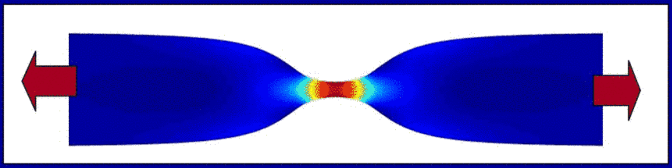
STZ Theory of Deformation in Amorphous Solids



J.S. Langer
KITP, September 6, 2005

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What I'd like to talk about

- Main objective of STZ theory
- Basic assumptions
- Zero-temperature theory
- General theory in terms of effective disorder temperature
- Comparison with metallic glass data
- Shear banding
- Theory of super-Arrhenius transition rates
- Universal yield strain

What I'll try to talk about

- Main objective of STZ theory
- Basic assumptions
- Zero-temperature theory (brief summary)
- General theory in terms of effective disorder temperature (brief summary)
- Comparison with metallic glass data
- Shear banding
- Theory of super-Arrhenius transition rates (maybe)
- Universal yield strain

Main Objective

- Tractable, quantitatively predictive model of deformation in amorphous solids, and also in foams, colloidal suspensions, and (maybe) dense granular materials.

- Analog of Navier-Stokes equations – but for deformable amorphous solids.

Continuum Theory of Large-Scale Deformation

$$\rho \frac{dv_i}{dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} s_{ij}$$

v_i = material velocity; p = pressure;
s_{ij} = deviatoric stress; d/dt includes advection.

$$\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) = \frac{\mathcal{D}}{\mathcal{D}t}\left(-\frac{p}{2K}\delta_{ij} + \frac{1}{2\mu}s_{ij}\right) + D_{ij}^{pl}(s, \ldots)$$

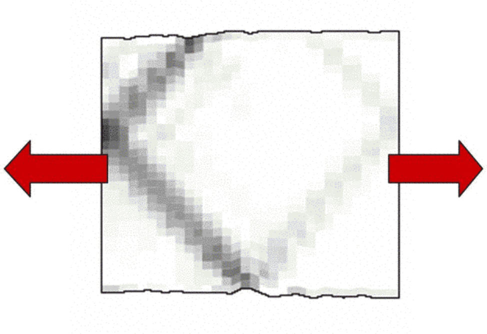
Rate-of-deformation tensor

Elastic part

Plastic part ($\dot{\varepsilon}^{pl}$)

$\frac{\mathcal{D}}{\mathcal{D}t}$ includes advection and rotation.

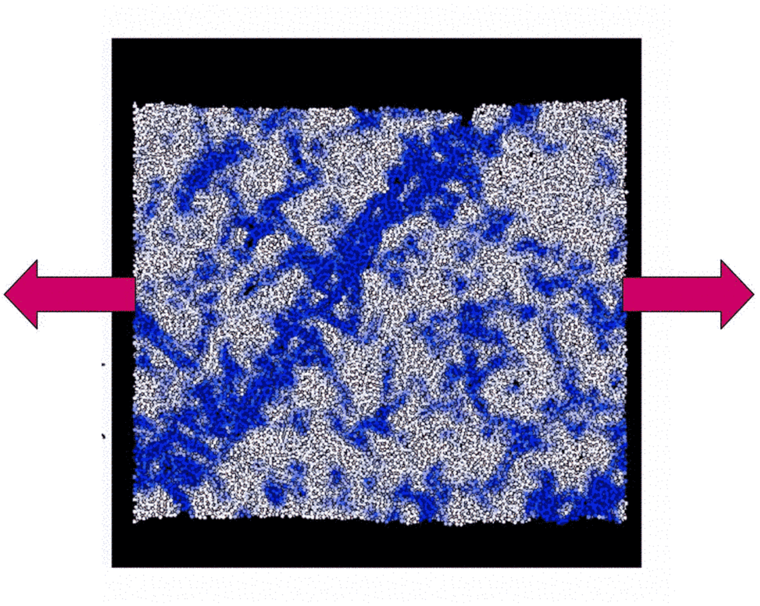
STZ constitutive relations: Expression for D_{ij}^{pl} in terms of internal state variables plus equations of motion for those state variables.



Eastgate STZ simulation: Free rough surfaces top and bottom.
Gray scale shows dissipation rate in nascent shear bands.

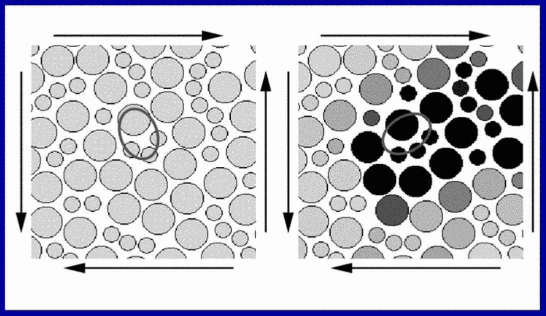
M. Falk, MD Simulation of Tensile Deformation

STZ Activity



Solid-Like Starting Point

- Irreversible atomic rearrangements occur at localized STZ's – "flow defects" – in an otherwise elastic solid.



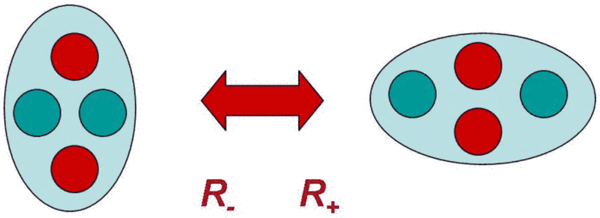
- STZ's do not diffuse, but may be created and annihilated by thermal fluctuations or during deformation.

STZ Model

- Localized two-state systems whose populations and orientations determine response to applied forces.
- STZ’s carry information about the history of recent deformations.
- Equations of motion for STZ’s must be consistent with basic symmetries and the laws of thermodynamics.

Low-Temperature STZ Theory

Simple Two-State Version



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

$s =$ deviatoric (shear) stress

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

STZ 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 a traceless, symmetric tensor Δ_{ij}

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

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

$R_+(s) = R_-(-s) =$ Stress-dependent rate factor

$\Gamma(s, \Lambda, \Delta) =$ STZ annihilation and creation rate

Pechenik's hypothesis: Γ = energy-dissipation rate per STZ. Equations of motion plus second law of thermodynamics determine Γ uniquely as a function of s and the internal state variables.

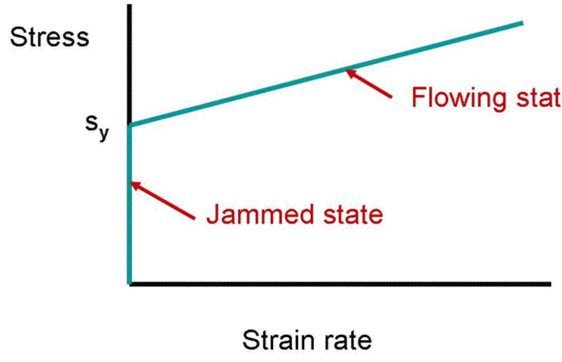
$$\Gamma \propto \frac{(\dot{\varepsilon}^{pl})^2}{\Delta^2{}_{max} - \Delta^2}; \quad \Delta^2{}_{max} \approx \Lambda^2.$$

STZ Dynamics

- Equations of motion for Λ and Δ, and the formula for Γ(s,Λ,Δ), follow from equations of motion for n_+ and n_- , and from physical models of the rate function R(s).
- Main result: Exchange of dynamic stability between jammed steady-state solution at small s, and flowing steady-state solution at large s, at a yield stress s_y.

Steady-State Solutions

Zero Temperature



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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

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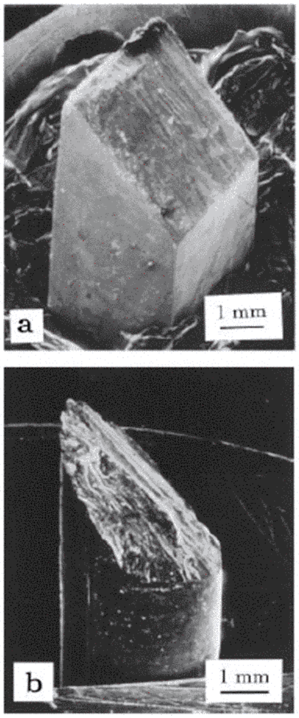
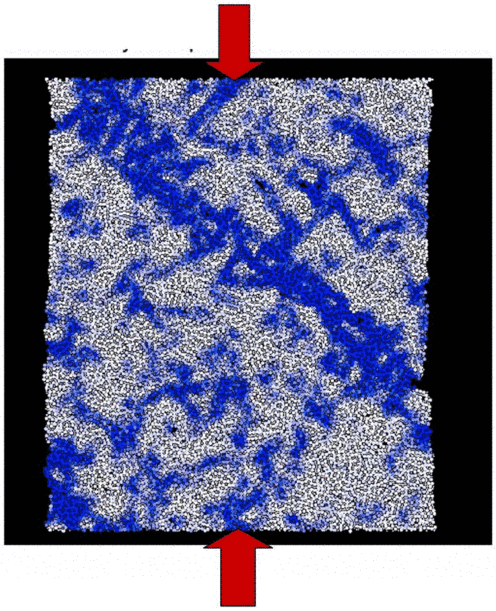
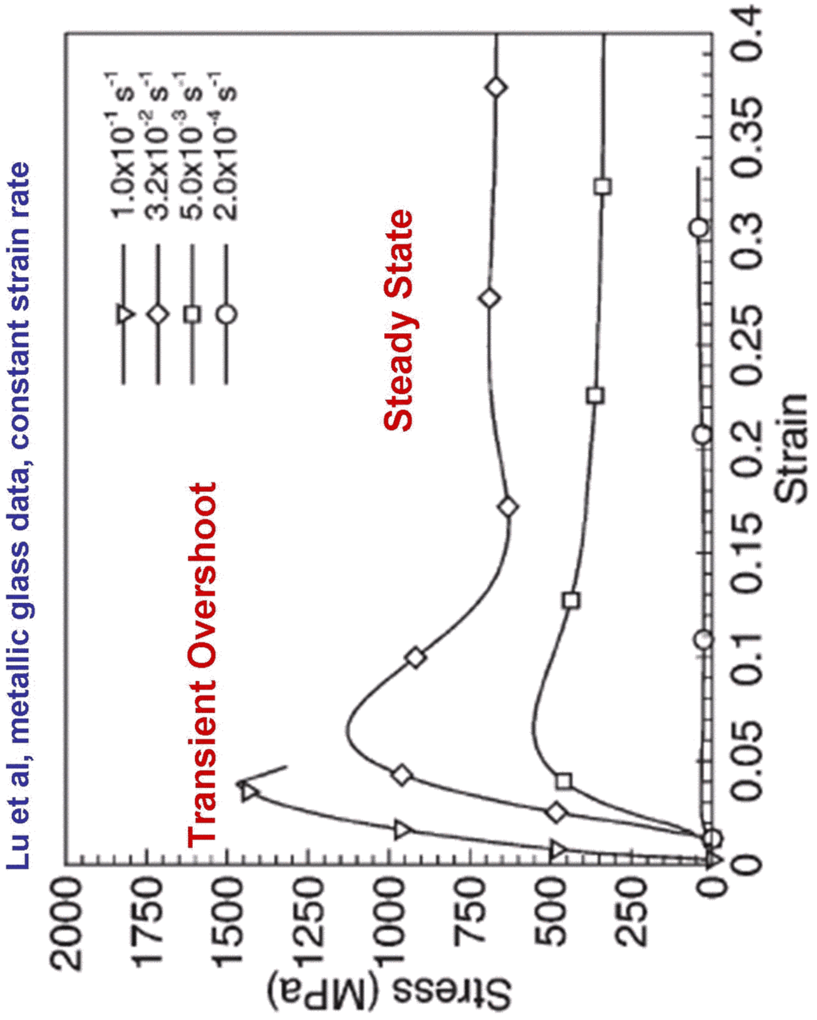
Earlier paper: Kato, Kawamura, Inoue and Chen, "Newtonian to non-Newtonian master flow curves of a bulk glass alloy Pd Ni Cu P," Applied Physics Letters 73, 3665 (1998)

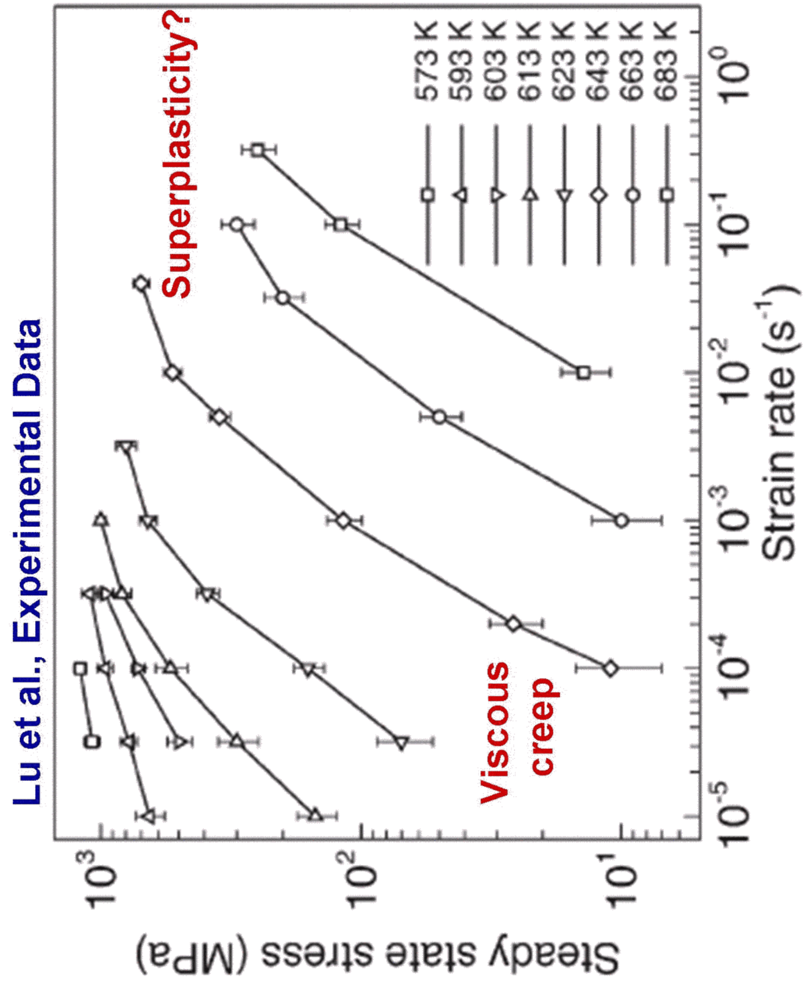


W.Johnson et al, Bulk Metallic Glass



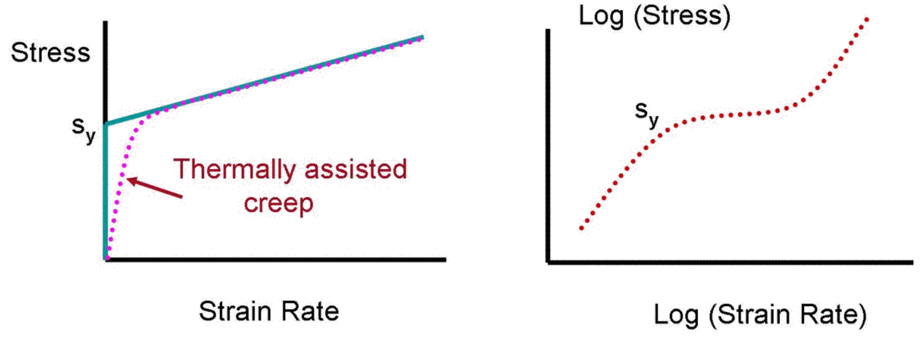
M. Falk, MD Simulation


Lu et al, metallic glass data, constant strain rate
Transient Overshoot
Steady State
1.0x10^-1 s^-1
3.2x10^-2 s^-1
5.0x10^-3 s^-1
2.0x10^-4 s^-1
Stress (MPa)
2000
1750
1500
1250
1000
750
500
250
0
Strain
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4


Lu et al., Experimental Data
Superplasticity?
Viscous creep
573 K
593 K
603 K
613 K
623 K
643 K
663 K
683 K
Steady state stress (MPa)
10^3
10^2
10^1
Strain rate (s^-1)
10^-5
10^-4
10^-3
10^-2
10^-1
10^0

Steady-State Solutions

Non-Zero Temperature



Generalization of STZ Theory to Nonzero Temperatures

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

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

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

E_{STZ} = STZ formation energy

We need:

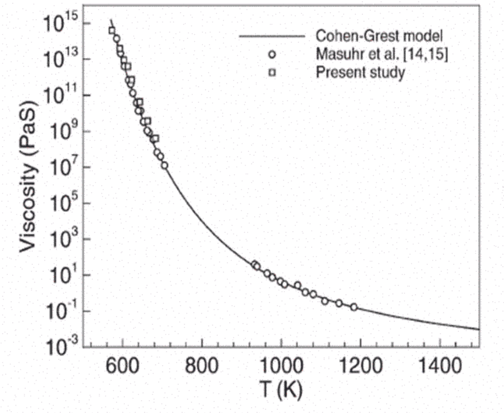
*** A way to deduce the function ρ(T)**

*** 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.

e.g. Vogel-Fulcher: $\ln\rho(T) \approx -\frac{const}{T-T_0}$

"Super-Arrhenius" rate factor

Effective Disorder Temperature

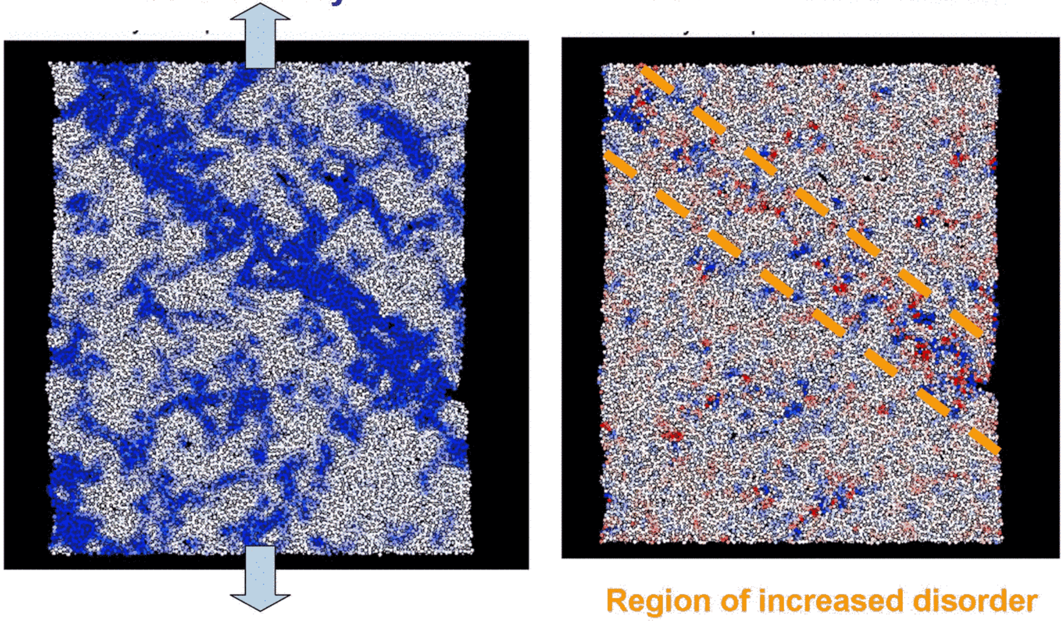
Basic Idea: During irreversible plastic deformation of an amorphous solid, molecular rearrangements drive the slow configurational degrees of freedom (inherent states) out of equilibrium with the heat bath.

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

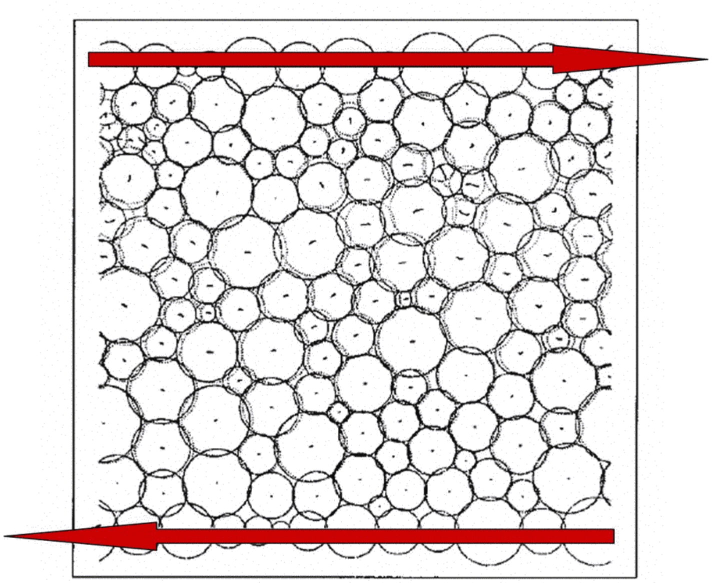


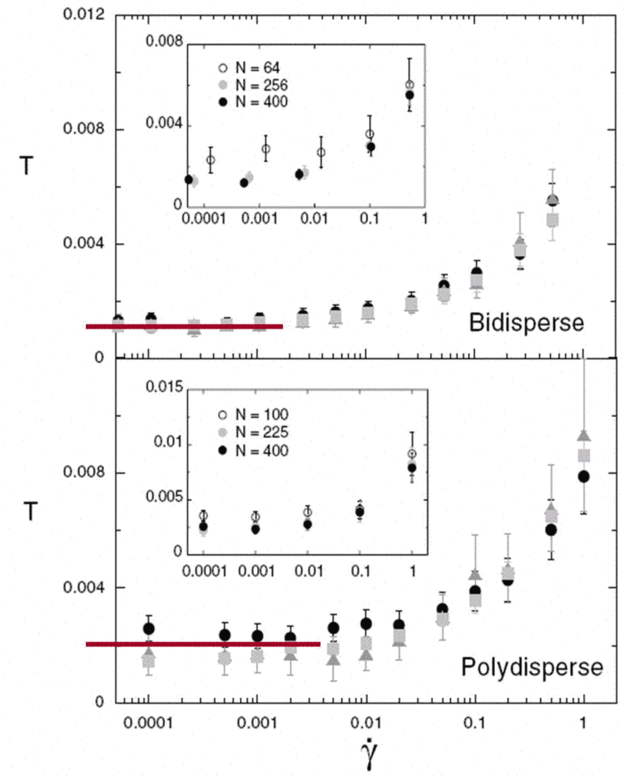
STZ Activity

Dilation Contraction

Region of increased disorder

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





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.

$$\boxed{\chi \to \chi_\infty}$$

Equation of Motion for χ

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

Energy dissipated during deformation, drives χ toward χ_∞.

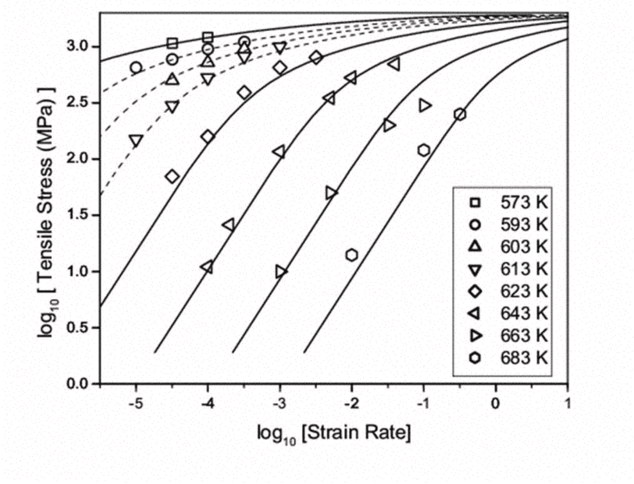
Thermal fluctuations drive T_{eff} toward T.

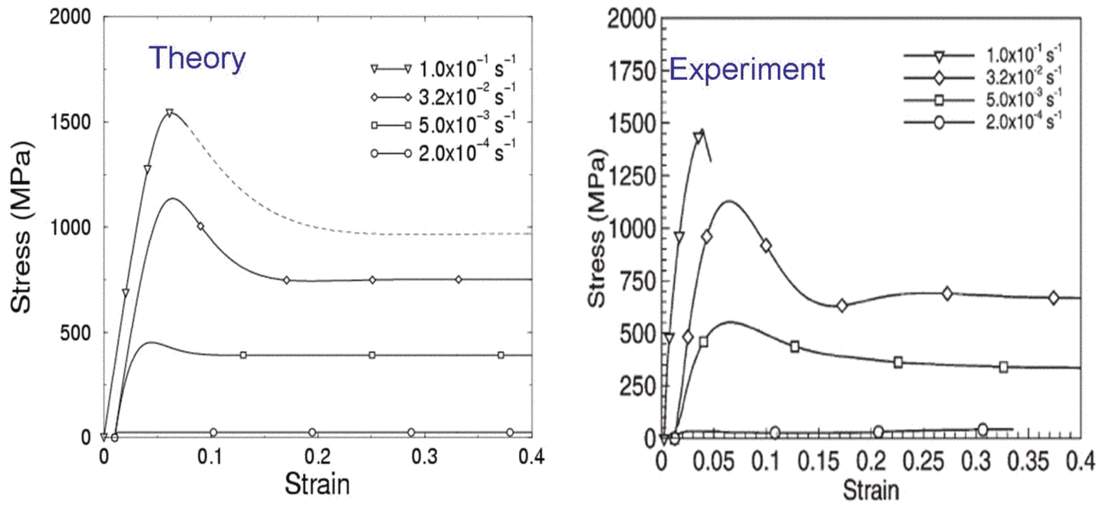
κ = adjustable parameter (= 2 to fit metallic glass data)

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





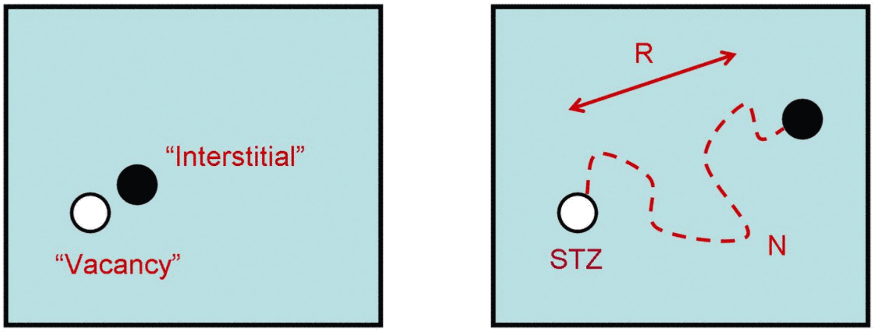
Comparison between (defect-dynamics) theory and experiment for transient behavior at different constant strain rates

Origin of Super-Arrhenius Rate Factors

- JSL and A. Lemaitre, PRL 05
- JSL pre-preprint

A very old problem. What does the STZ model have to say about it?

Thermally Activated Formation of a Density Fluctuation -- e.g. an STZ -- in a Disordered Material



- - - - - - = chain of displacements containing N links, extending a distance R.

Probability of forming a chain of length *N*, extension *R*

$$W(N,R) \propto q^N e^{-Ne_0/kT} \underset{\overset{\nearrow}{\text{Random walk}}}{e^{-R^2/2N}} \underset{\overset{\nwarrow}{\text{Localization}}}{e^{-\gamma R}} \underset{\overset{\nwarrow}{\text{Self-exclusion}}}{e^{-U/kT}}$$

q = number of choices per step

e_0 = energy per step

$\gamma(T)$ = disorder strength ~ $(T_{eff}/T)^2$

U = exclusion energy ~ $kT_{\text{int}}(\tilde{N}^2/R^3)$ (a la Flory)

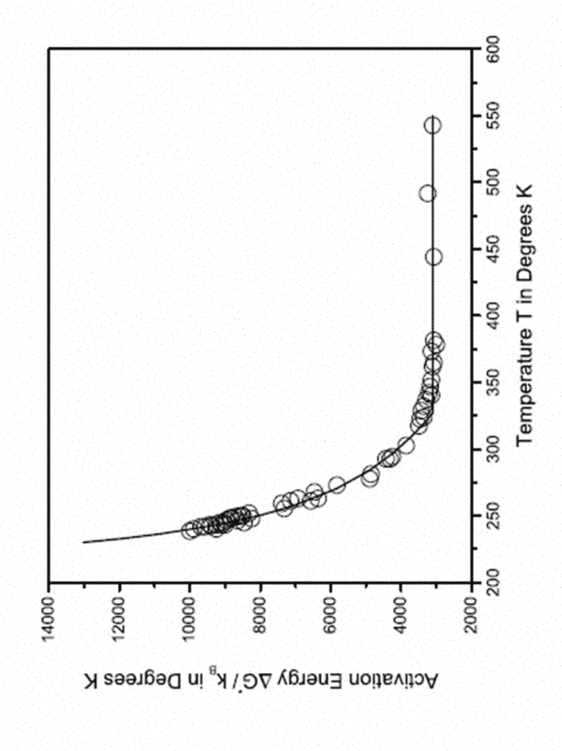
Minimize -*ln W* with respect to *R*, then find maximum as a function of *N*. That is, compute the free energy barrier for activating an indefinitely long chain of displacements.

The result (for temperatures low enough that *N* is large) is:

$$-\ln W^* \propto \frac{\gamma(T)^{3/2}(T\,T_{\text{int}})^{1/2}}{T-T_0} \quad (T_0 = e_0/(k\,ln\,q))$$

which is essentially the familiar Vogel-Fulcher formula.

Super-Arrhenius Activation Energy for Ortho-Terphenyl



Super-Arrhenius Activation Energy for Metallic Glass Vitreloy I