DYNAMICS OF SHEAR-TRANSFORMATION ZONES IN AMORPHOUS SOLIDS

J.S. Langer, UCSB

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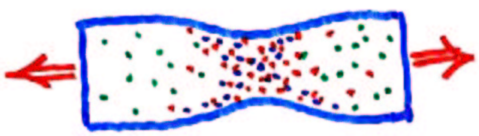
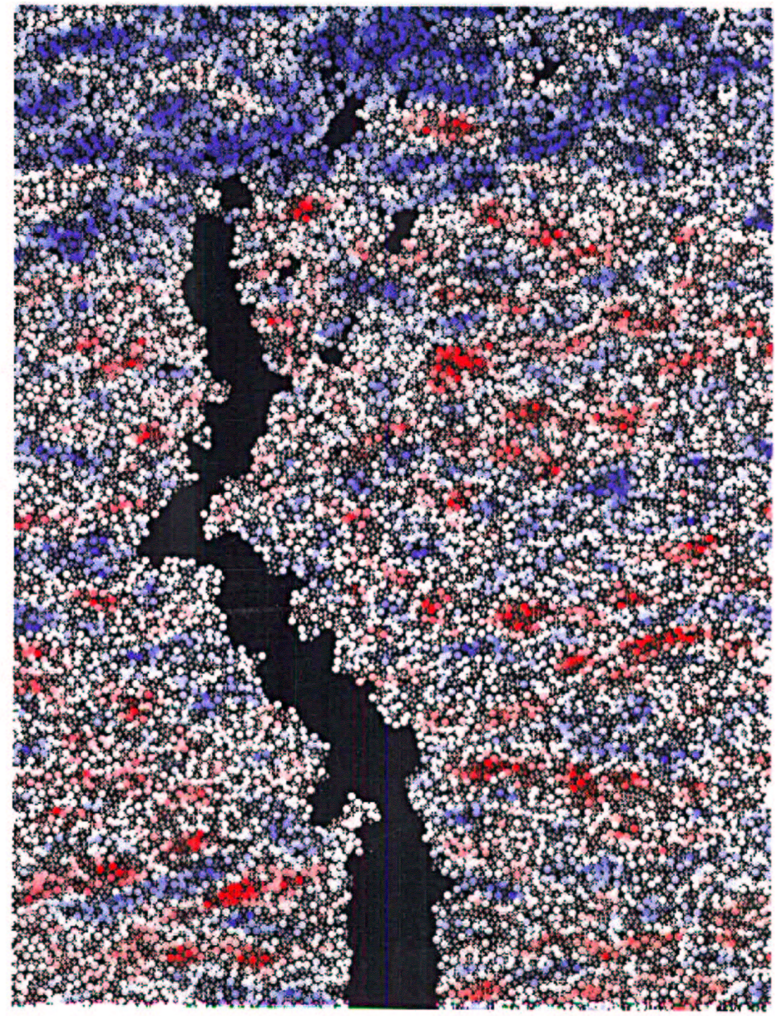


Collaborators: M. Falk, L. Pechenik, A. Lemaitre, L. Eastgate, C. Malon
A. Foglia

M. Falk

Closeup of Crack Tip In Brittle Fracture

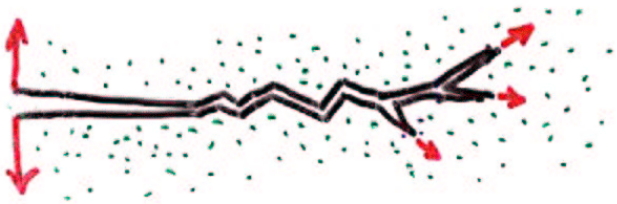
10^5 Molecule 2D Compressed LJ Solid with distribution of molecular radii colored by σ_{yy} – red = compression, blue = tension



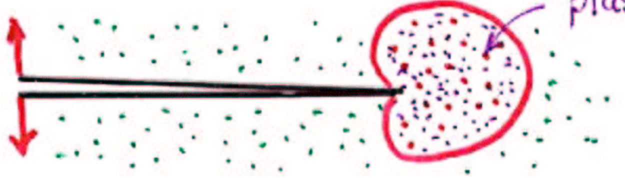
FUNDAMENTAL PUZZLES IN FRACTURE DYNAMICS

How can we understand brittle and ductile behaviors, especially in noncrystalline solids?

What is the origin of dynamic instabilities in brittle fracture?

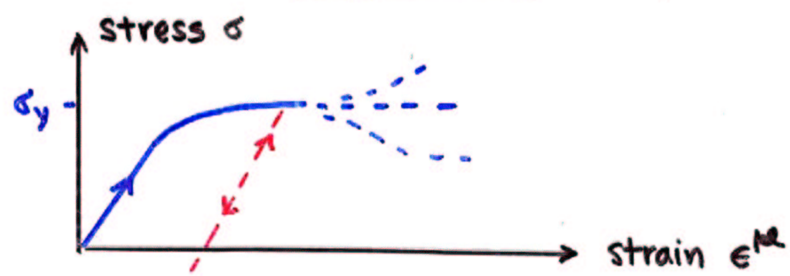


If there is always a plastic yield stress, how can a (higher)? breaking stress be transmitted to a crack tip?



CONVENTIONAL DESCRIPTIONS OF PLASTICITY

Time - Independent



Rate - Dependent

What would be a suitable form for a theory of plasticity?

Equations of Motion

$$\frac{d\epsilon^{pl}}{dt} = F(\sigma, \Delta, \ldots)$$

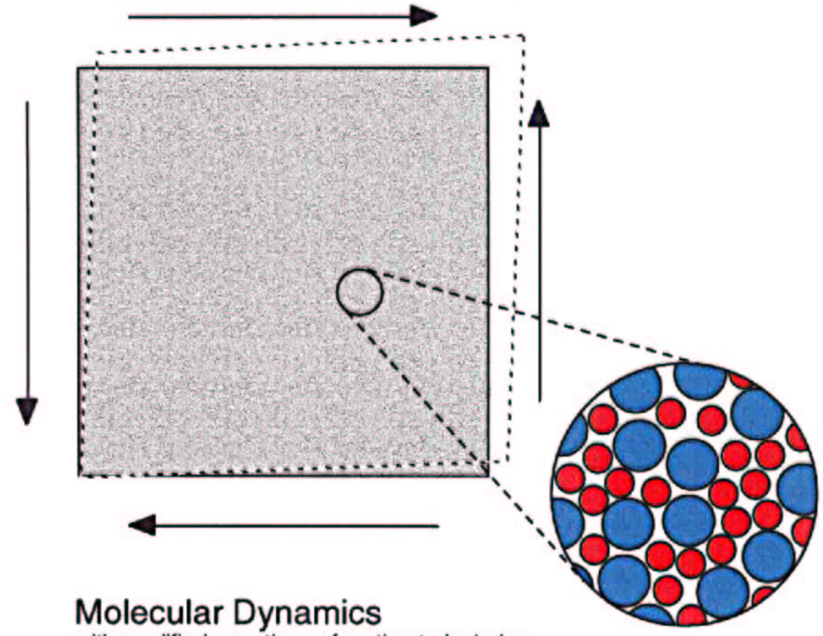
$$\frac{d\Delta}{dt} = G(\sigma, \Delta, \ldots)$$

$\sigma =$ **stress;** $\epsilon^{pl} =$ **plastic strain**

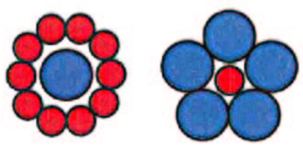
$\Delta_{,..} =$ **internal state variables (<u>not</u> including ϵ^{pl})**

Later, we must generalize these equations to include elasticity, boundary conditions, etc. – and construct a theory of large-scale deformations.

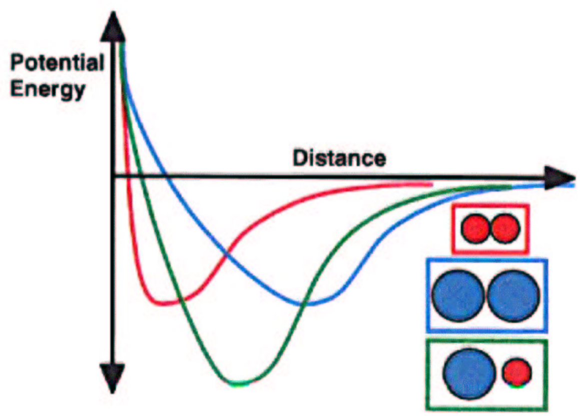
2-D 2-Component LJ Solid Under Applied Simple Shear



Molecular Dynamics
with modified equations of motion to include:
- Thermostat
- Pressure-Stress Barostat

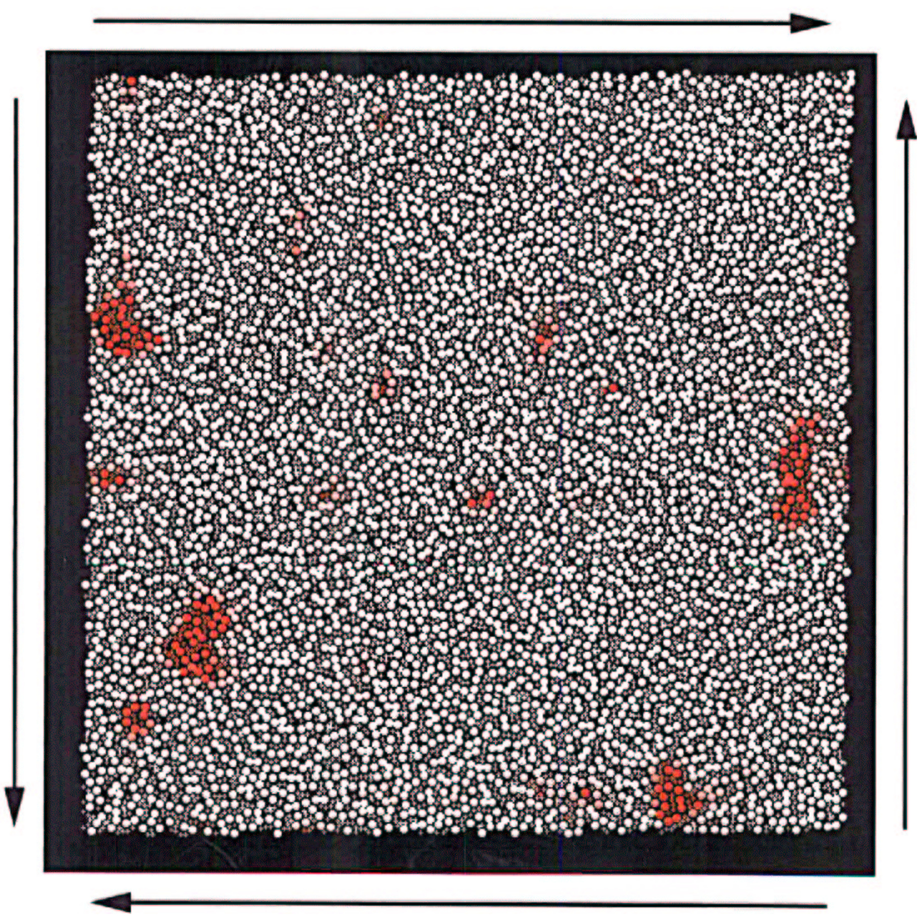


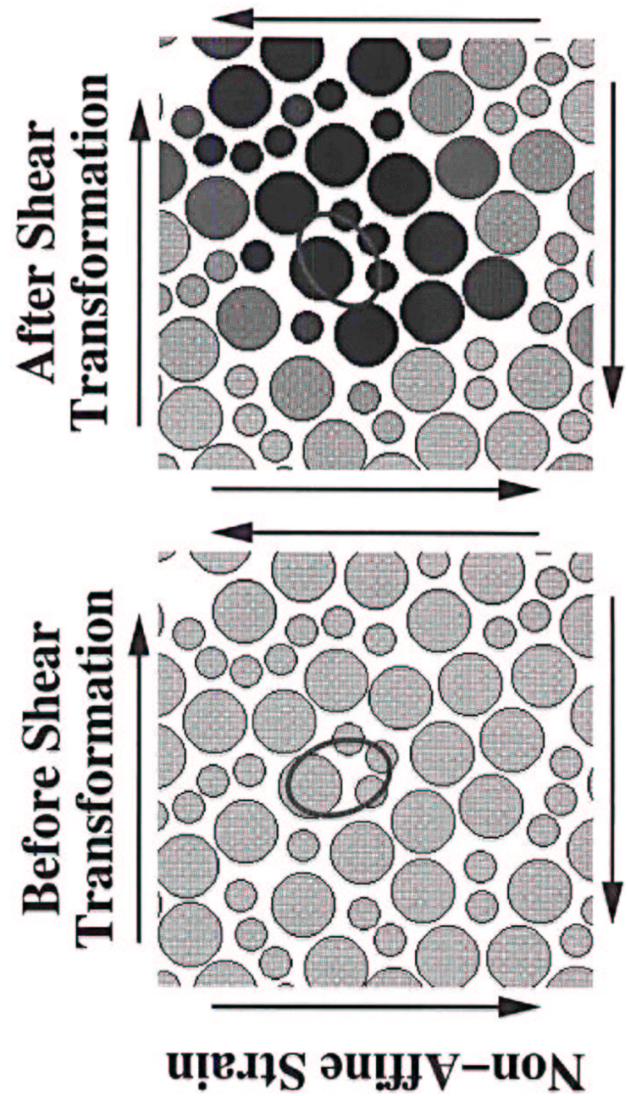
Quasicrystalline Ground State



Periodic Cell Under Applied Pure Shear Stress

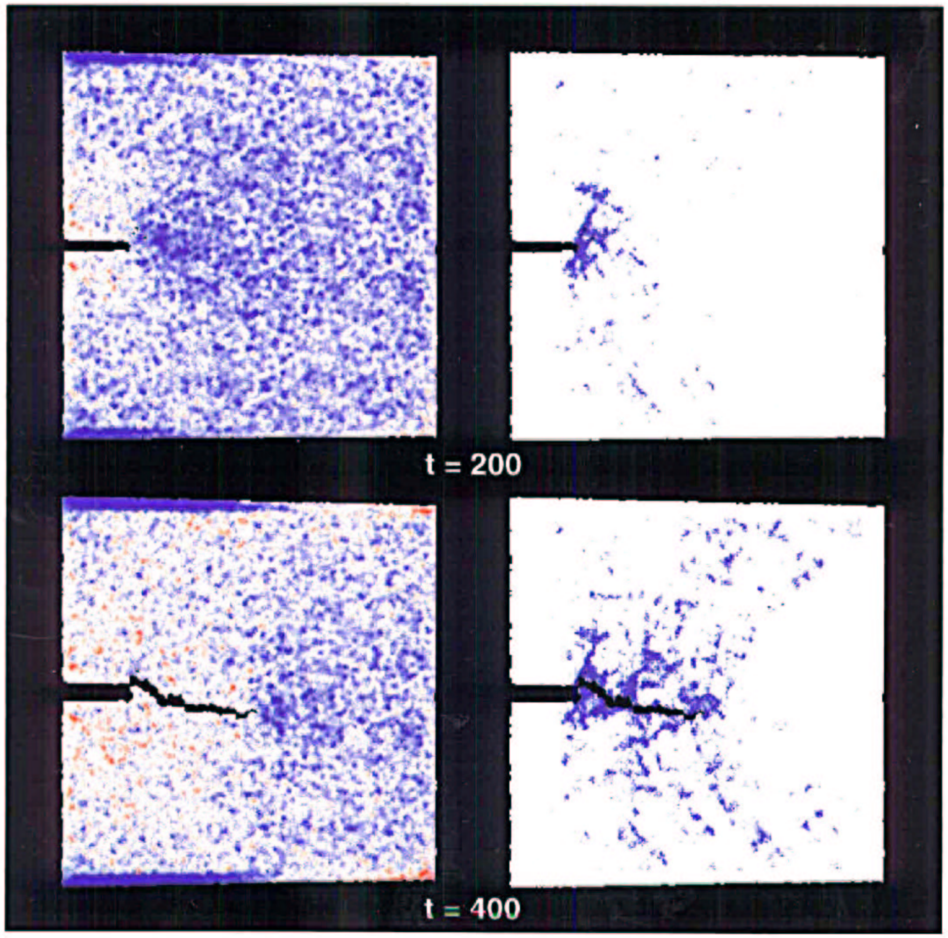
red regions denote areas of
local deviation from affine deformation





Brittle Crack

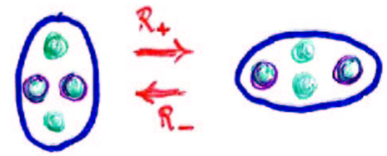
Local Hydrostatic Stress | **Local Non–Affine Rearrangement**



Dynamics of Shear-Transformation Zones (STZ's)

M. Falk and JSL, PRE 1998

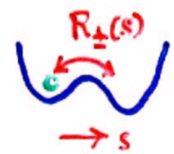
Simple Two-State Version



Plastic strain rate: $\dot{\epsilon}^{pl} \sim R_+ n_+ - R_- n_-$

$n_\pm =$ density of $\pm$ STZ's $\qquad s =$ deviatoric stress

Transition rates:



$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \Gamma(s,\dots)(A_{cr} - A_{ann} n_\pm)$$

$\Gamma(s,\dots) \hat{=}$ STZ creation and annihilation rates

$\sim$ Energy dissipation rate (Pechenik)

STZ ORDER PARAMETERS
(Internal State Variables)

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

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

$$n_\infty = \frac{2A_{cr}}{A_{ann}}$$ = steady-state density of STZ's

Are there other relevant dynamical state variables?

QUASILINEAR EQUATIONS OF MOTION

(do not account properly for memory effects)

$$\Lambda \to 1\,; \qquad s/s_y \to \tilde{\sigma}$$

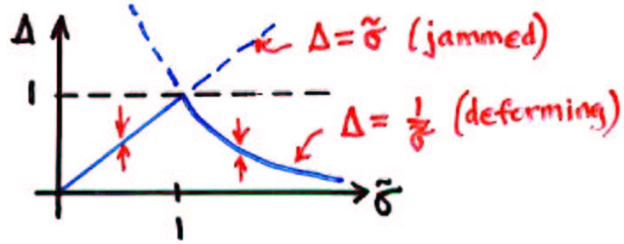
s_y = yield stress = combination of material parameters and couplings

$$\dot{\epsilon}^{pl} \sim \tilde{\sigma} - \Delta \sim$$ ("effective stress")

$$\Gamma(\tilde{\sigma}, \Delta) = \frac{(\tilde{\sigma} - \Delta)^2}{1 - \Delta^2} \sim$$ dissipation rate

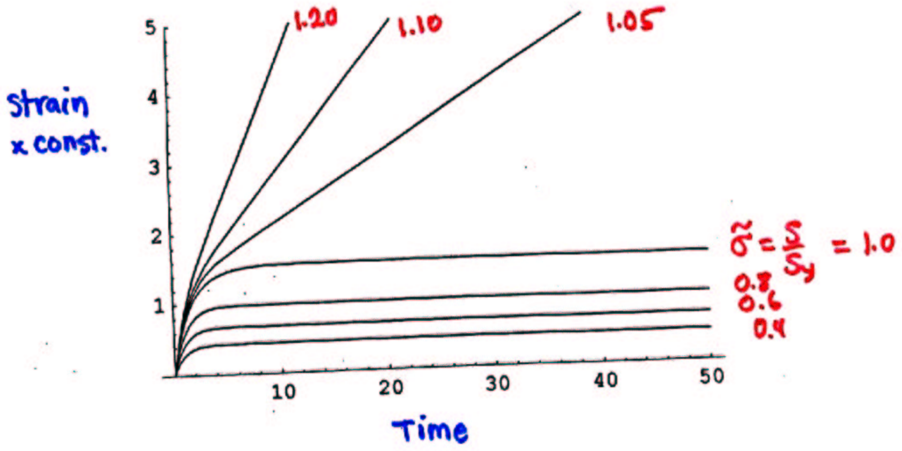
$$\dot{\Delta} \sim \frac{(\tilde{\sigma} - \Delta)(1 - \tilde{\sigma}\Delta)}{1 - \Delta^2}$$

Dynamic interpretation of the yield stress: Exchange of stability between non-deforming jammed states at low stresses and plastically deforming states at higher stresses.



QUASI-LINEAR STZ THEORY

"Creep Tests" (constant stress)



Energy Balance (Pechenik + JSL)

STZ STATE VARIABLES

Λ ~ density of STZ's

Δ ~ orientational bias

Strain rate $\dot{\epsilon} \sim \Lambda \tilde{\sigma} - \Delta$

$$\dot{\Delta} = \Lambda \tilde{\sigma} - \Delta - \Gamma(\tilde{\sigma}, \Lambda, \Delta)\,\Delta$$

$$\dot{\Lambda} = \Gamma(\tilde{\sigma}, \Lambda, \Delta)(1 - \Lambda)$$

$\tilde{\sigma}$ = deviatoric stress / yield stress

$\Gamma(\tilde{\sigma}, \Lambda, \Delta)$ ~ STZ creation and annihilation rates

What is $\Gamma(\tilde{\sigma}, \Lambda, \Delta)$?

(Original F-L conjecture $\Gamma \sim \dot{\epsilon} \cdot s$ - i.e. plastic work; but $\dot{\epsilon} \cdot s < 0$ during unloading.)

Energy balance: $\tilde{\sigma}\dot{\epsilon} \sim \frac{d}{dt}\psi(\Lambda,\Delta) + Q(\tilde{\sigma},\Lambda,\Delta)$ *

$\psi(\Lambda,\Delta)$ = recoverable energy associated with the STZ degrees of freedom.

$Q(\tilde{\sigma},\Lambda,\Delta)$ = dissipation rate ≥ 0 (2nd Law)

Pechenik's conjecture: $Q(\tilde{\sigma},\Lambda,\Delta) = a(\Lambda)\,\Gamma(\tilde{\sigma},\Lambda,\Delta)$

Use $\frac{d\psi}{dt} = \frac{\partial\psi}{\partial\Lambda}\dot{\Lambda} + \frac{\partial\psi}{\partial\Delta}\dot{\Delta}$ and solve * for Γ.

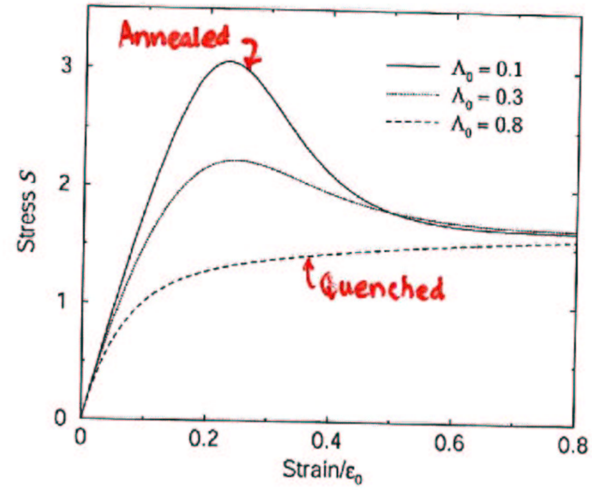
The result is:

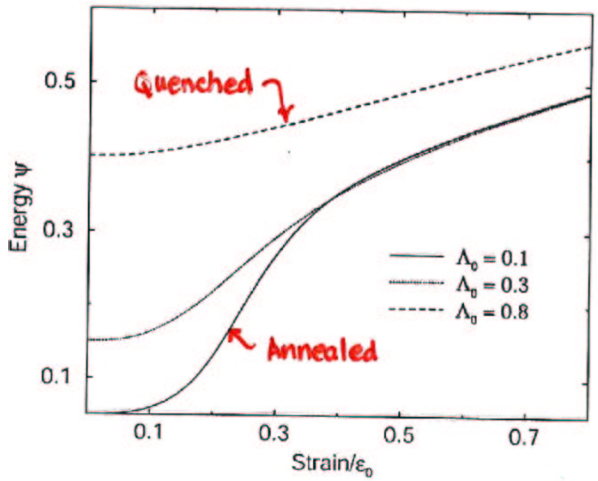
$$\Gamma(\tilde{\sigma},\Lambda,\Delta) = \frac{2\Lambda(\Lambda\tilde{\sigma}-\Delta)^2}{(1+\Lambda)(\Lambda^2-\Delta^2)}$$

$$a(\Lambda) = \Lambda$$

$$\psi(\Lambda,\Delta) = \frac{\Delta^2}{2\Lambda} + \frac{1}{2}\Lambda$$

Constant strain rate simulations





O.A. Hasan and M. C. Boyce, Polymer 34, 5085, (1993)

Constant stain rate loading of polystyrene(PS) sample

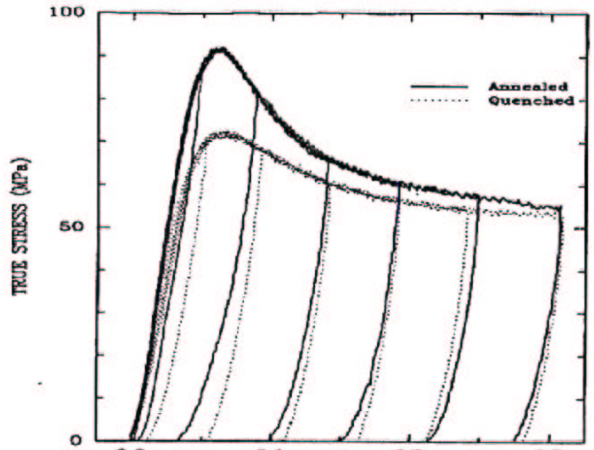


Figure 2 Annealed and quenched PS loaded to different strains at temperature 296 K and strain rate −0.001 s^{-1}

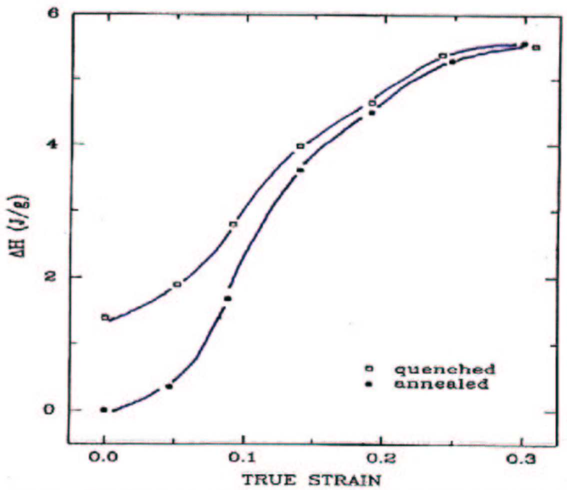


Figure 4 Change in enthalpy of annealed and quenched PS with increasing strain ($\rho = 1.06$ g cm^{-3})

DISORDER TEMPERATURE

(Lemaitre)

Steady-state density of STZs $\sim n_\infty \sim \dfrac{\text{Creation rate}}{\text{Annihil'n rate}} \sim e^{-1/\chi}$

χ ~ disorder temperature → T in equilibrium?

$$\dot{\chi} = c_1 Q - c_2 e^{-\varkappa/\chi}$$

Rate of energy dissipation by plastic deformation

Slow, spontaneous relaxation $\sim \Lambda^{\varkappa}$

Results:

Constant strain rate : $\dot{\epsilon}^{pl} \sim \frac{1}{\tilde{\sigma}} (\tilde{\sigma}^2 - 1)^{\varkappa/\varkappa - 1}$

$\chi \sim -\dfrac{\varkappa}{\ln \dot{\epsilon}^{pl}}$ for $\dot{\epsilon}^{pl} \to 0$

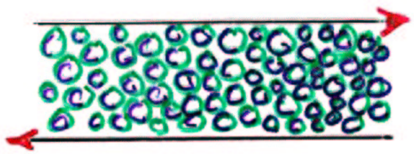
Stress relaxation for $\tilde{\sigma} >> 1$; ϵ^{tot} fixed

$\tilde{\sigma}(t) \sim \exp[-\text{const} \times t^{\beta}]$

$\beta = 1 - \frac{1}{\varkappa}$

Effective Temperatures

Ono et al., "Effective Temperatures of a Driven System Near Jamming," PRL 89, 095703 (2002).



Numerical simulation of a sheared foam: Temperature, computed in several independent ways, goes to a non-zero constant in the limit of vanishing shear rate !! $(\dot{\epsilon} \to 0)$

This result is implied by STZ-like theories, essentially by dimensional analysis:

Viscosity $\eta \sim s_y / \dot{\epsilon}$

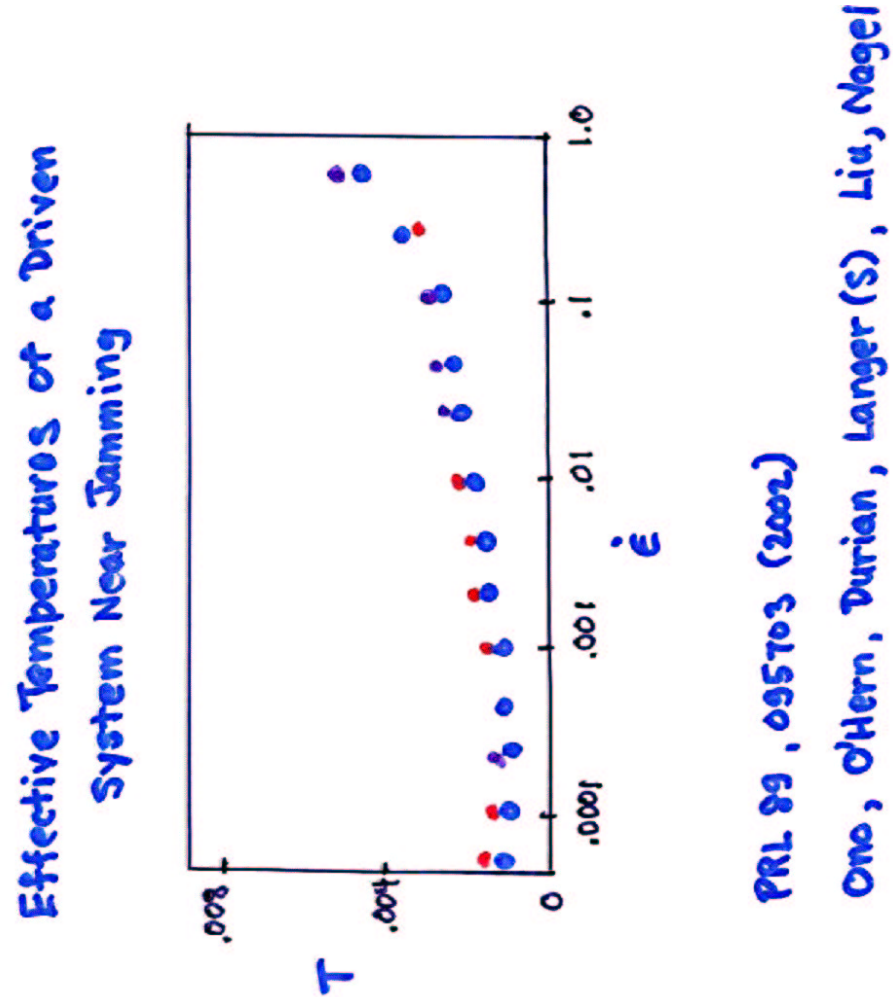
Diffusion constant $D \sim \ell^2 \dot{\epsilon}$

$\ell \sim$ jump size $\sim$ bubble size

Response-fluctuation theorem

$$D \sim \frac{T_{eff}}{\eta \ell} \Rightarrow T_{eff} \sim s_y \ell^3$$

What is the meaning of this non-equilibrium effective temperature?



CONCLUDING REMARKS

There is a wide range of deep, urgent problems to be solved in theories of deformable solids and solid-like materials.

Solving these problems will require new ideas about the physics of driven, out-of-equilibrium systems.

Solving these problems also will require a much closer interaction between experiment, theory, and numerical simulation than exists today.