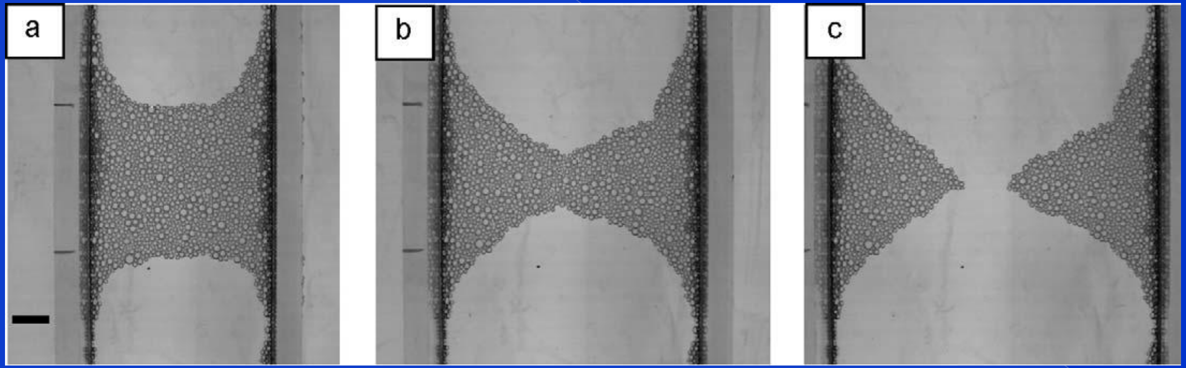
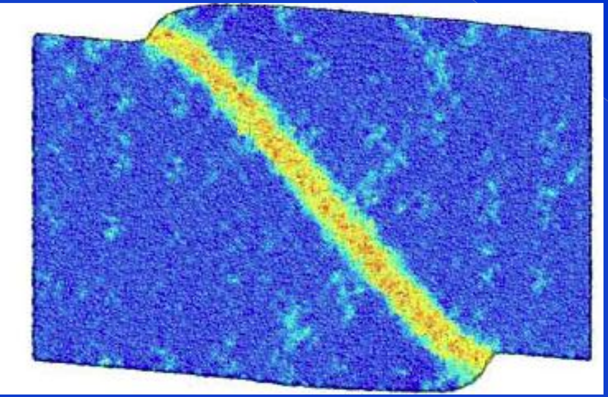
Continuum physics of deforming glasses: From oscillatory shear to fracture

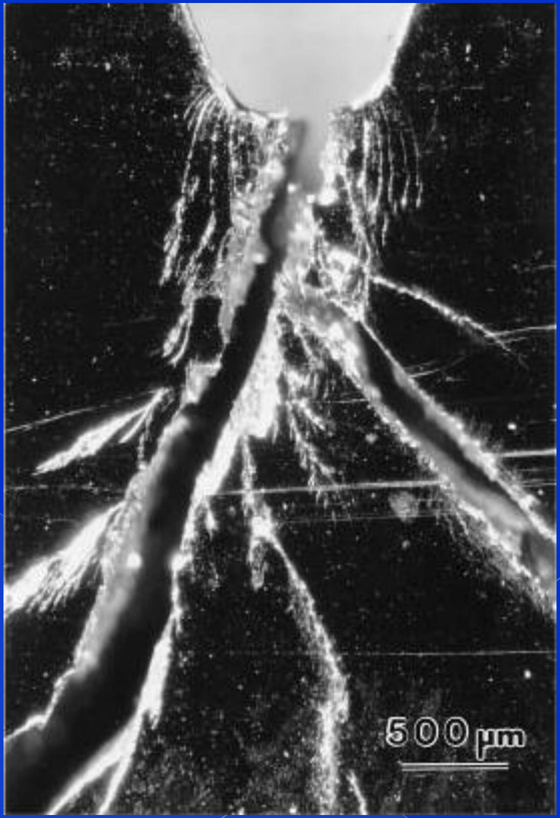
Eran Bouchbinder
Weizmann Institute of Science



Arciniaga, Kuo and Dennin
Colloids and Surfaces A (2011)



Cao, Cheng and Ma
Acta Materialia (2009)

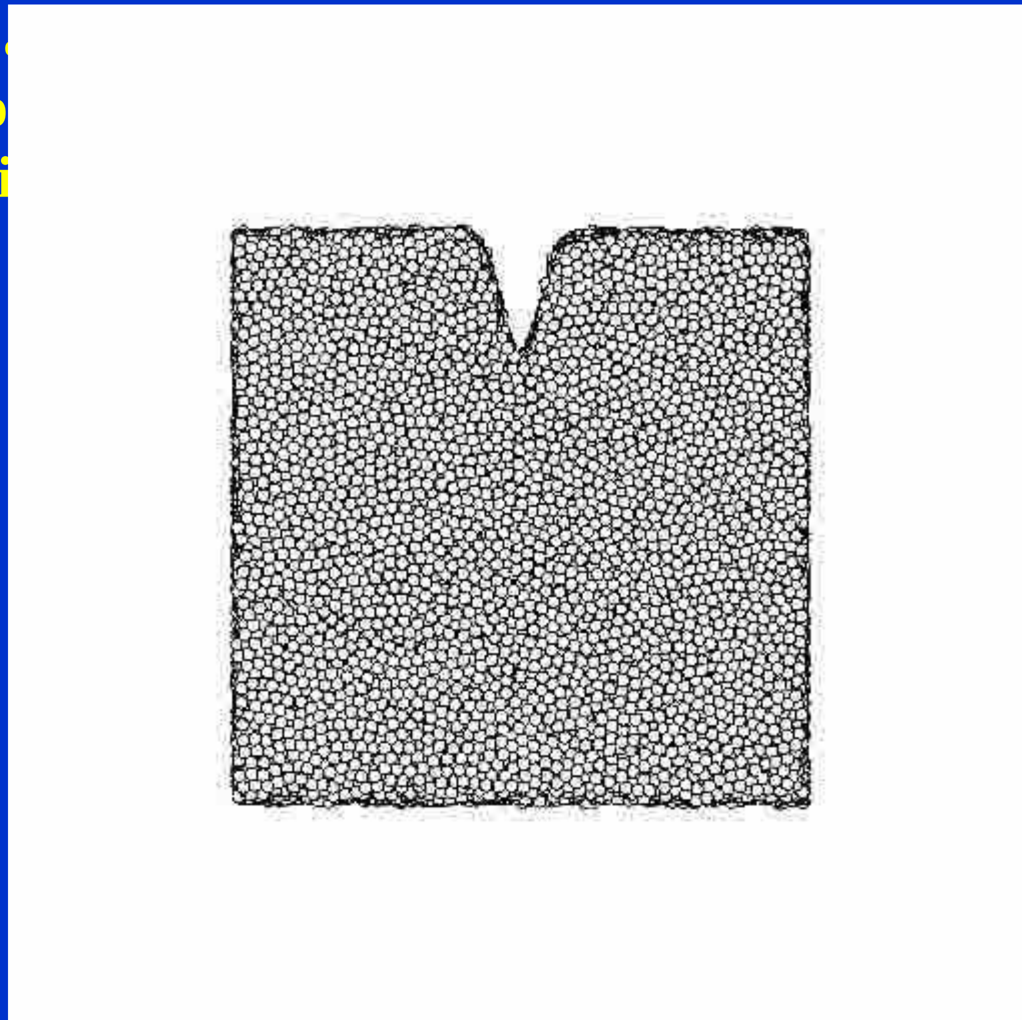


Lowhaphandu and Lewandowski
Scripta Materialia (1998)

Work with:
Jim Langer (UCSB)
Chris Rycroft (Harvard)
Nathan Perchikov (Weizmann)

The challenge (as we see it)

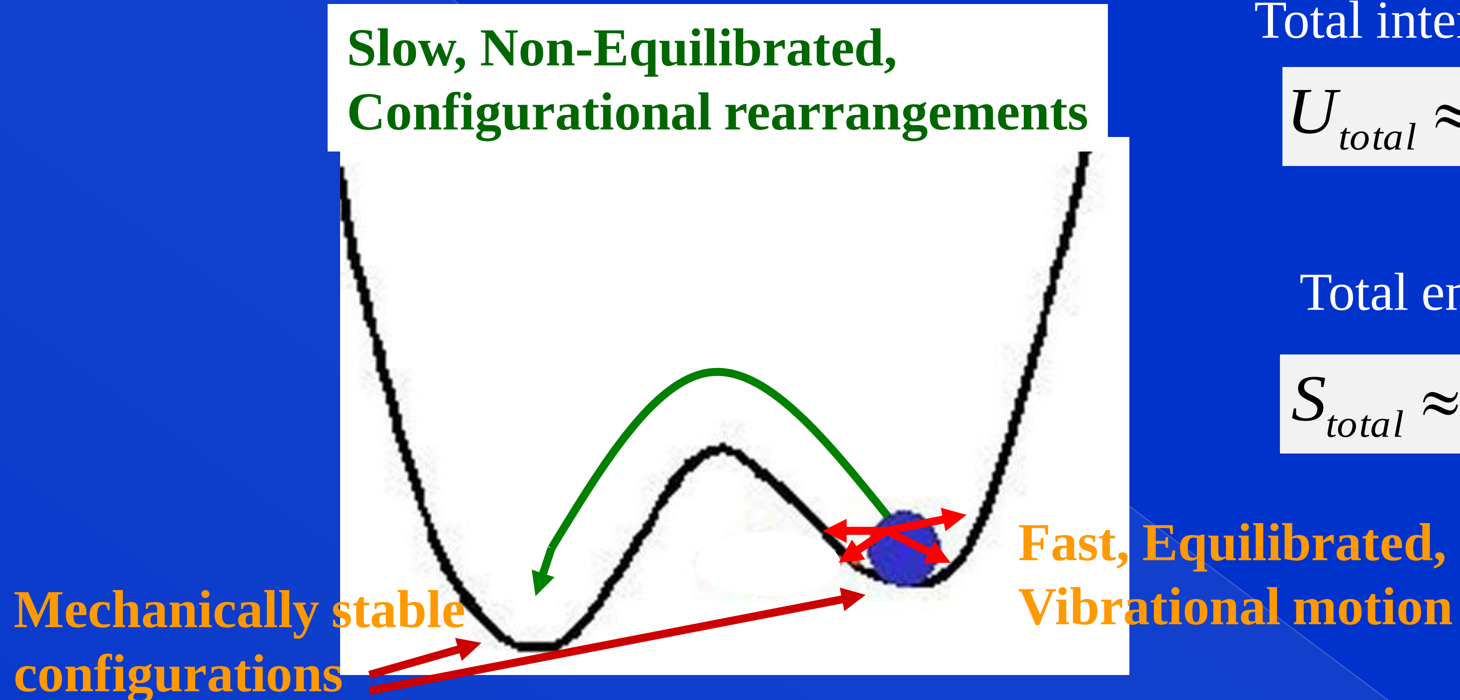
To develop … ing glasses, with a focus on no … cking instabilities, shear-bandi…



N. Bailey et al. PRB 69, 144205 (2004)
Simulation of Cu-Mg Metallic Glass

Theoretical approach: Nonequilibrium thermodynamics

Basic idea 1: Separable Configurational + Kinetic/Vibrational Subsystems



Total internal energy:

$$U_{total} \approx U_C + U_K$$

Total entropy:

$$S_{total} \approx S_C + S_K$$

Weak coupling between these two subsystems, Timescales separation, Quasi-ergodicity due to external driving forces

EB & JS Langer, Physical Review E 80, 031131 (2009)
EB & JS Langer, Physical Review E 80, 031132 (2009)

Basic idea 2: The degrees of freedom relevant to irreversible deformation can be described by non-equilibrium coarse-grained internal variables

$$U_{total} \approx U_C(S_C, E_{ij}, \Lambda, m_{ij}) + U_K(S_K, E_{ij})$$

Define two different temperatures:

$$\chi = \left(\frac{\partial U_C}{\partial S_C}\right) \qquad T = \left(\frac{\partial U_K}{\partial S_K}\right)$$

"Effective" temperature, non-equilibrium degrees of freedom

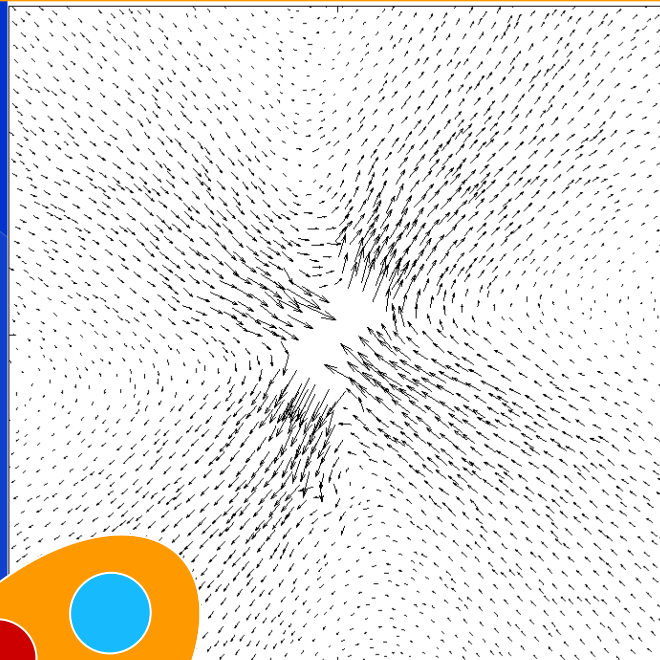
Ordinary, equilibrium temperature

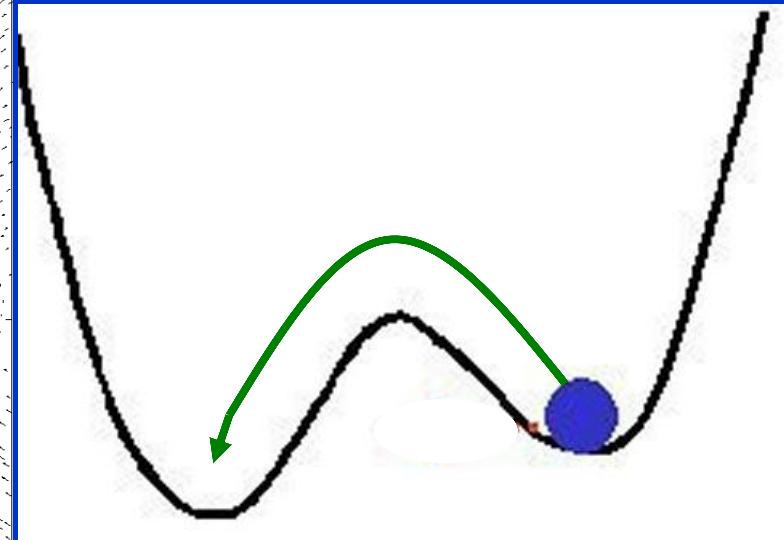
Early ideas in the glass/granular materials community:
Edwards, Cugliandolo, Kurchan, Coniglio, Barrat, Berthier and more

χ **is a thermodynamic temperature, e.g. it appears in equations of state, it controls the probability of configurational fluctuations etc.**

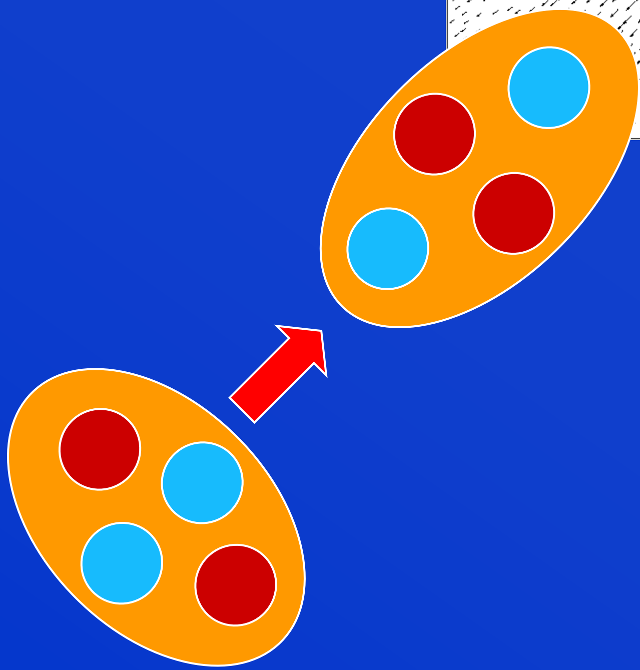
EB & JS Langer, Physical Review E 80, 031131 (2009)
EB & JS Langer, Physical Review E 80, 031132 (2009)

Theoretical approach: Constitutive law





Potential Energy Landscape



Shear-Transformation-Zones (STZ)

Λ Probability to observe an STZ (average normalized density)

m_{ij} Normalized orientational bias of STZ

ML Falk & JS Langer, Physical Review E 57, 7192 (1998)
EB, JS Langer & I Procaccia, Physical Review E 75, 036107 (2007)
EB & JS Langer, Physical Review E 80, 031133 (2009)
ML Falk & JS Langer, Annu. Rev. Condens. Matter Phys. 2, 353 (2011)
K Kamrin & EB, J. Mech. Phys. Solids , In press (2014)

The Equations (dimensionless, simple shear, low T)

$$\dot{\gamma}^{pl}(s,T,\Lambda,m) = \Lambda\, e^{-1/T} \cosh\left(\frac{\Omega s}{T}\right)\left[\tanh\left(\frac{\Omega s}{T}\right) - m\right]$$

STZ density

Stress-biased thermal activation

STZ flips dynamics

s can change for ve

$$\Lambda = e^{-1/\chi}$$

Generalized Boltzmann factor controls STZ density

$$\dot{m} = \frac{2\,\dot{\gamma}^{pl}}{\Lambda}\,(1 - m\,s)$$

Orientational order dynamics

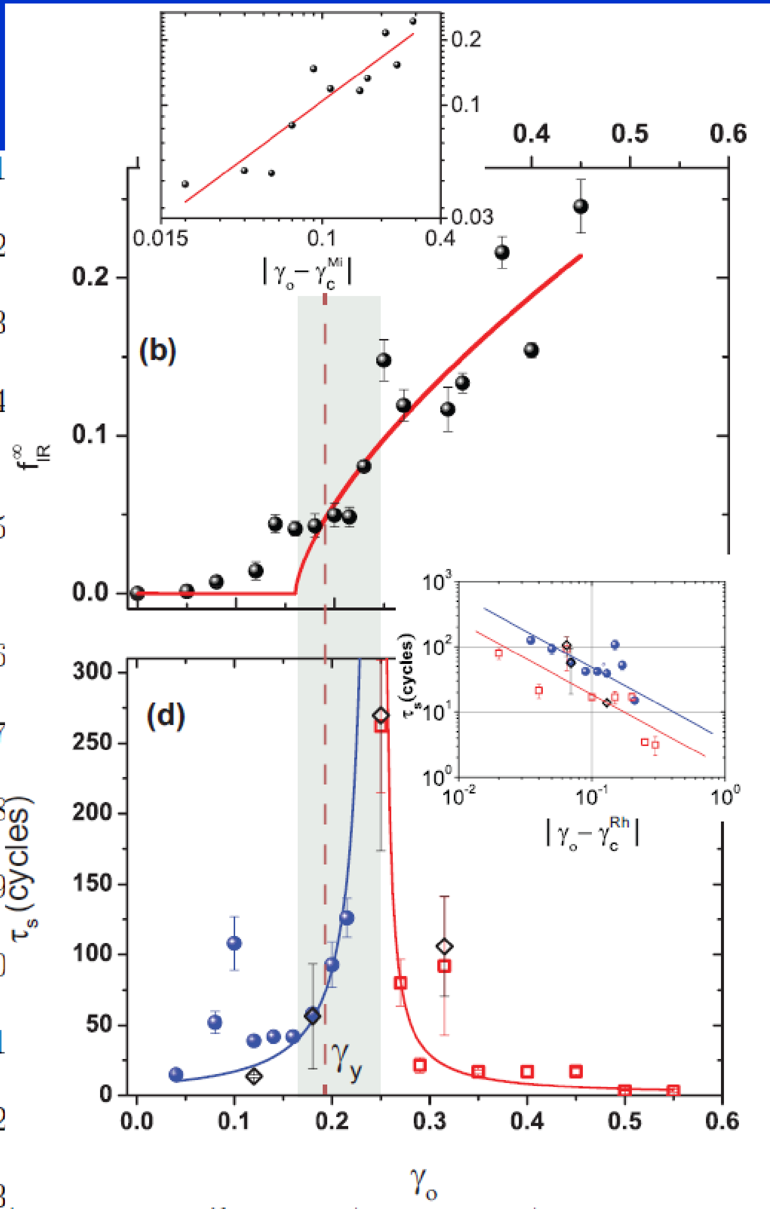
$$c_0\dot{\chi} = 2\,s\,\dot{\gamma}^{pl}\,(\chi_\infty - \chi) + \kappa_c\nabla^2\chi$$

Configurational heat equation

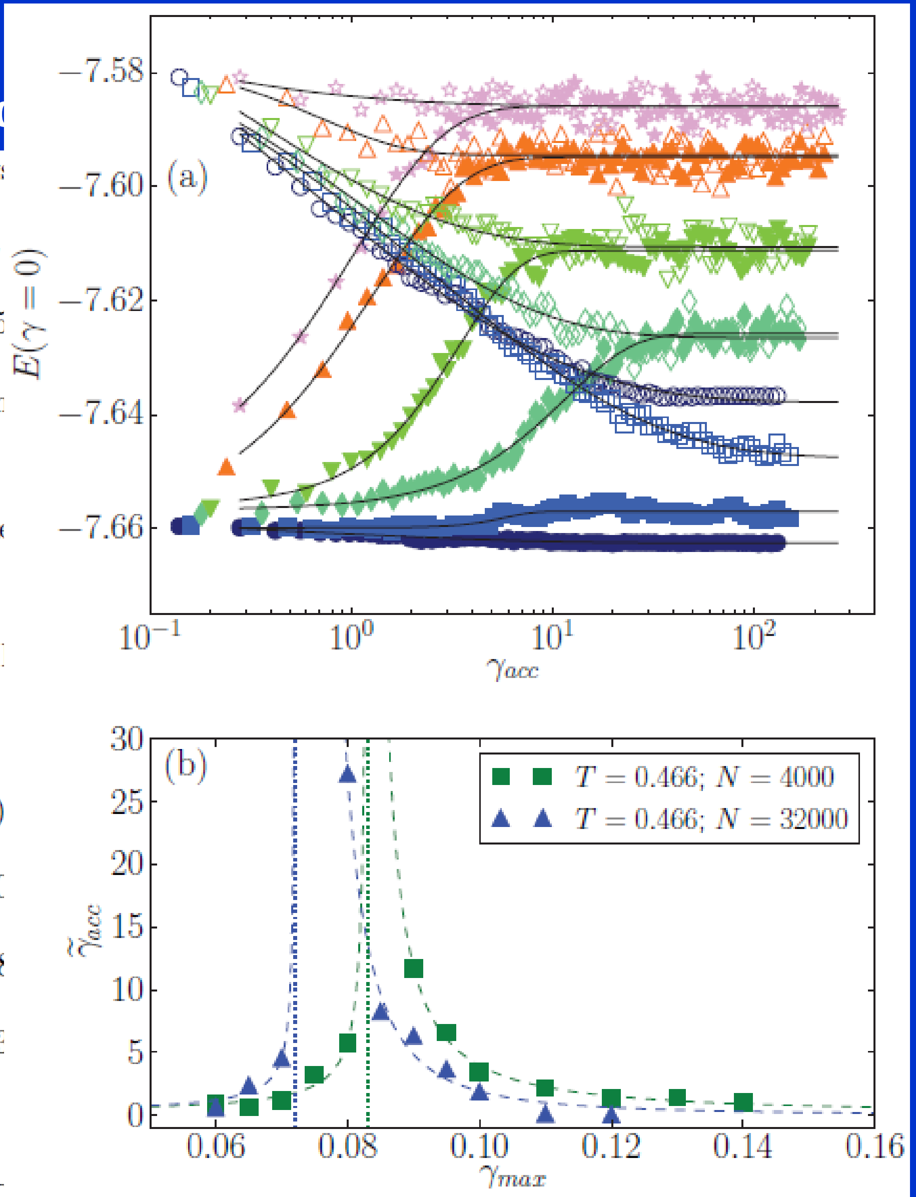
Elasto-plastic rates decomposition

$$\dot{\gamma} = \dot{\gamma}^{el} + \dot{\gamma}^{pl} \quad\Longrightarrow\quad \dot{s} = 2\mu\left[\dot{\gamma} - \dot{\gamma}^{pl}\right]$$

Application I: Variable-amplitude oscillatory shear



Hima Nagamanasa et al., Physical Review E (2014)



Fiocco et al., Physical Review E (2013)

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[3 … , 2555

[4 … I. Der

[5 … Hecke

[6 … Rev. I

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[8 … (2013)

[9 … 02030

[10 … v. E 8

[11 … , 0283

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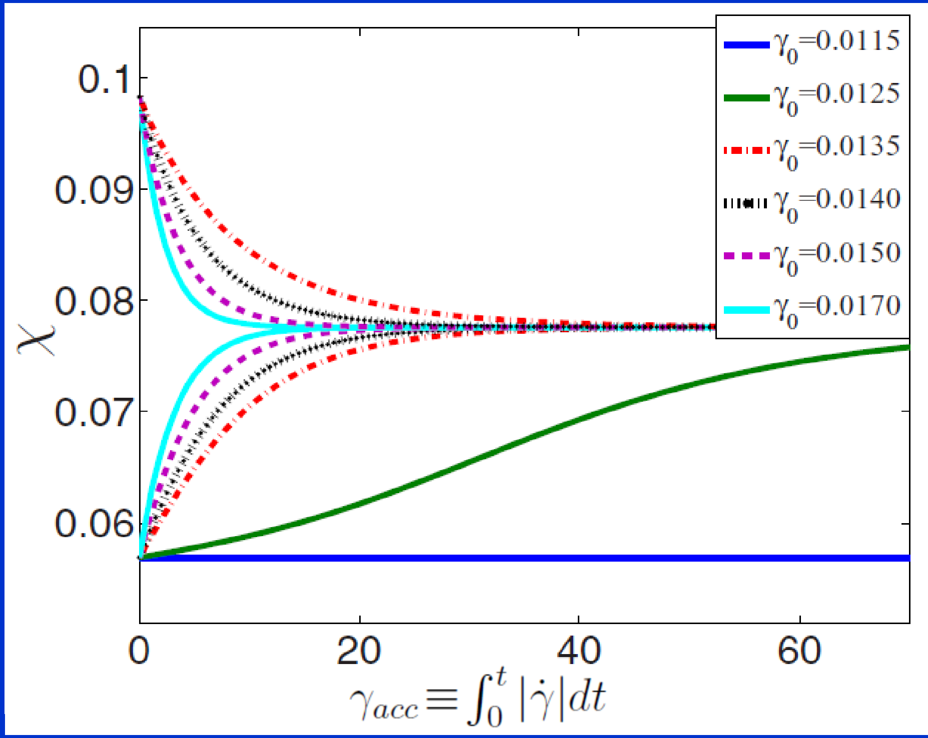
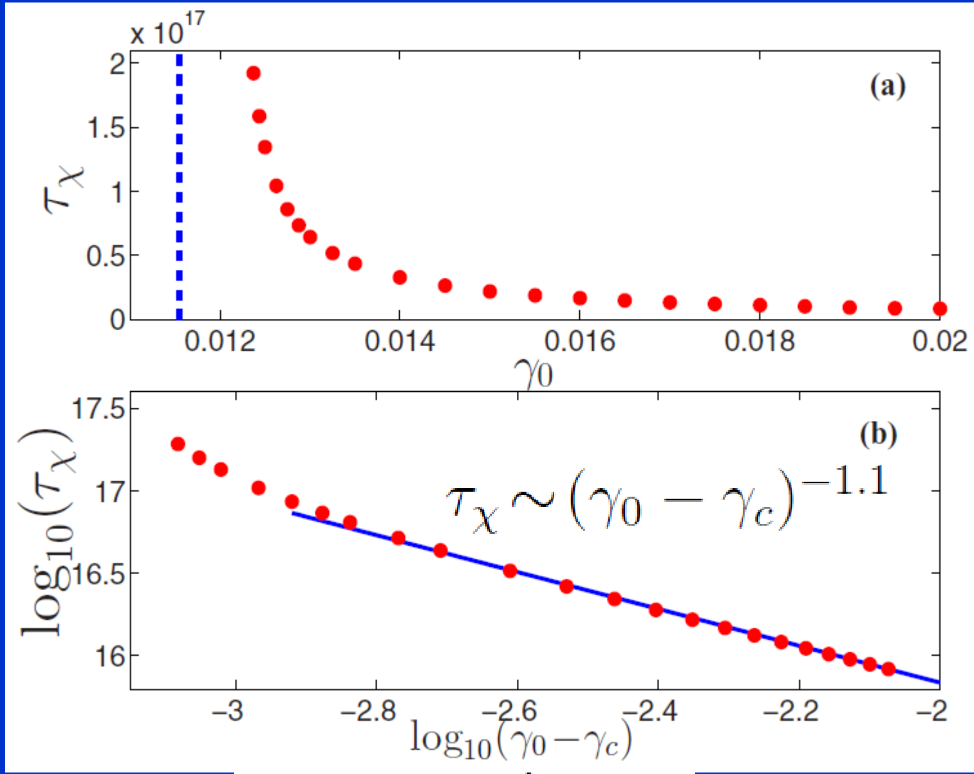
[13 … l R. C

062308 (2014).

… nary LJ glass

Variable-amplitude oscillatory shear: Results





$$c_0 \dot\chi = 2\, s\, \dot\gamma^{pl} \left(\chi_\infty - \chi\right)$$

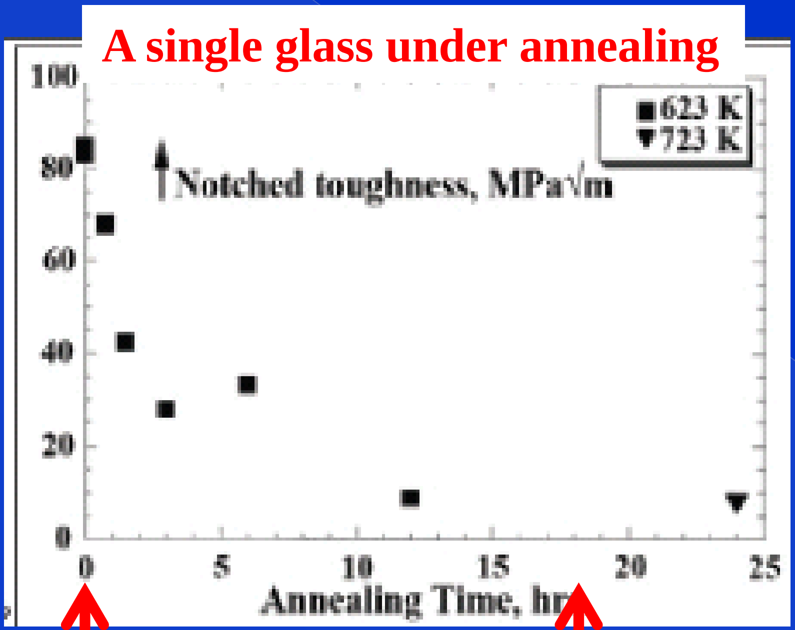
$$\mathcal{A} \equiv \lim_{t\to\infty} \oint s \dot\gamma \, dt$$

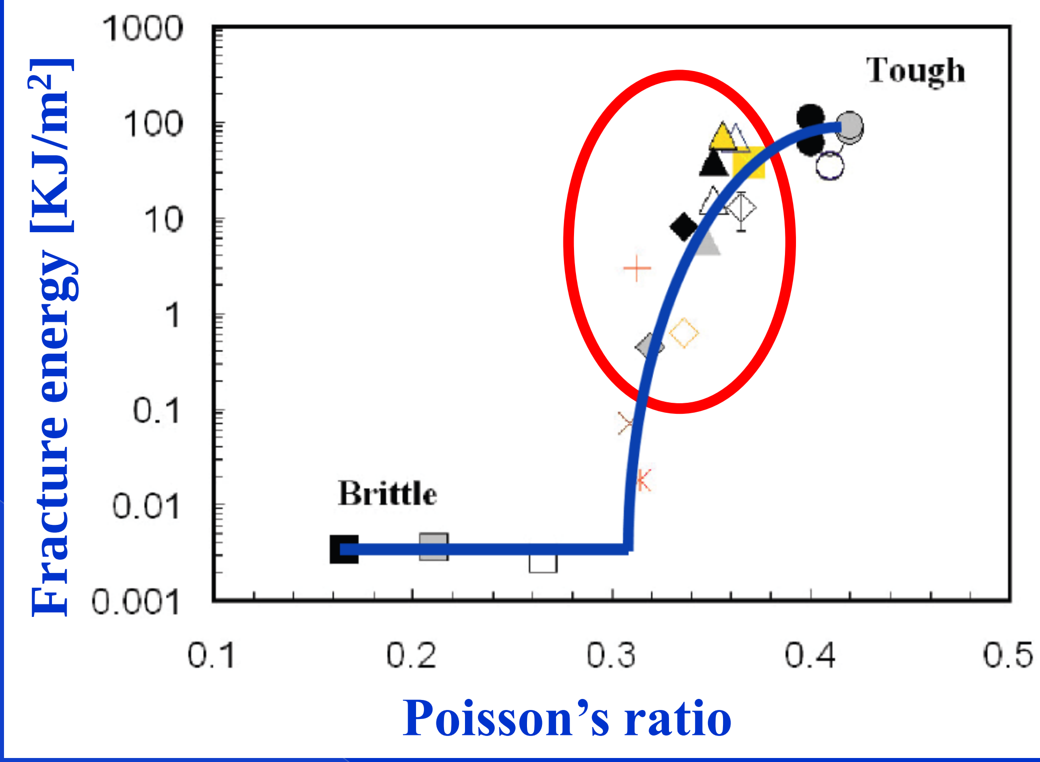
$$c_0 \dot\chi \simeq 2$$

$$\dot\gamma^{pl} = e^{-1/\chi}\, e^{-1/T} \cosh\left(\frac{\Omega s}{T}\right) \left[\tanh\left(\frac{\Omega s}{T}\right) - m\right]$$

N. Perchikov & EB, Physical Review E 89, 062307 (2014)

Application II: Ductile-to-brittle transition





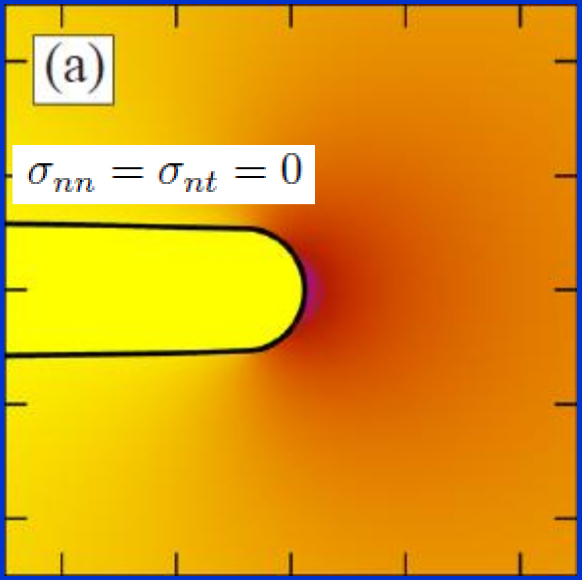
High initial χ

Low initial χ

$$\chi > T$$

CH Rycroft & EB, Phys. Rev. Lett. 109, 194301 (2012)

Notch Fracture Toughness



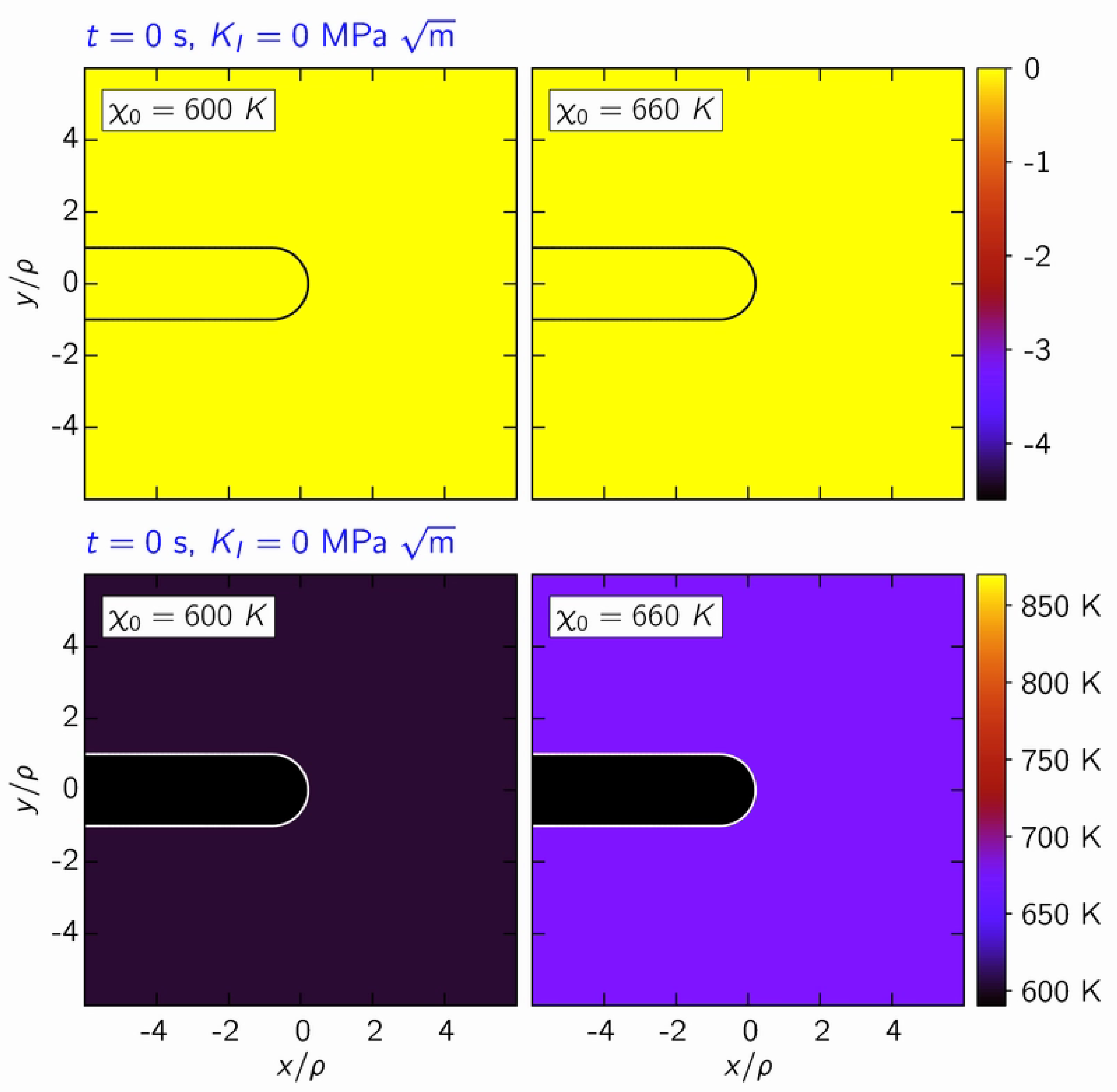
Serious computational challenges were involved, especially in achieving realistic loading rates

An Eulerian projection method for quasi-static elastoplasticity
CH Rycroft, Y. Sui & EB, arxiv 1409.2173 (2014)

$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ bulk metallic glass (Vitreloy 1)

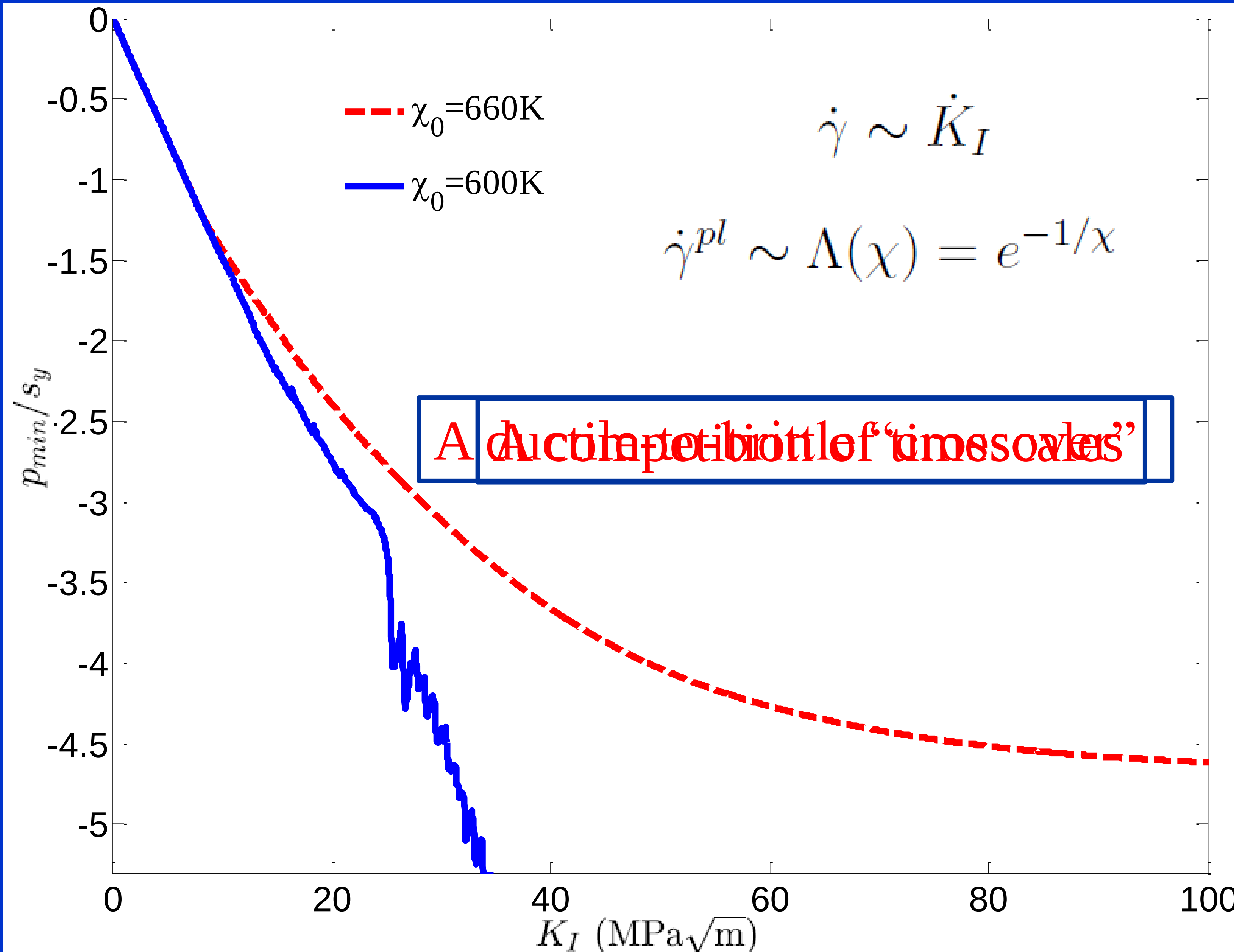
Parameters determined from independent sources	
$\tau_0 \sim 10^{-13}$ sec	Molecular vibration timescale
$s_y \sim 1$ GPa	Shear yield stress
$K,\ \mu \sim 100$ GPa	Elastic moduli
$e_z \sim 1$ eV	STZ formation energy
$\chi_\infty \sim 1.4 T_g$	Steady state of χ
$T \sim 0.5 T_g$	Test temperature

Results



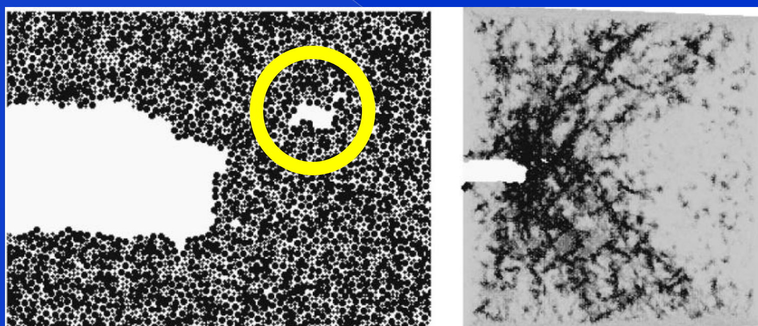
$t = 0$ s, $K_I = 0$ MPa $\sqrt{m}$
$\chi_0 = 600\ K$
$\chi_0 = 660\ K$
0
-1
-2
-3
-4
y/ρ
4
2
0
-2
-4
$t = 0$ s, $K_I = 0$ MPa $\sqrt{m}$
$\chi_0 = 600\ K$
$\chi_0 = 660\ K$
850 K
800 K
750 K
700 K
650 K
600 K
x/ρ

Results (cont'd)



Initiation criterion: A cavitation instability

MD simulation

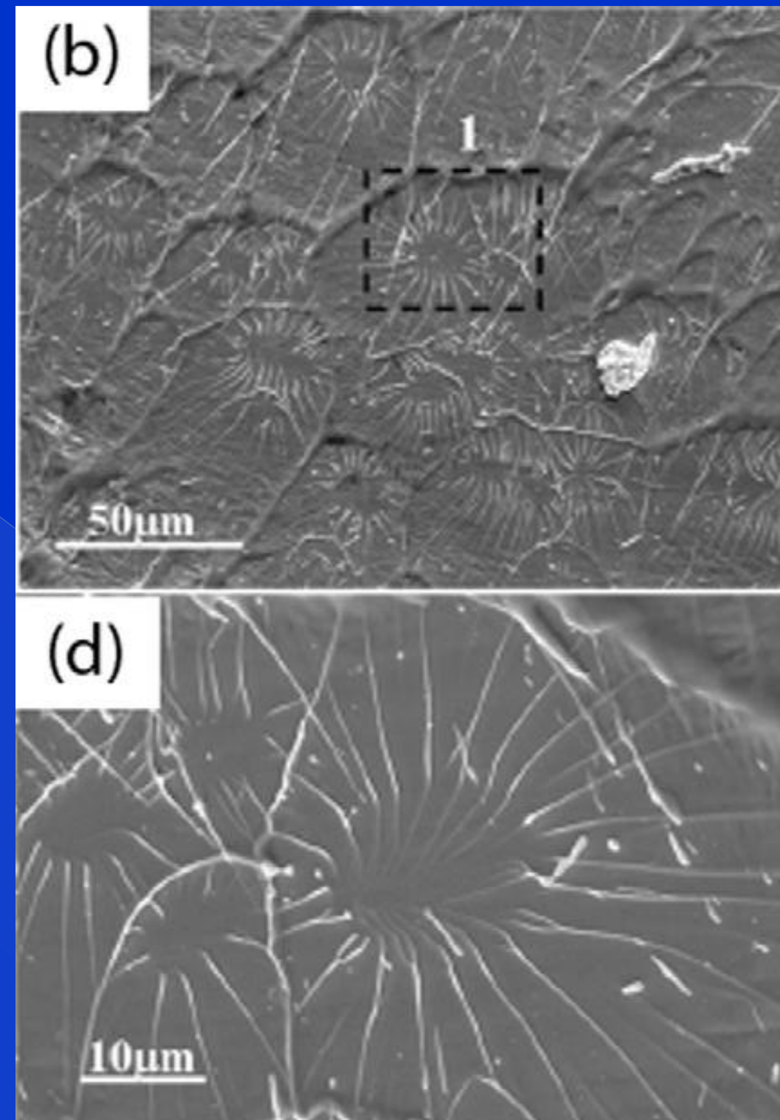


M. L. Falk, PRB 60, 7062 (1999)

$$\sigma_c = \frac{2}{\sqrt{3}}\left[1 + \log\left(\frac{2\,E}{3\sqrt{3}\,s_y}\right)\right] s_y$$

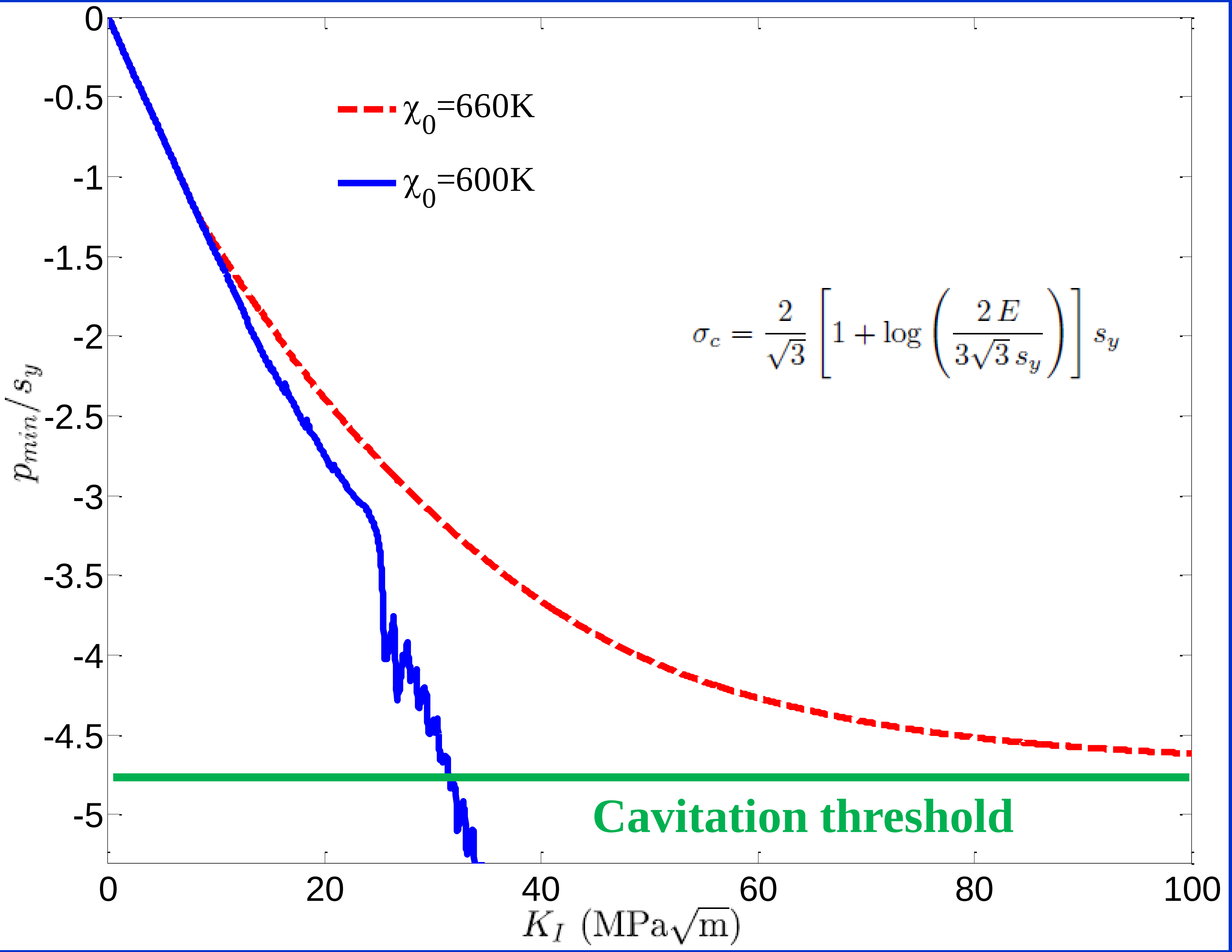
Huang et al., JMPS 39, 223 (1991)

Experiment

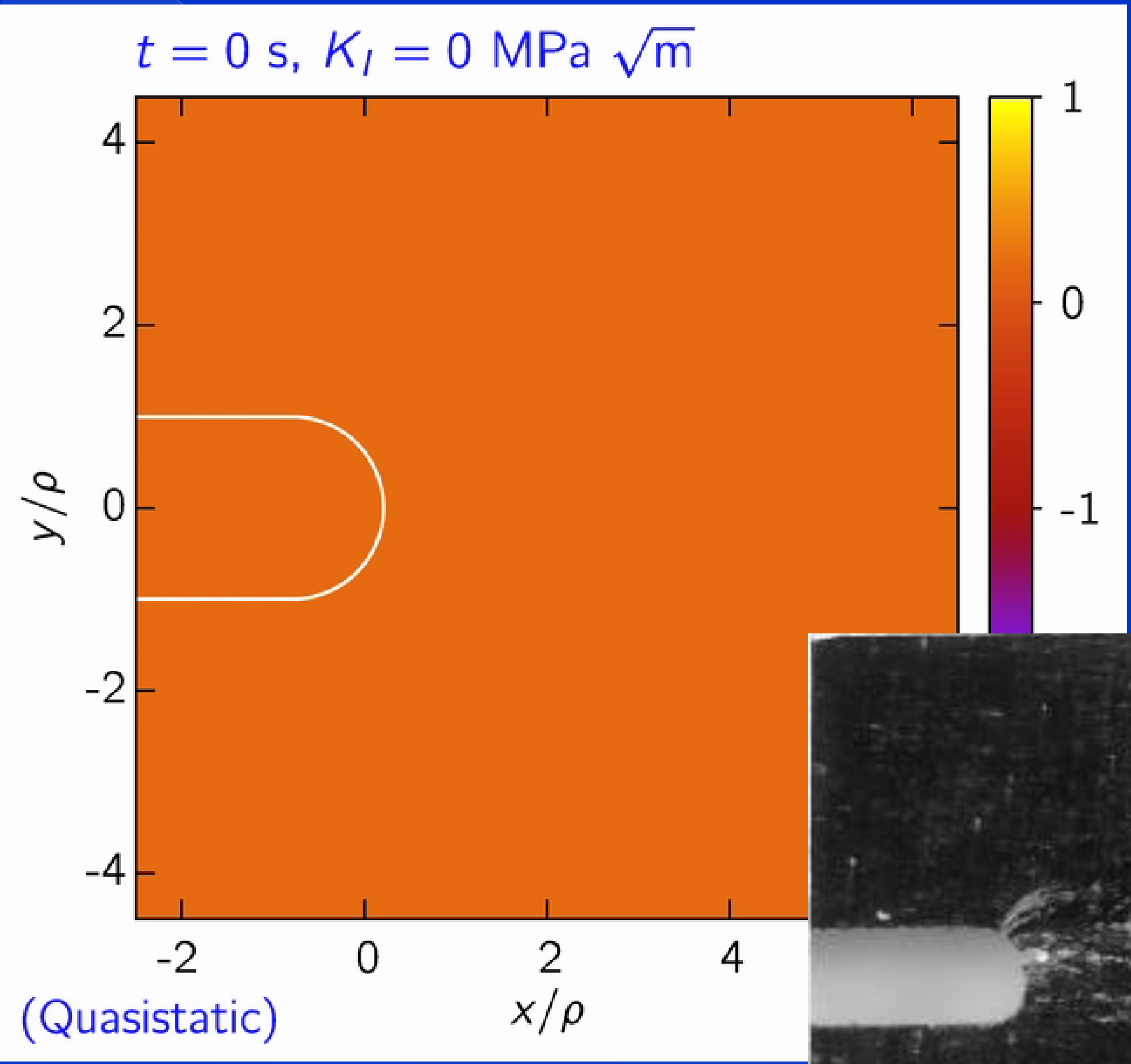


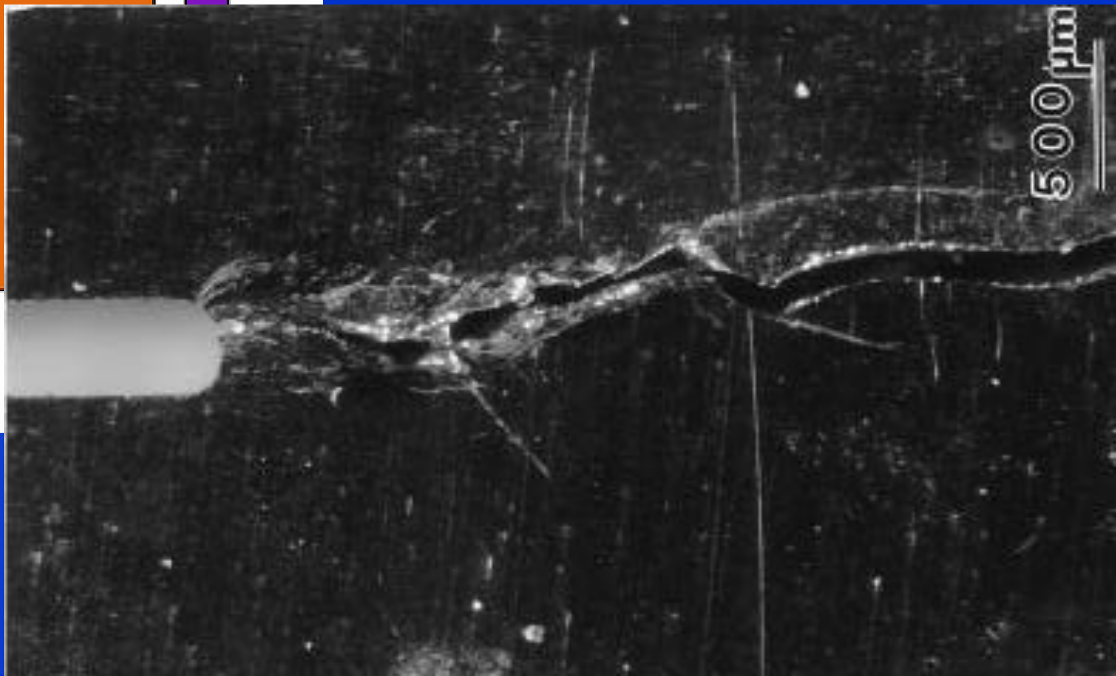
Jiang et al., Philosophical Magazine 2008, 88 407

Results (cont'd)

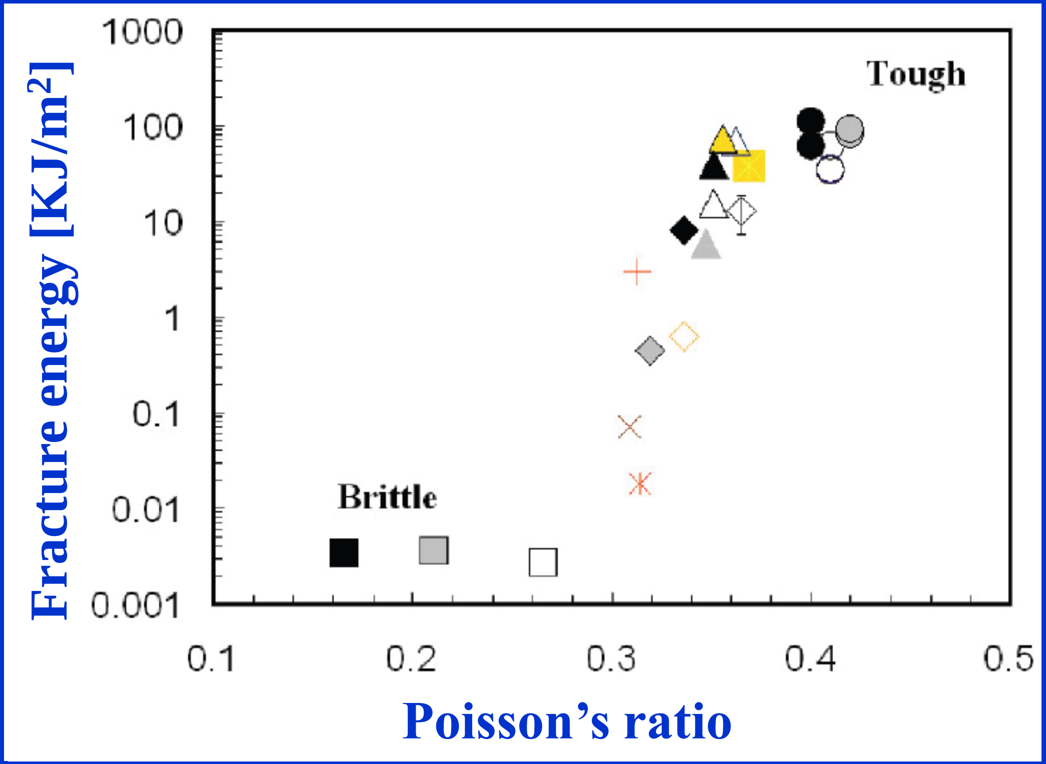


Does local cavitation lead to global failure?





Final comment



$$\nu(\chi)$$

$$\dot{\gamma}^{pl} \sim \Lambda(\chi) = e^{-1/\chi}$$

Summary

The macroscopic theory of glassy deformation based on Shear-Transformation-Zones (STZ) has been discussed.

The theory incorporates coarse-grained internal state variables and characterizes the structural state of the deforming glass by a temperature that may differ from the bath temperature.

We discussed two recent applications of the theory:

- The theory predicts salient features of the variable-amplitude oscillatory shear response of amorphous materials, as observed in recent experiments and computer simulations.

- The theory offers an explanation for an observed annealing-induced ductile-to-brittle transition and may open the way for a better understanding of the toughness of metallic glasses.