Non-equilibrium Thermodynamics of Driven Disordered Materials

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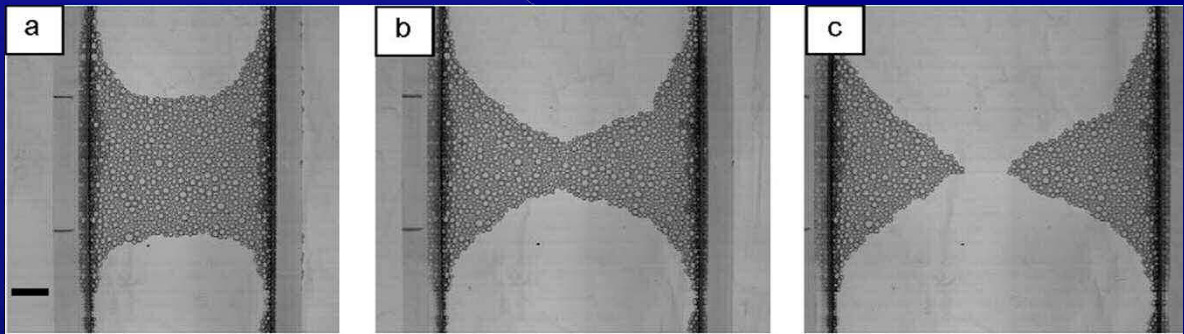
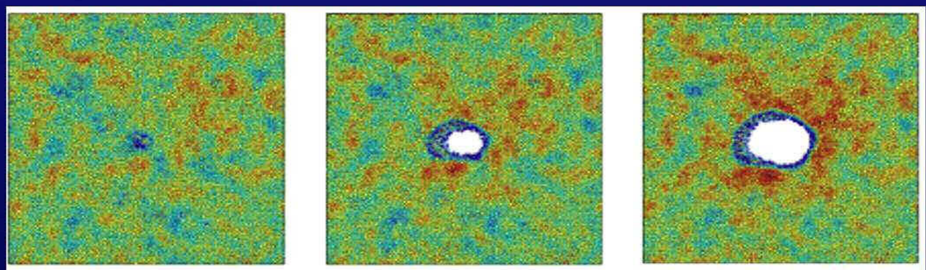
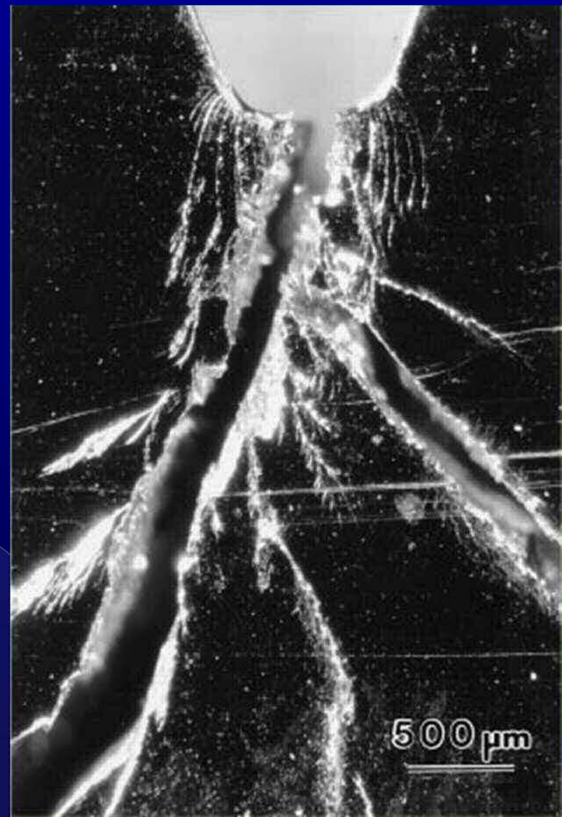


Dennin s group, UCI (2011)



Murali et al., PRL 107, 215501 (2011)

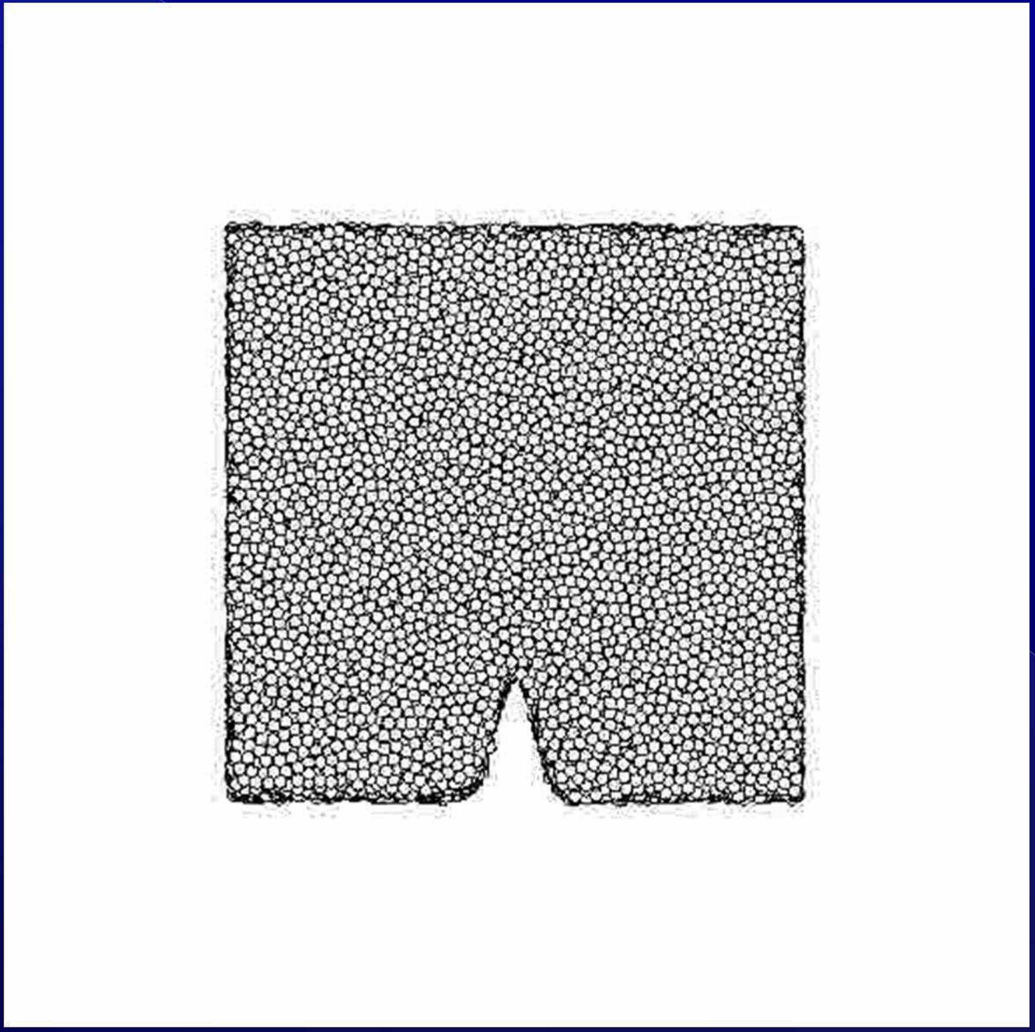


Lowhaphandu and Lewandowski
Scripta Materialia 38, 1811 (1998)

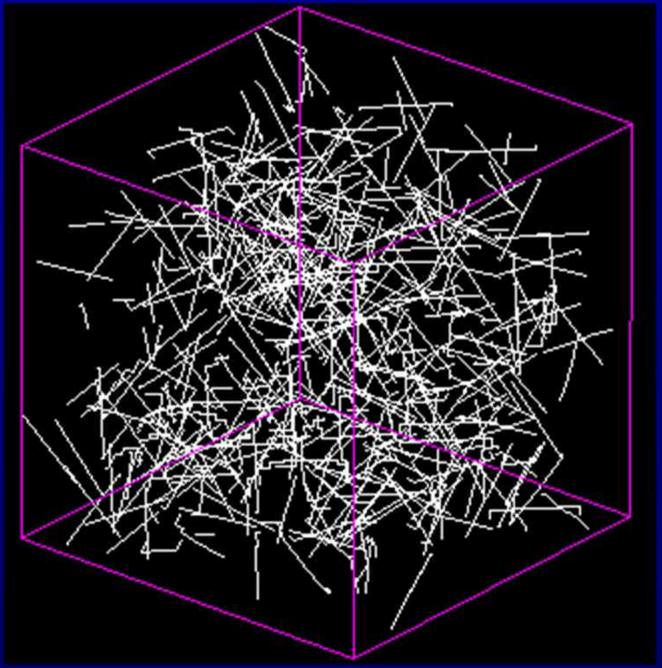
Work with: James Langer (UCSB)
Chris Rycroft (UC Berkeley)

Microscopic picture

MOTIVATION



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



Devincre
3-D dislocation dynamics simulation

The basic question

Can one develop a continuum thermodynamic framework that allows an effective macroscopic description of the collective dynamics of such microscopic objects?

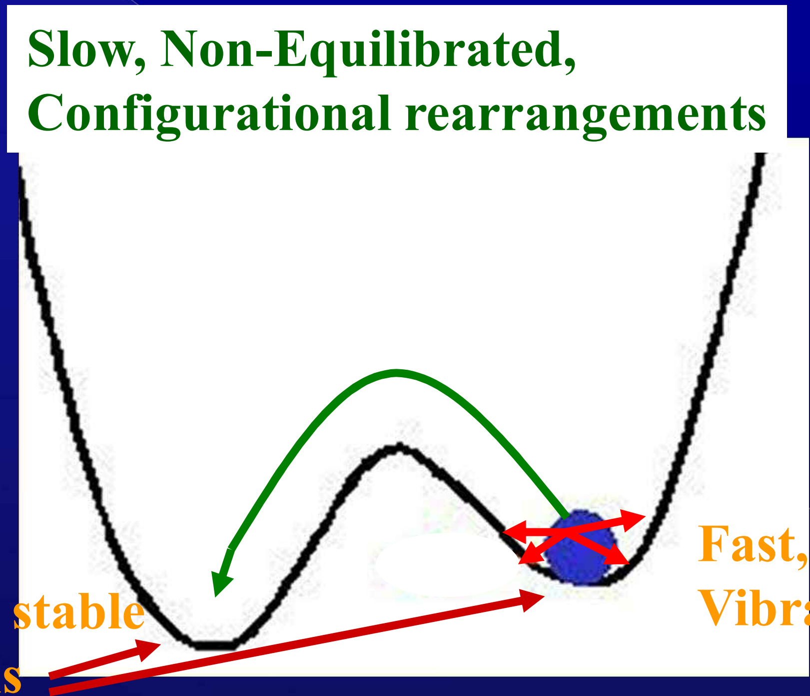
We need concepts and theoretical tools to bridge over the widely separated scales.

Fundamental properties shared by these systems:

These are all driven, strongly dissipative, systems, whose dynamics involve configurational changes that are weakly coupled to thermal fluctuations

Our approach

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 non-equilibrium state of the system can be characterized by coarse-grained internal variables

$$U_C(S_C, E, \{\Lambda_\alpha\}) \longrightarrow S_C(U_C, E, \{\Lambda_\alpha\})$$

The elastic part of the deformation

A small number of coarse-grained internal variables (order parameters), describe internal degrees of freedom that may be out of equilibrium

Non-equilibrium entropy $S_C(U_C, E, \{\Lambda_\alpha\}) = \ln \Omega_C(U_C, E, \{\Lambda_\alpha\})$

A constrained measure of the number of configurations

When $\{\Lambda_\alpha\} \to \{\Lambda_\alpha^{eq}\}$ $S_C(U_C, E, \{\Lambda_\alpha\}) \to S_C(U_C, E)$

in the thermodynamic limit

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

Basic idea 2: The non-equilibrium state of the system can be
(cont d) characterized by coarse-grained internal variables

$$U_{total} \approx U_C(S_C, E, \{\Lambda_\alpha\}) + U_K(S_K, E)$$

Define two different temperatures:

$$\chi = \left(\frac{\partial U_C}{\partial S_C}\right)_{E,\{\Lambda_\alpha\}} \qquad \theta = \left(\frac{\partial U_K}{\partial S_K}\right)_E$$

Effective temperature, non-equilibrium degrees of freedom

Ordinary, equilibrium temperature

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

χ **is a true 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)

The Laws of Thermodynamics

The 1st law: $V\sigma : \dot{\varepsilon} = \dot{U}_{tot} \quad \Rightarrow \quad V\sigma : \dot{\varepsilon}^{pl} = \chi \dot{S}_C + \theta \dot{S}_K + \sum_\alpha \frac{\partial U_C}{\partial \Lambda_\alpha} \dot{\Lambda}_\alpha$

Using $\dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{pl}$ and $\sigma = \frac{1}{V} \frac{\partial U_C}{\partial E}$

The 2nd law: $\dot{S}_C + \dot{S}_K \geq 0$ define $W\left(\dot{\varepsilon}^{pl}, \{\dot{\Lambda}_\alpha\}\right) = V\sigma : \dot{\varepsilon}^{pl} - \sum_\alpha \frac{\partial U_C}{\partial \Lambda_\alpha} \dot{\Lambda}_\alpha$

$$\theta \dot{S}_K = \alpha_K W + A(\chi - \theta), \quad A \geq 0.$$

$$W\left(\dot{\varepsilon}^{pl}, \{\dot{\Lambda}_\alpha\}\right) \geq 0$$

Configurational heat equation:

$$C_V^{eff} \dot{\chi} \approx \chi \dot{S}_C = \alpha_C W - A(\chi - \theta)$$

$$\alpha_K, \alpha_C > 0 \qquad \alpha_K + \alpha_C = 1$$

Sollich & Cates, arXiv:1201.3275 (2012)

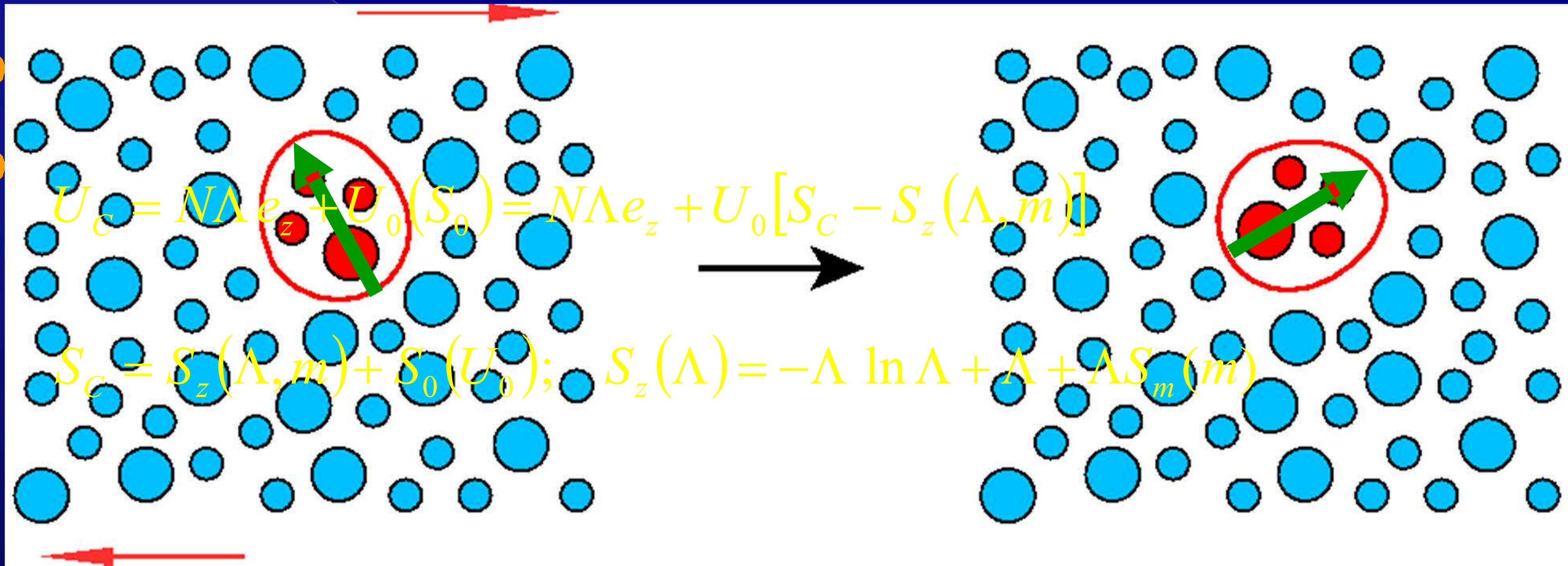
Constitutive Laws: The Physics that comes after Thermodynamics

Example: Amorphous Plasticity

Two steps:

Step

Step



$$U_C = N\Lambda e_z + U_0(S_0) = N\Lambda e_z + U_0[S_C - S_z(\Lambda, m)]$$

$$S_C = S_z(\Lambda, m) + S_0(U_0); \quad S_z(\Lambda) = -\Lambda \ln \Lambda + \Lambda + \Lambda S_m(m)$$

Density of zones (STZ) Λ

Averaged orientation m (magnetization)

F. Spaepen, Acta Metall. 25, 407 (1977), AS Argon, Acta Metall. 27, 47 (1979)
ML Falk & JS Langer, Physical Review E 57, 7192 (1998)
EB & JS Langer, Physical Review E 80, 031133 (2009)
ML Falk & JS Langer, Annu. Rev. Condens. Matter Phys. 2, 353 (2011)

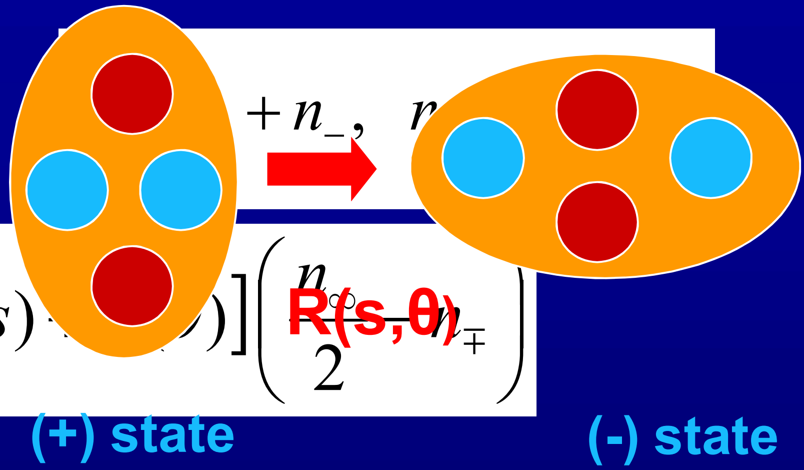
Amorphous plasticity

Step 2 **Derive equations of motion consistent with the laws of thermodynamics**

$$\tau_0 \dot{\varepsilon}^{pl} = R(s,\theta)\, n_+ - R(-s,\theta)\, n_-$$

$$\ldots + n_-, \quad n \ldots$$

$$\tau_0 \dot{n}_\mp = R(\pm s,\theta)\, n_\pm - R(\mp s,\theta)\, n_\mp + \left[\Gamma(s) \ldots\right]\left(\frac{n_\infty}{2} - n_\mp\right)$$



Plug in the 1st and 2nd laws

$$W\left(\dot{\varepsilon}^{pl}, \{\dot{\Lambda}_\alpha\}\right) \geq 0$$

The upshot of the analysis:

$$\Lambda \sim e^{-e_z/\chi}$$

$$\Gamma(s) \sim \frac{W}{s_0}$$

$$\tau_0 c_{eff} \dot{\chi} \;=\; e^{-e_z/\chi}\left[\Gamma(s)(\chi_\infty - \chi) + \rho(\theta)(\theta - \chi)\right]$$

The final equations

$$\tau_0 \dot{\varepsilon}^{pl} \quad = \quad e^{-e_z/\chi} \mathcal{C}(s,\theta) \left[\mathcal{T}(s,\theta) - m(s,\theta) \right]$$

$$\mathcal{C}(s) = \frac{1}{2} \left[R(s) + R(-s) \right]$$

$$\mathcal{T}(s) = \frac{R(s) - R(-s)}{R(s) + R(-s)}$$

$$R(s,\theta) = e^{-\Delta(s)/\theta}$$

$$\left[\mathcal{T}(s) - m(s) \right] \left[1 - \frac{s\, m(s)}{s_0} \right] = \frac{\rho(\theta)}{2\, \mathcal{C}(s)}$$

$$\tau_0 c_{eff} \dot{\chi} \quad = \quad e^{-e_z/\chi} \left[\Gamma(s)(\chi_\infty - \chi) + \rho(\theta)(\theta - \chi) \right]$$

$$\dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{pl} = \frac{\dot{s}}{\mu} + \dot{\varepsilon}^{pl}$$

Properties of the model

The yielding transition

$$\tau_0 \dot{\varepsilon}^{pl} \quad = \quad e^{-e_z/\chi} \mathcal{C}(s,\theta) \left[\mathcal{T}(s,\theta) - m(s,\theta) \right]$$

$$[\mathcal{T}(s) - m(s)] \left[1 - \frac{s\, m(s)}{s_0} \right] = \frac{\rho(\theta)}{2\mathcal{C}(s)}$$

$$s < s_0 \quad m(s) = \mathcal{T}(s)$$

$$s > s_0 \quad m(s) = \frac{s_0}{s}$$

$$\Rightarrow s_0 = s_y$$

Entropic interpretation of the yielding transition

$$\Gamma(s) \sim \frac{W}{s_0}$$

Properties of the model (cont d)

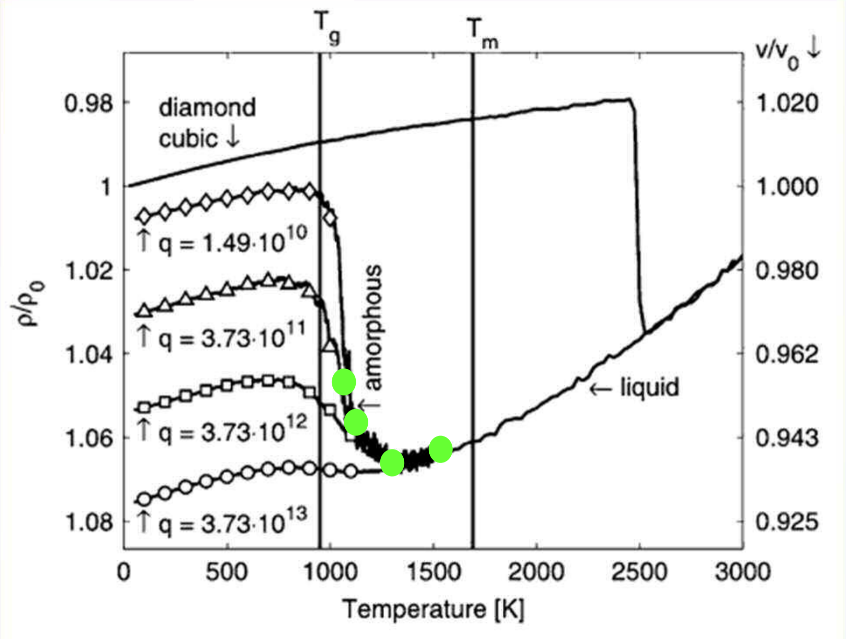
Stress-strain curves and history dependence

$$\dot{s} = \mu\left(\dot{\varepsilon} - \tau_0^{-1} e^{-e_z/\chi}\mathcal{C}(s,\theta)\left[\mathcal{T}(s,\theta) - m(s,\theta)\right]\right)$$

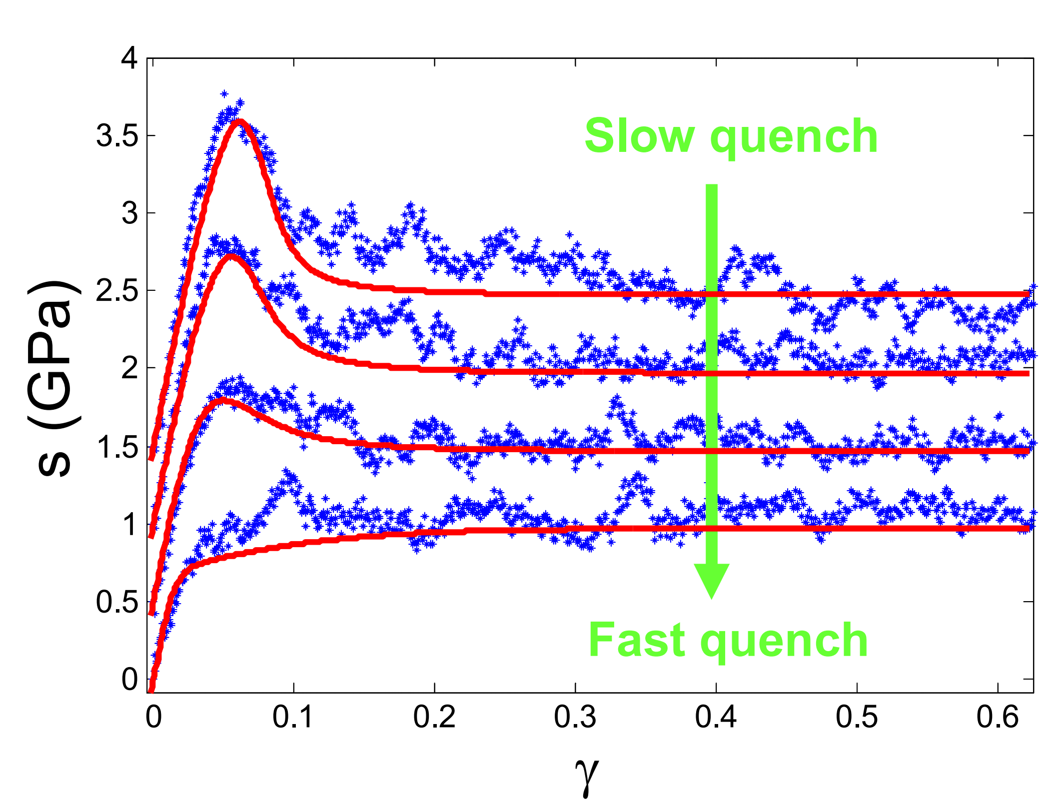
$$\tau_0 c_{eff}\dot{\chi} \;=\; e^{-e_z/\chi}\left[\Gamma(s)(\chi_\infty - \chi) + \rho(\theta)(\theta - \chi)\right]$$

$\chi(0) =$ 1174,1237,1392,1572K

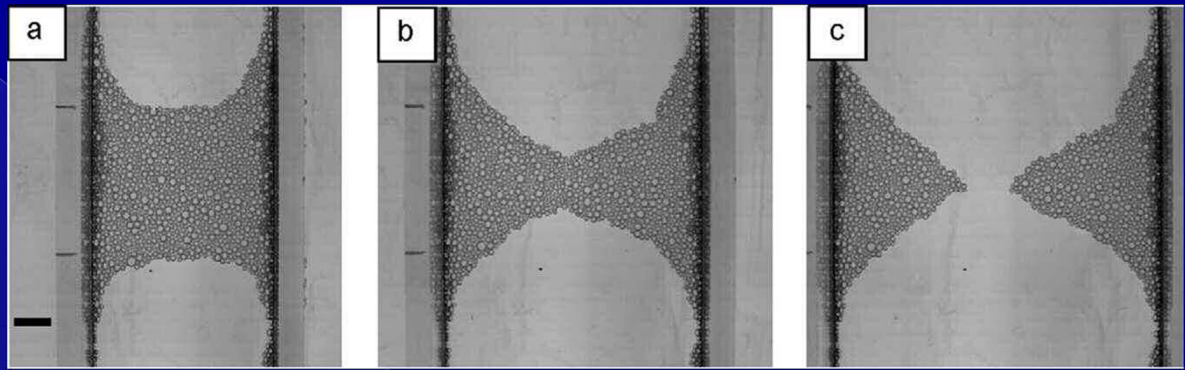
$e_z =$ 1.3eV



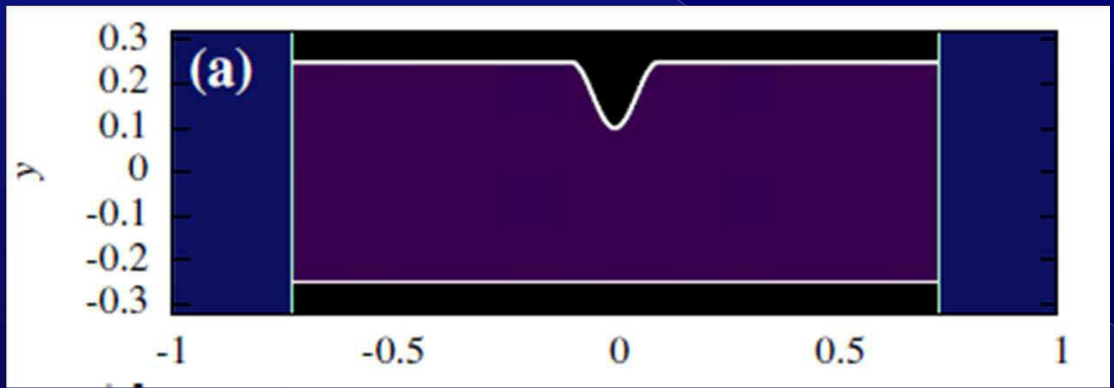
Demkowicz & Argon, PRL 93, 025505 (2004)



Application: The necking instability

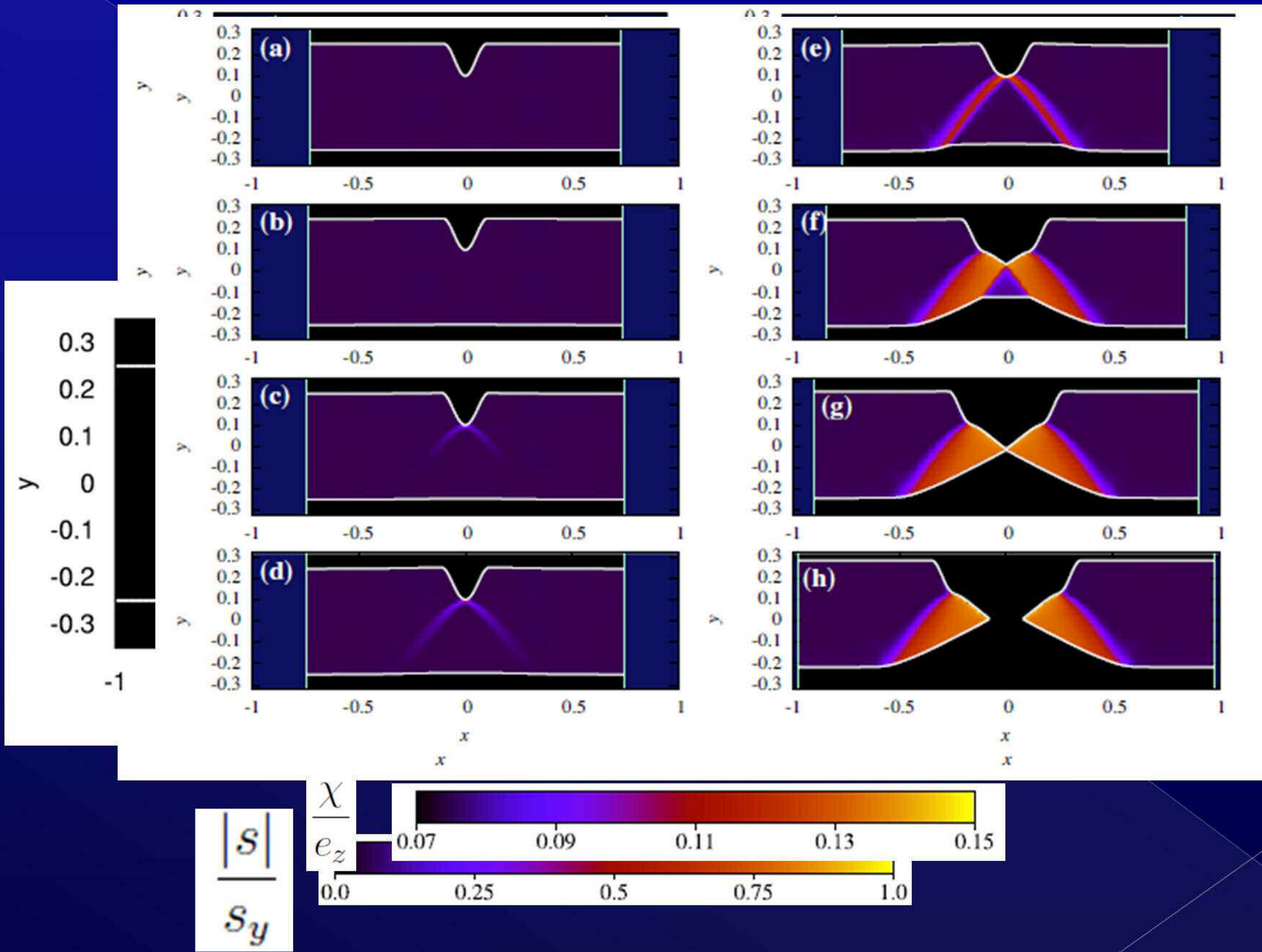


Dennin s group (2011)



CH Rycroft and F Gibou, J. Comp. Phys. 231 (2012) 2155

Necking (cont d)



CH Rycroft and F Gibou, J. Comp. Phys. 231 (2012) 2155

Application: Crack initiation (fracture toughness)

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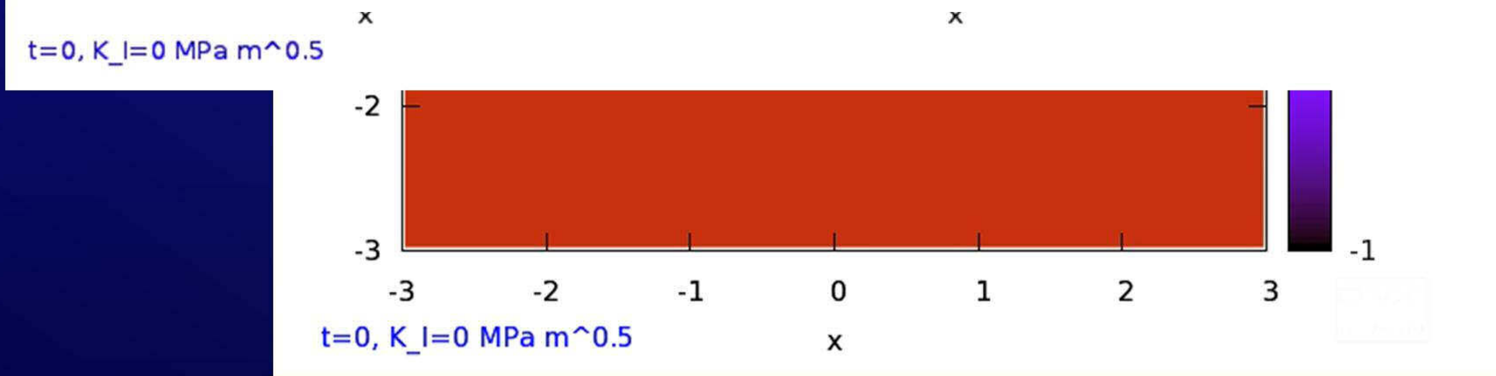
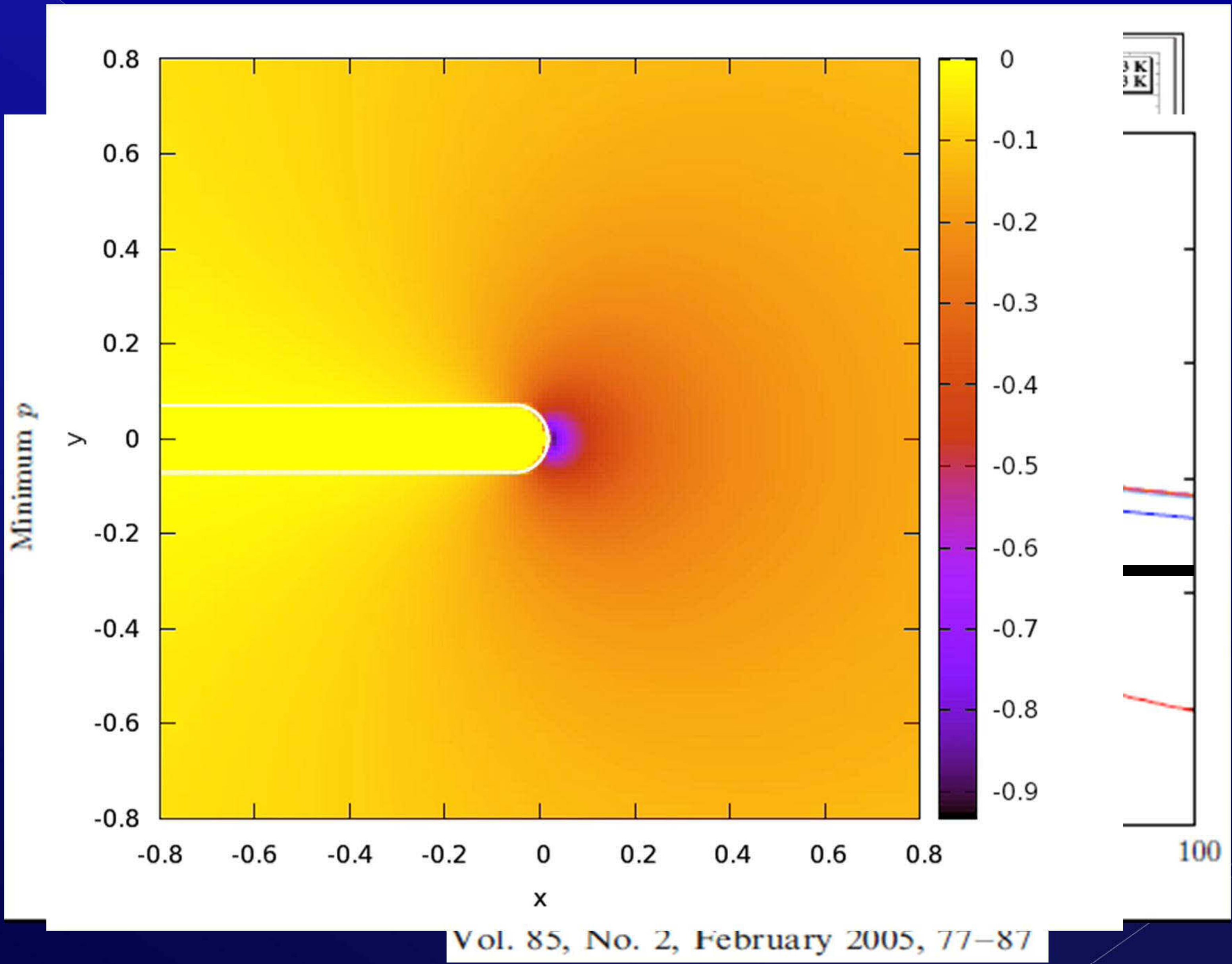
Deformation behavior of the $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ bulk metallic glass over a wide range of strain-rates and temperatures

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



CH Rycroft & EB, work in progress (2012)

Fracture toughness (cont d)



CH Rycroft & EB, work in progress (2012)

More applications

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Thermodynamic theory of dislocation-mediated plasticity

J.S. Langer[a,*], Eran Bouchbinder[b], Turab Lookman[c]

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Nonequilibrium thermodynamics of the Kovacs effect†

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Thermodynamic Interpretation of Soft Glassy Rheology Models

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(Dated: 15 Jan 2012)

arXiv:1201.3275v1

Summary and prospects

A non-equilibrium thermodynamics framework for driven disordered systems was developed

Many problems can be addressed within this framework (we focused here on amorphous plasticity)

Open questions: Limitations? Range of validity of the adopted approximations? What roles play the mechanical noise associated with χ in activated dynamics? χ diffusion?