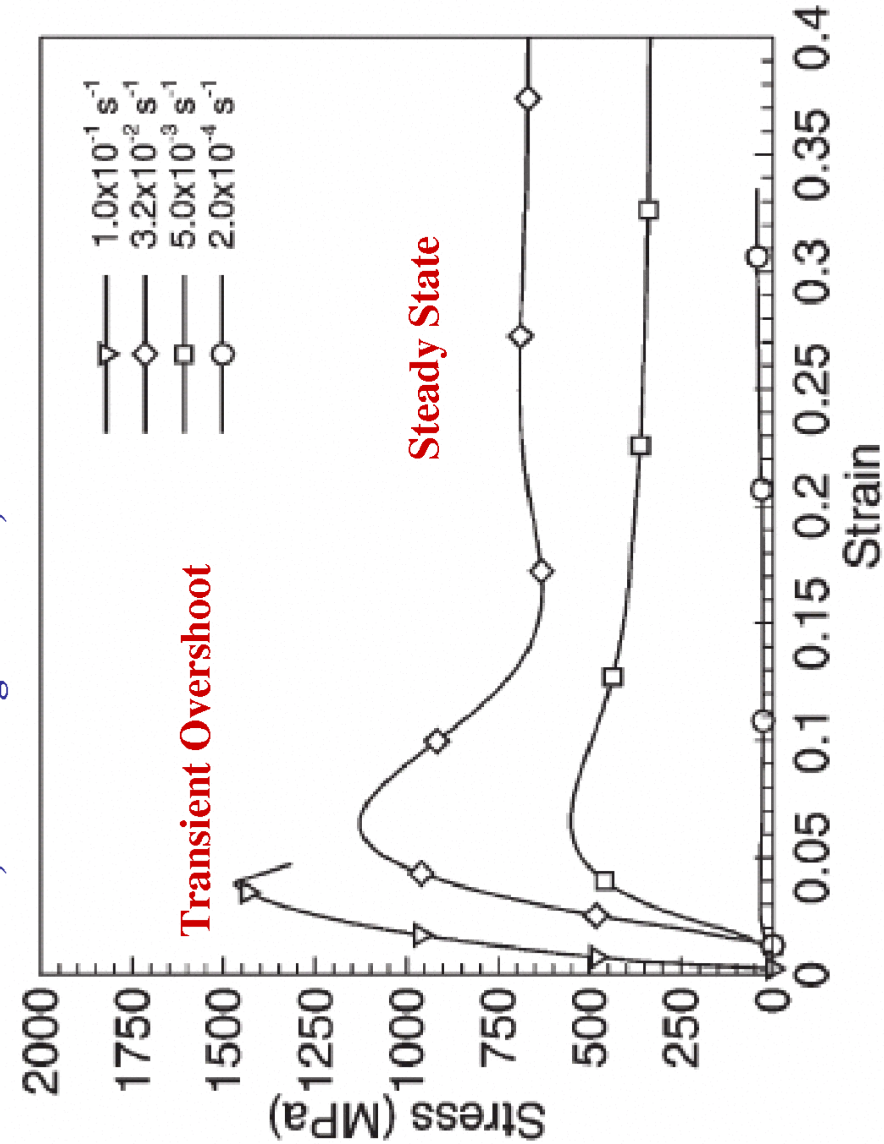


M. Falk, MD Simulation

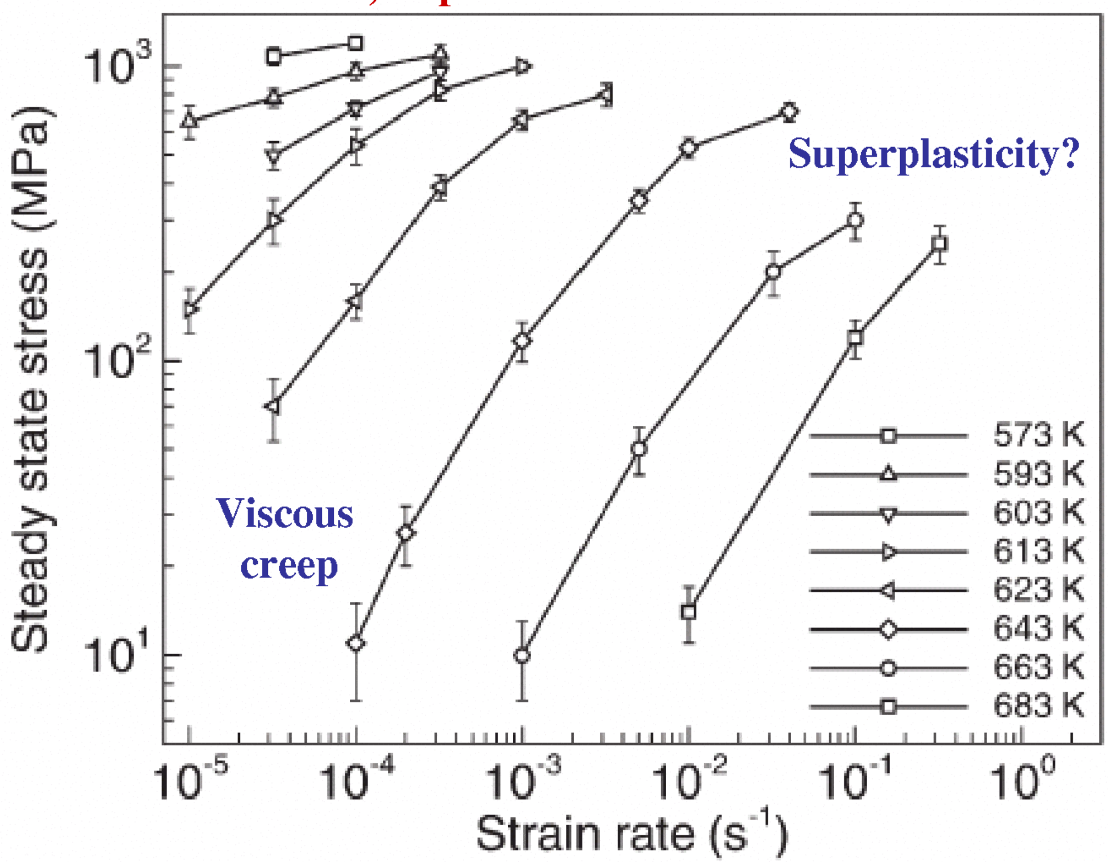


W.Johnson et al, Bulk Metallic Glass

Lu et al, metallic glass data, constant strain rate



Lu et al., Experimental Data

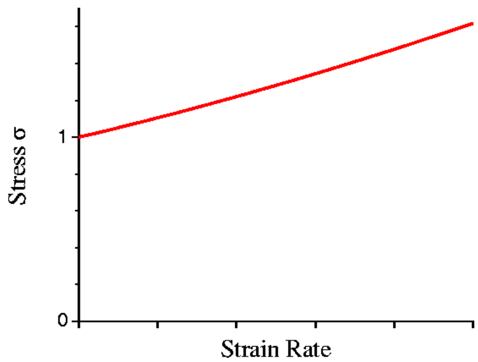


EFFECTS OF THERMAL FLUCTUATIONS

- Falk, Langer, and Pechenik, Phys. Rev. E (2004), “Defect Dynamics.”
- JSL, Phys. Rev. E (2004), “Effective Temperature.”
- Langer and Lemaitre, PRL (2005), STZ theory of super-Arrhenius rate factors.

Steady-State Solutions

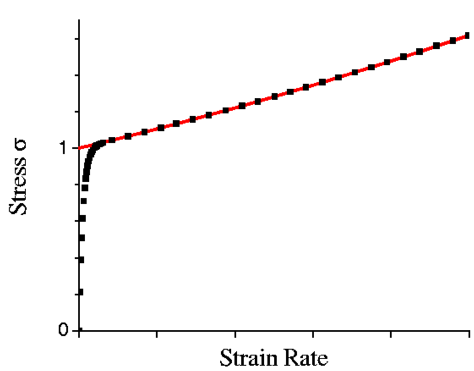
Low-temperature limit: $$\dot{\varepsilon}^{pl} \propto \begin{cases} \sigma - \dfrac{1}{\sigma} & \text{for } \sigma > 1; \\ 0 & \text{for } 0 < \sigma < 1. \end{cases}$$

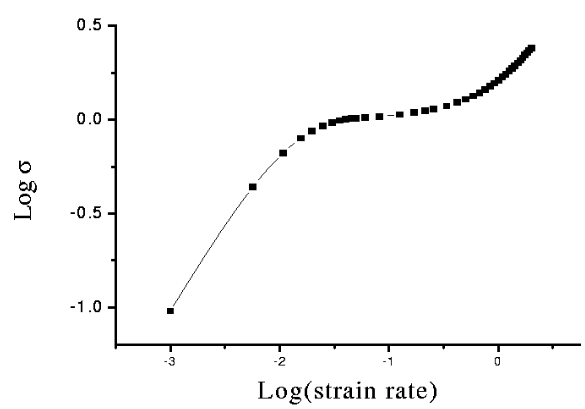


Steady-State Solutions

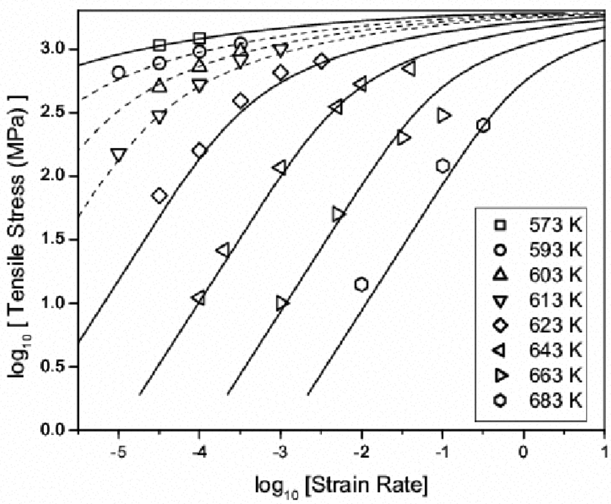
Low-temperature limit: $$\dot{\varepsilon}^{pl} \propto \begin{cases} \sigma - \dfrac{1}{\sigma} & \text{for } \sigma > 1; \\ 0 & \text{for } 0 < \sigma < 1. \end{cases}$$

Thermally assisted creep below the yield stress:





Comparison between Metallic Glass Data and Effective-Temperature Theory



Generalization of STZ Theory to Nonzero Temperatures

$$\dot{n}_{\pm} = R_{\pm} n_{\pm} - R_{\mp} n_{\mp} + \left[\Gamma(s,\ldots) + \rho(T)\right]\left(\frac{n_{\infty}}{2} e^{-1/\chi} - n_{\pm}\right)$$

$\rho(T)$ = thermally assisted (super-Arrhenius) fluctuation rate

$\chi = \dfrac{k_B T_{eff}}{E_{STZ}}$ = dimensionless effective disorder temperature

E_{STZ} = STZ formation energy

We now need:

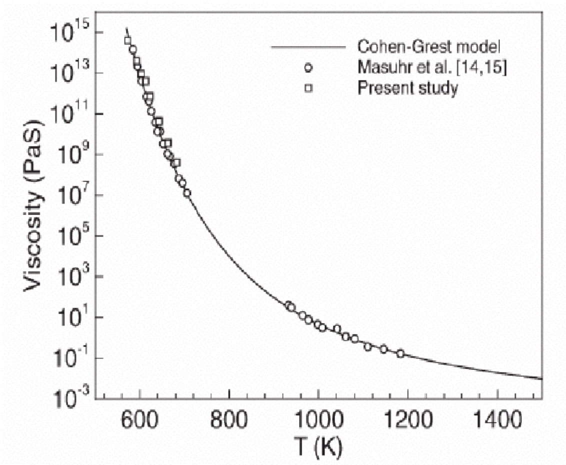
* A way to deduce the function ρ(T)

* An interpretation, and an equation of motion for χ

Newtonian viscosity: Limit of vanishing shear rate

$$\dot{\varepsilon}^{pl} \approx n_{eq}(T)\,\rho(T)\,s; \quad n_{eq} \approx exp(-E_{STZ} / k_B T)$$

$$\eta_N = \lim_{s \to 0} \frac{s}{\dot{\varepsilon}^{pl}} \propto \frac{s_y}{\rho(T)} exp(E_{STZ} / k_B T)$$



Measured viscosities provide estimates of E_{STZ} and $\rho(T)$ up to a scale factor.

Effective Disorder Temperature

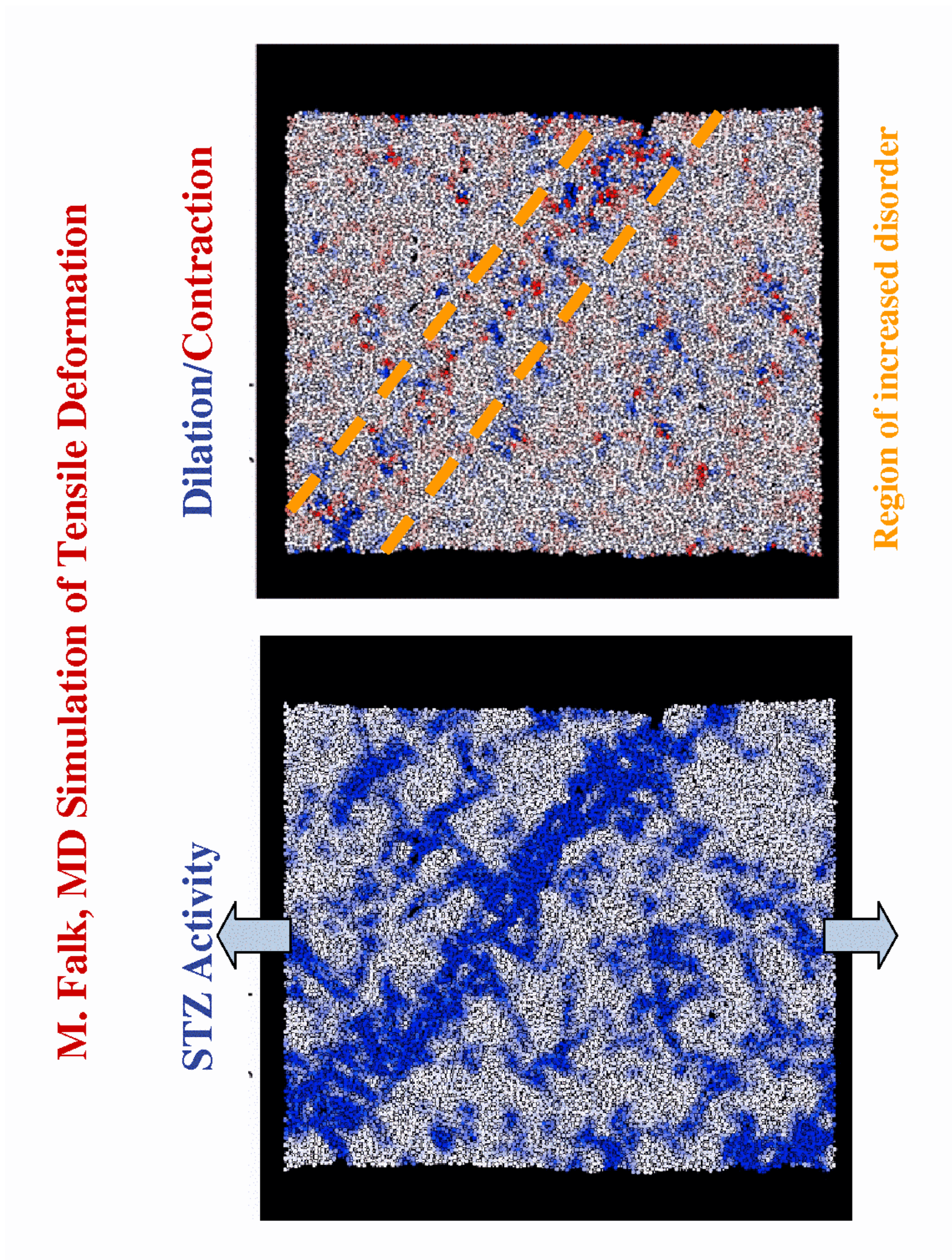
Basic Idea:

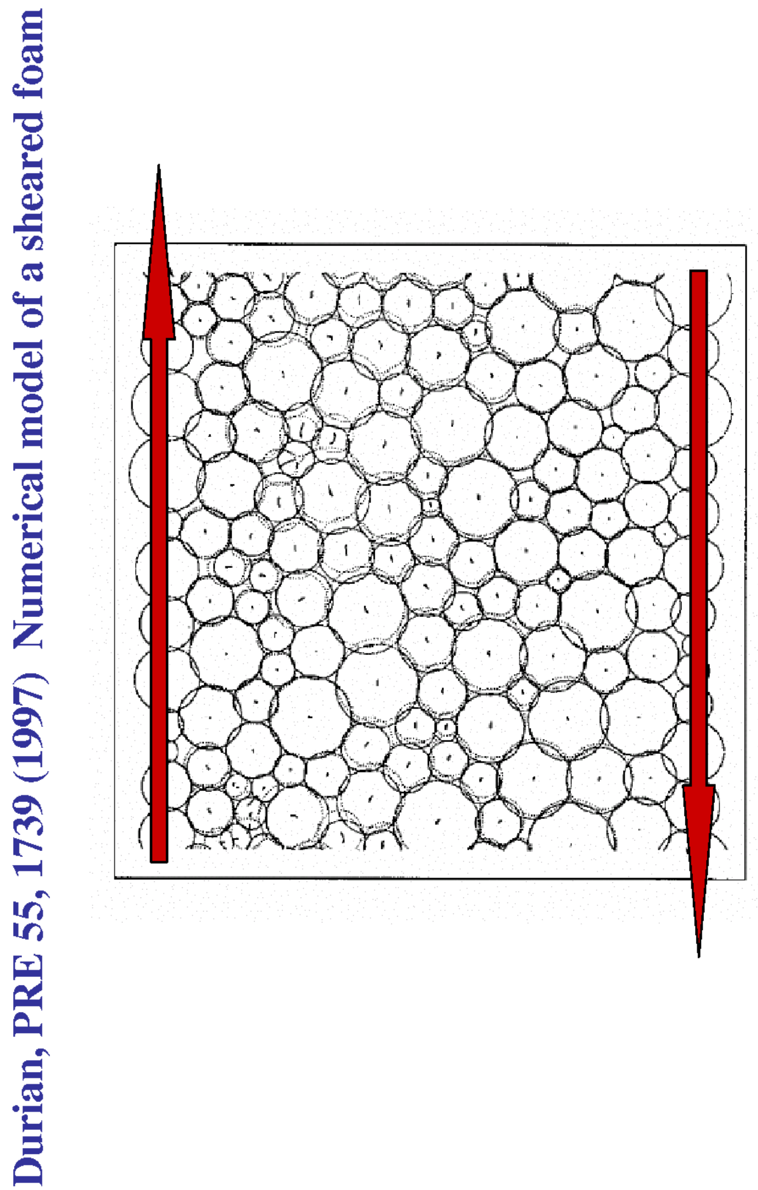
During irreversible plastic deformation of an amorphous solid, molecular rearrangements drive the slow configurational degrees of freedom (inherent states) out of equilibrium with the heat bath.

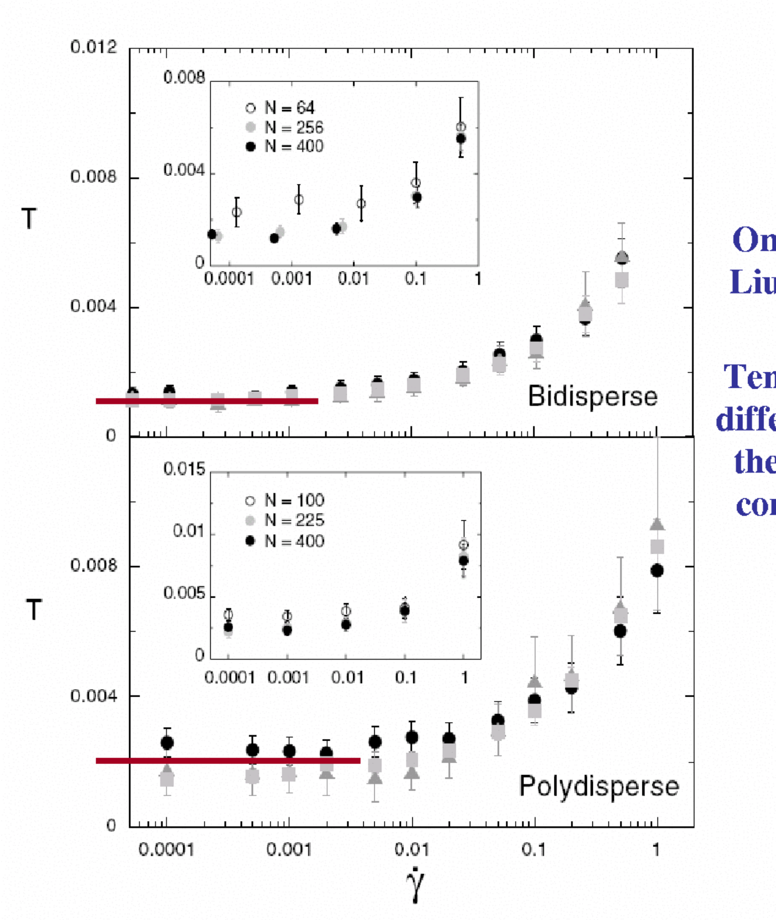
Because those degrees of freedom maximize an entropy, their state of disorder should be characterized by a temperature.

The STZ's are density fluctuations well out in the wings of the disorder distribution; therefore

$$n_{STZ} \propto exp(-E_{STZ} / k_B T_{eff}) = exp(-1/\chi)$$


M. Falk, MD Simulation of Tensile Deformation
Dilation/Contraction
Region of increased disorder
STZ Activity


Numerical model of a sheared foam
Durian, PRE 55, 1739 (1997)



Sheared Foam

Ono, O'Hern, Durian, (S.) Langer, Liu, and Nagel, PRL 095703 (2002)

Temperature, measured in several different ways (response-fluctuation theorems, etc.), goes to a nonzero constant in the limit of vanishing shear rate.

$$\chi \to \chi_\infty$$

Effective temperature is implied by STZ-like theories.

Viscosity $\quad \eta \propto \dfrac{s_y}{\dot{\varepsilon}} \quad (s \to s_y \text{ as } \dot{\varepsilon} \to 0)$

Diffusion constant $\quad D \propto b^2\, \dot{\varepsilon}$

b ~ jump size ~ bubble size

Stokes-Einstein theorem $\quad D \propto \dfrac{T_{eff}}{\eta\, b}$

➡ $T_{eff} \propto s_y\, b^3$ ~ glass temperature?

$$\chi_\infty \cong \frac{s_y\, b^3}{E_{STZ}}$$

Equation of Motion for χ

$$\dot{\chi} \propto e^{-1/\chi}\Gamma(s,\ldots)(\chi_\infty - \chi) + \kappa\,\rho(T)\,e^{-\beta/\chi}\left(\frac{k_B T}{E_{STZ}} - \chi\right)$$

Q, heat generated by deformation, drives χ toward χ_∞.

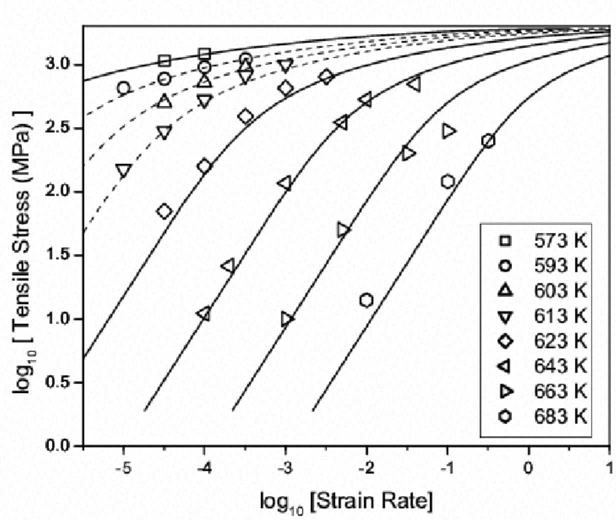
Thermal fluctuations drive T_{eff} toward T.

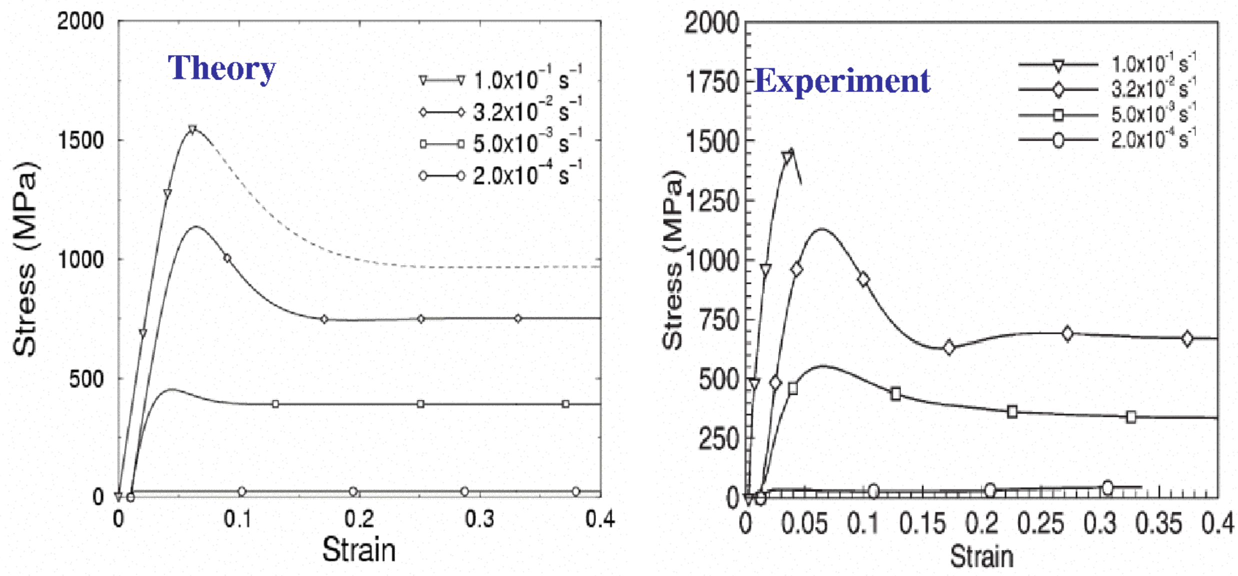
κ = adjustable parameter (= 2 to fit metallic glass data if β =1)

β =1 means that the equilibrating fluctuations occur at the STZ's.

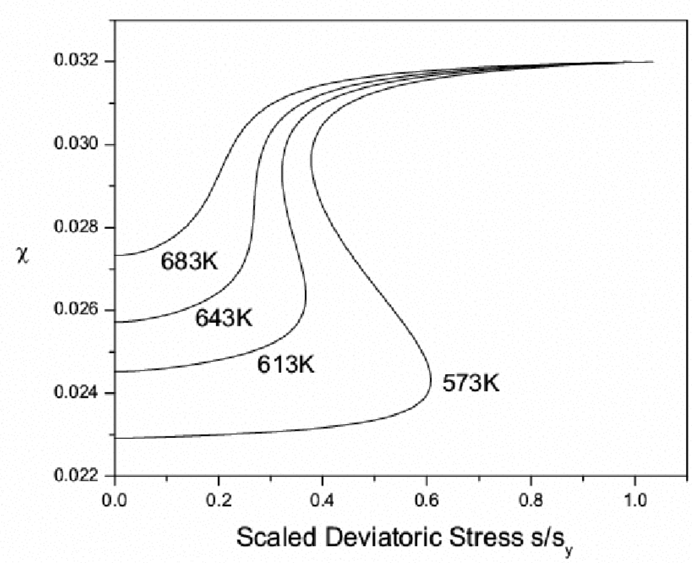
β < 1 means that they are more widely distributed, and is interesting.

Comparison between Metallic Glass Data and Effective-Temperature Theory

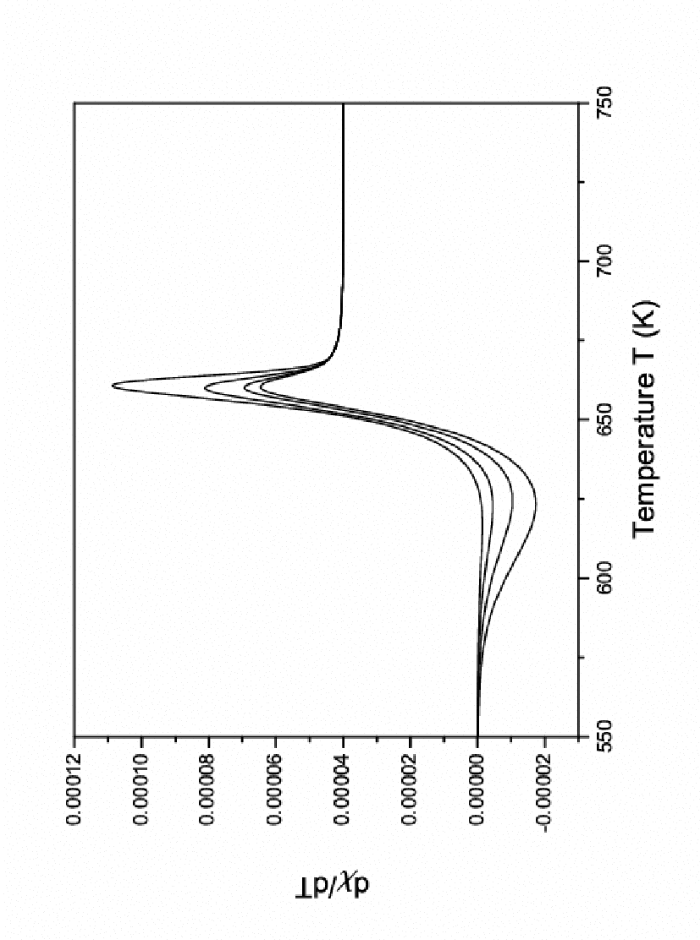




Comparison between (defect-dynamics) theory and experiment for transient behavior at different constant strain rates

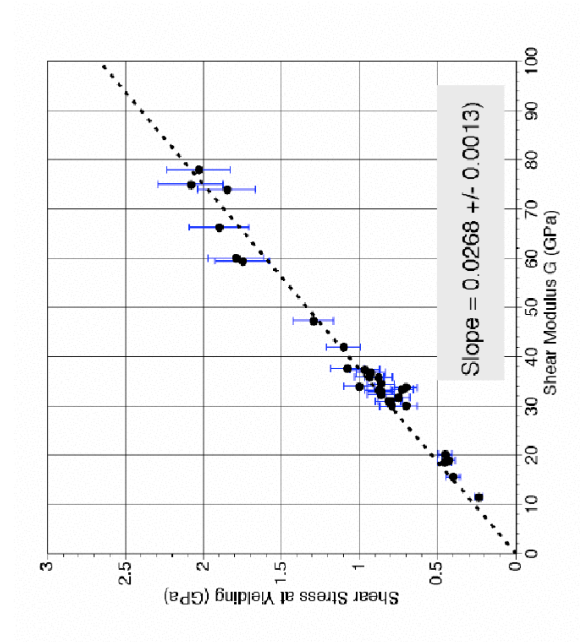


Steady-state dimensionless effective temperature χ as a function of stress, for β = 0.5. Note shear-banding instability implied by multi-valued curves at lower temperatures.

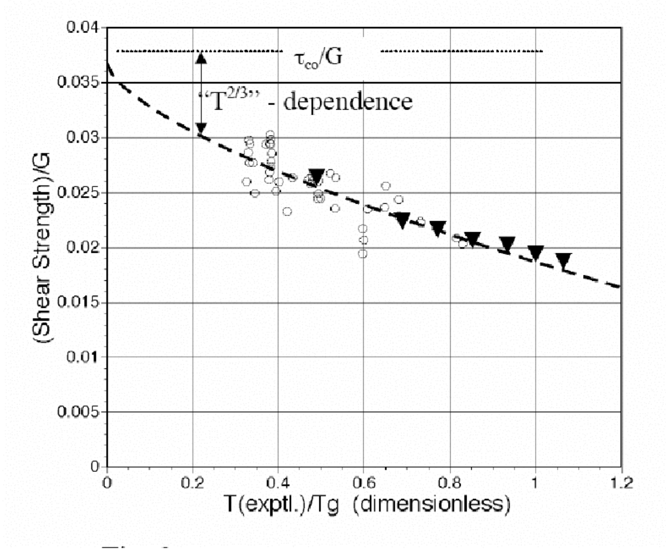


Simulated DSC scans for initial disorder corresponding to effective temperatures of 630K, 640K, 650K, and 660K.

W. Johnson, 2005: Evidence for a universal yield *strain*



W. Johnson, 2005: Temperature dependence of the yield strain



Universal Yield *Strain*

- **Implies that yielding depends more on geometry than details of the interatomic forces.**
- **If so, then the yielding behaviors of metallic (and other) glasses might be similar to those of dense granular materials.**
- **Then the appropriate effective temperature should describe volume, rather than energy, fluctuations (Edwards et al).**

Concluding Remarks

- The effective-temperature theory seems to work well, but needs to be developed further and tested by experiments.
- The deepest outstanding problem is to find a theory for the super-Arrhenius fluctuation rate $\rho(T)$. The STZ picture should give us clues about possible – intrinsically dynamic – mechanisms. (Langer and Lemaitre, PRL in press) JSL1
- Extension of STZ theory to (from) granular materials?

Slide 33

JSL1 J. Langer, 9/10/2004