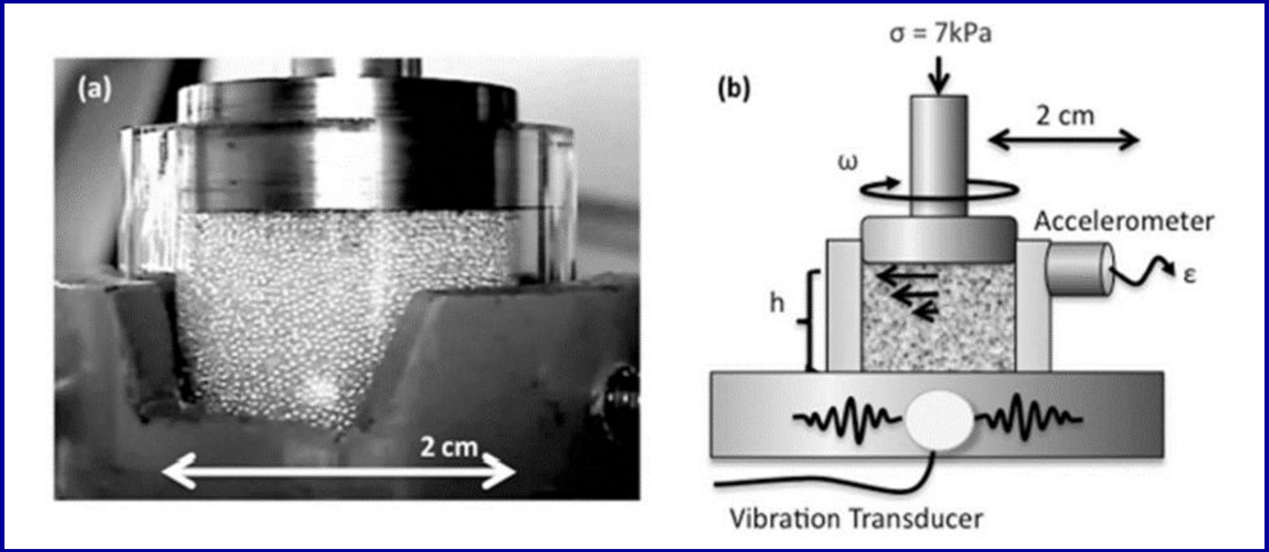
Recent Adventures in Nonequillibrium Statistical Thermodynamics: Driven Granular Materials



J.S. Langer
UC Santa Barbara
10/22/2014

Focus on realistic, “normal,” driven systems

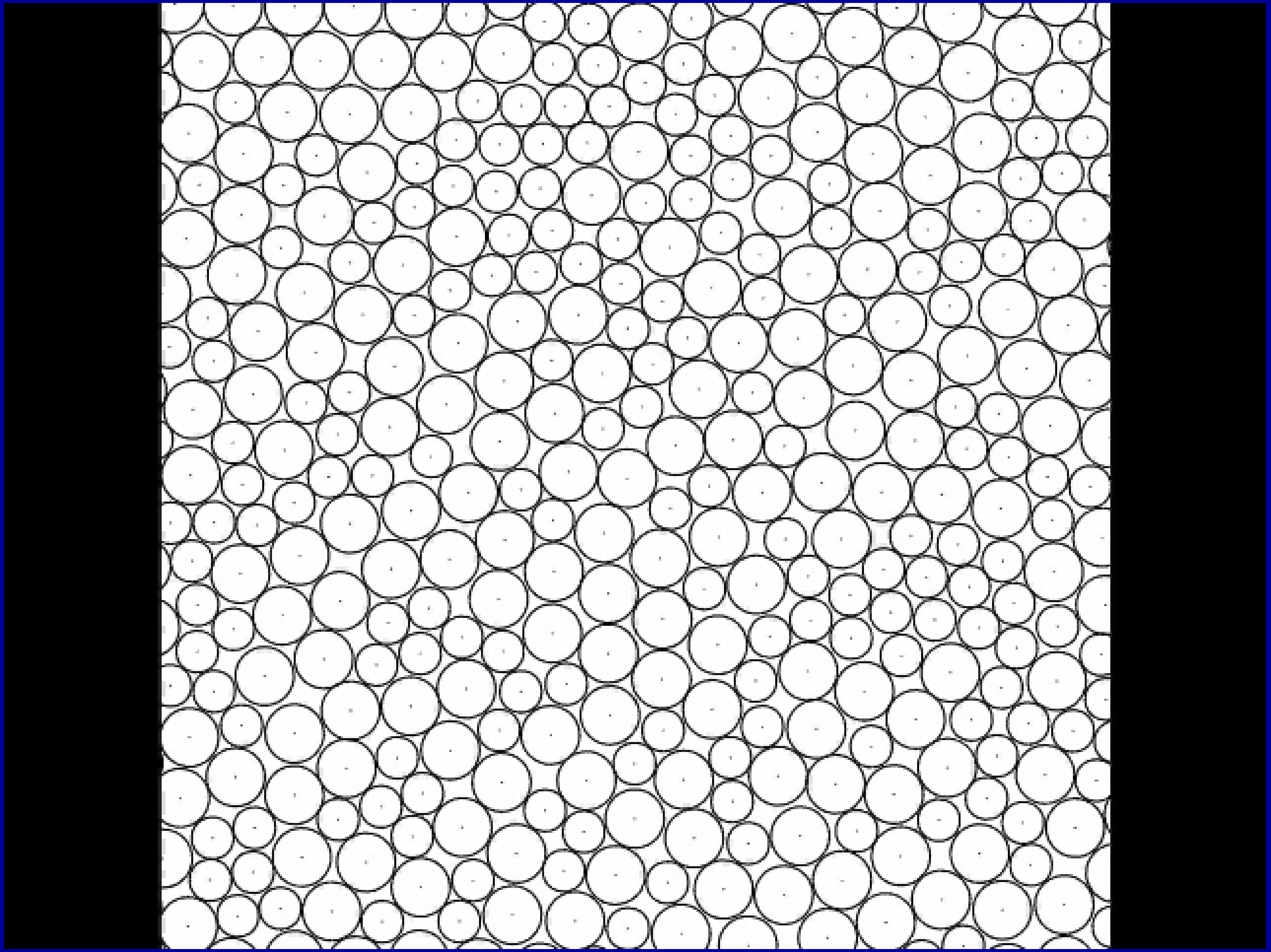
- E.g. dense, glass forming liquids, BMG’s, granular fault gouge, etc.
- Intrinsically noisy systems – thermal noise, or mechanical noise generated by external driving
- Local flow laws, independent of the system size. This does not preclude extended deformation such as shear banding or fracture. (But not “crackling”)

Two core theoretical ingredients

1. Localized flow defects – STZ's. Ephemeral, activated soft spots in solid-like amorphous materials.

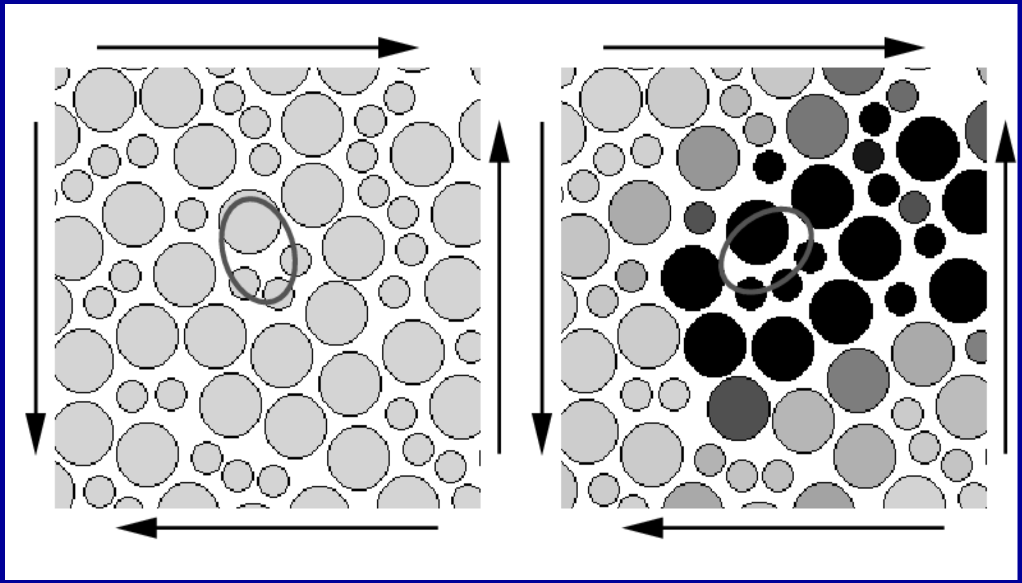
2. Thermodynamically defined effective temperature – a measure of configurational disorder – controls the density of STZ's and the ways by which noise is generated by external driving.

Visualize a slowly sheared glass



T. Haxton and A. Liu: MD simulation of 2D glass. The shear rate is constant but very small on the molecular time scale.

Shear-Transformation-Zones (STZ's)
M.Falk and JSL, 1998



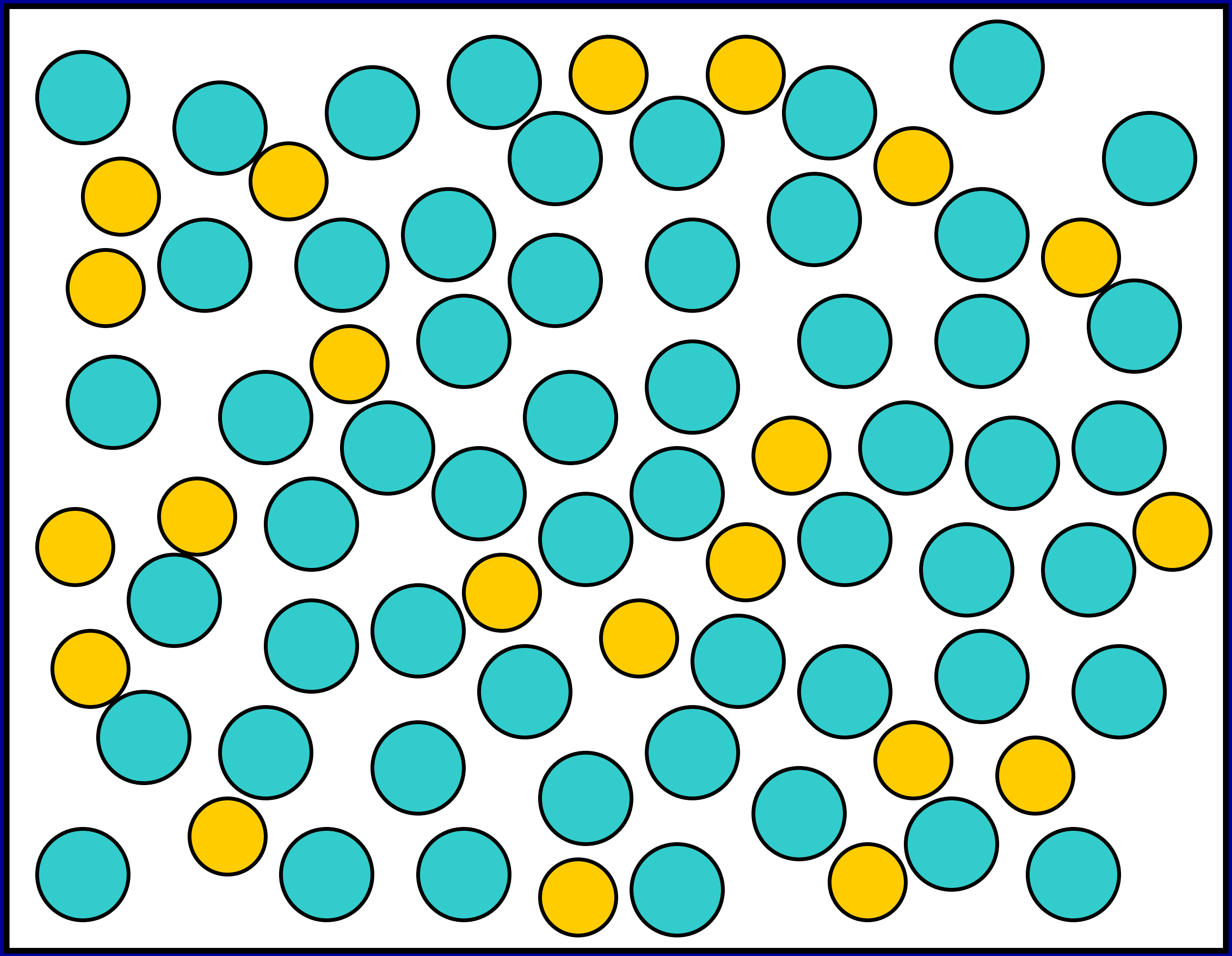
Detect local shear rearrangements by looking for non-affine displacements **(D^2_{min}** = measure of non-affinity)

Effective Disorder Temperature

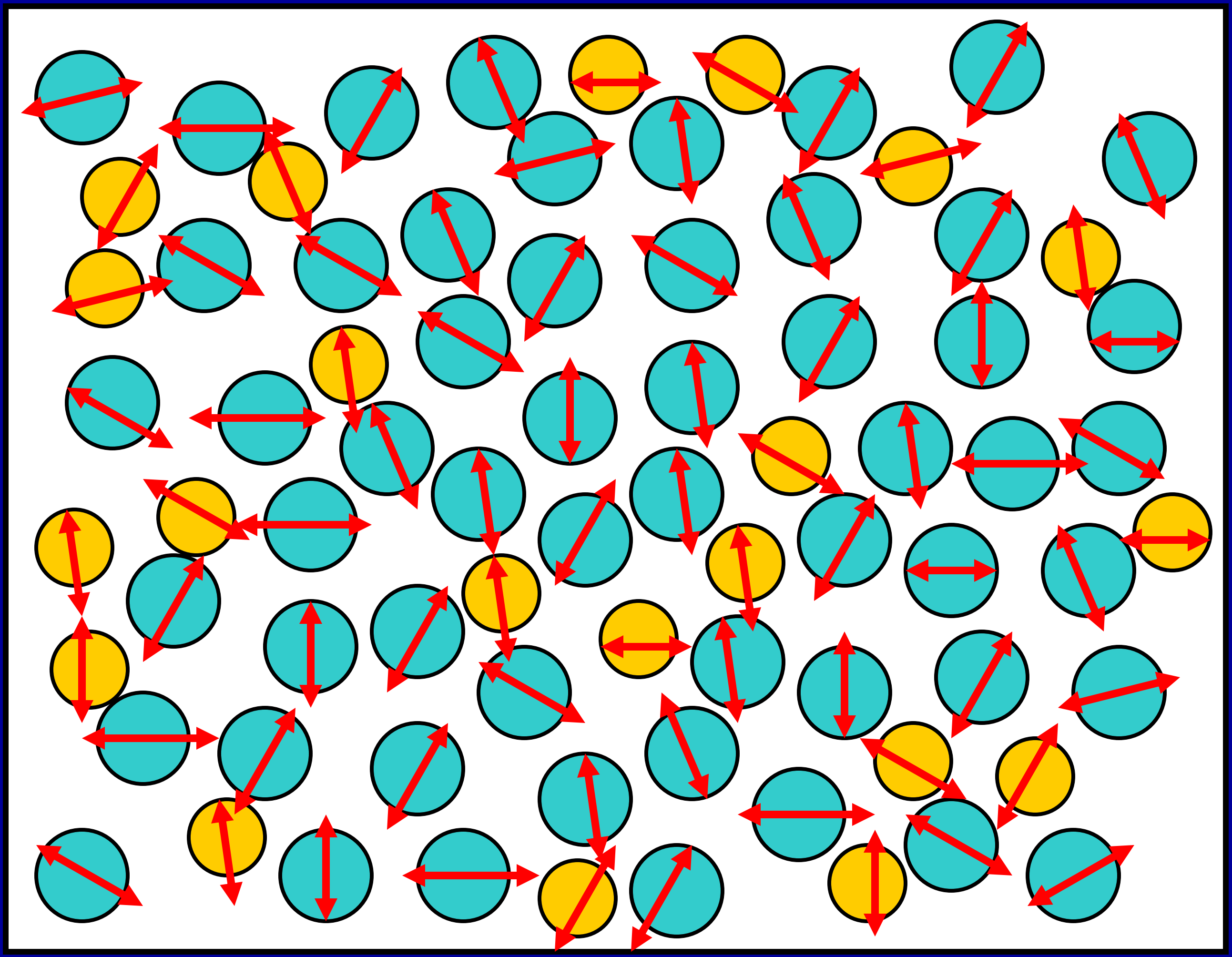
Two weakly coupled subsystems:

(1) Configurational subsystem, described by slowly varying inherent structures. These configurational degrees of freedom have an effective temperature $\chi = k_B T_{eff}$, which may not be the same as the ordinary temperature when the system is out of equilibrium.

(2) Kinetic-vibrational and thermal degrees of freedom, are rapidly fluctuating, have temperature $\theta = k_B T$, serve as a thermal reservoir.



Inherent structure with molecules in a mechanically stable configuration. The degree of disorder of this structure is described by its effective temperature, which may not be the same as its kinetic temperature.



Kinetic/vibrational degrees of freedom superimposed on the inherent structure. In a glassy system, these rapid motions are only weakly coupled to the slow configurational transitions from one inherent structure to another.

Thermodynamic definition of the effective temperature

Configurational energy = $U(S, \{\Lambda\})$.

Configurational entropy = S$(U, \{\Lambda\})$.

$\{\Lambda\}$ = set of order parameters, e.g. density of STZ's.

$$\left(\frac{\partial U}{\partial S}\right)_{\{\Lambda\}} = \chi = k_B\, T_{eff}$$

For hard, granular materials, replace energy *U* by volume *V*.

$$p\left(\frac{\partial V}{\partial S}\right)_{\{\Lambda\}} = p\,\mathrm{X} = k_B\, T_{eff} = \chi$$

X= compactivity (S.F. Edwards)

Flow laws have the form:

$$\dot{\gamma}^{pl} \propto \Lambda\, f(\sigma, \dots)$$

$\dot{\gamma}^{pl}$ = plastic strain rate; Λ = STZ density; σ = stress.

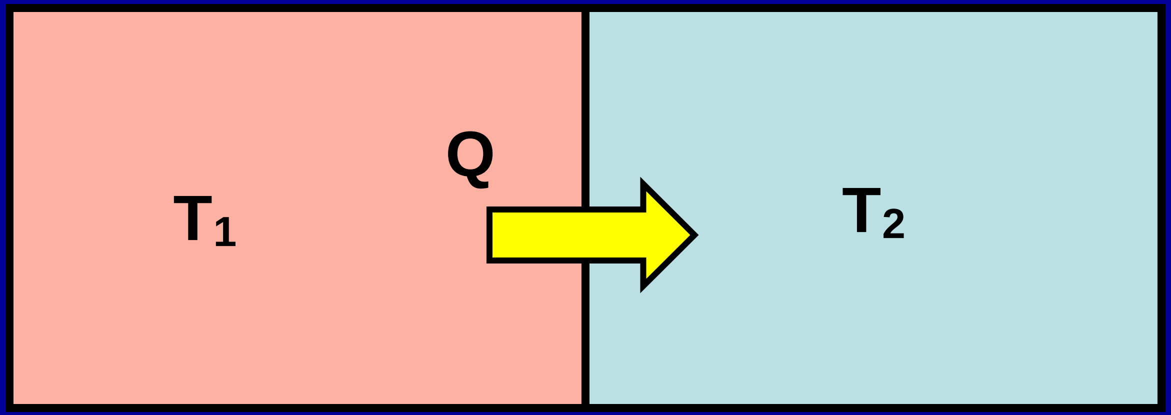
These relations are constrained by the second law:

$$\dot{S} + \dot{S}_R \geq 0$$

which, among other things, tells us that $\Lambda \propto e^{-\epsilon/\chi}$,
where ϵ = activation energy (or activation volume),
and that there must be a non-negative thermal conductivity *K*
coupling the configurational degrees of freedom to the thermal reservoir:

$$\theta \dot{S}_R = Q = K(\chi - \theta)$$

A textbook analogy



Spatially separated subsystems – each in internal equilibrium – in weak thermal contact with each other:

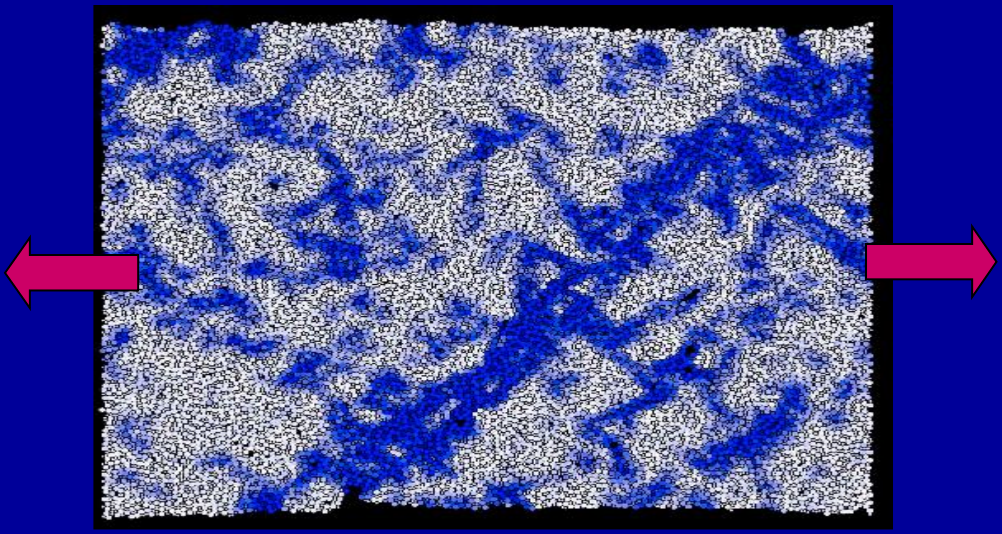
If $T_1 > T_2$, then heat Q flowing from the hotter to the cooler subsystem increases the entropy of the system as a whole.

$$\dot{S}_{tot} = \frac{\dot{U}_1}{T_1} + \frac{\dot{U}_2}{T_2} = \dot{U}_1\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \geq 0$$

Therefore $Q = -\dot{U}_1 = A(T_1 - T_2); \quad A \geq 0$

The effective temperature plays a key role in many of the most interesting nonequilibrium phenomena.

For example, shear banding: Larger χ means more STZ's; thus larger flow at fixed stress, or smaller stress at fixed flow. This slip-weakening instability can produce shear-banding. (Manning, JSL and Carlson, 2007).



The effective temperature plays a key role in many of the most interesting nonequilibrium phenomena.

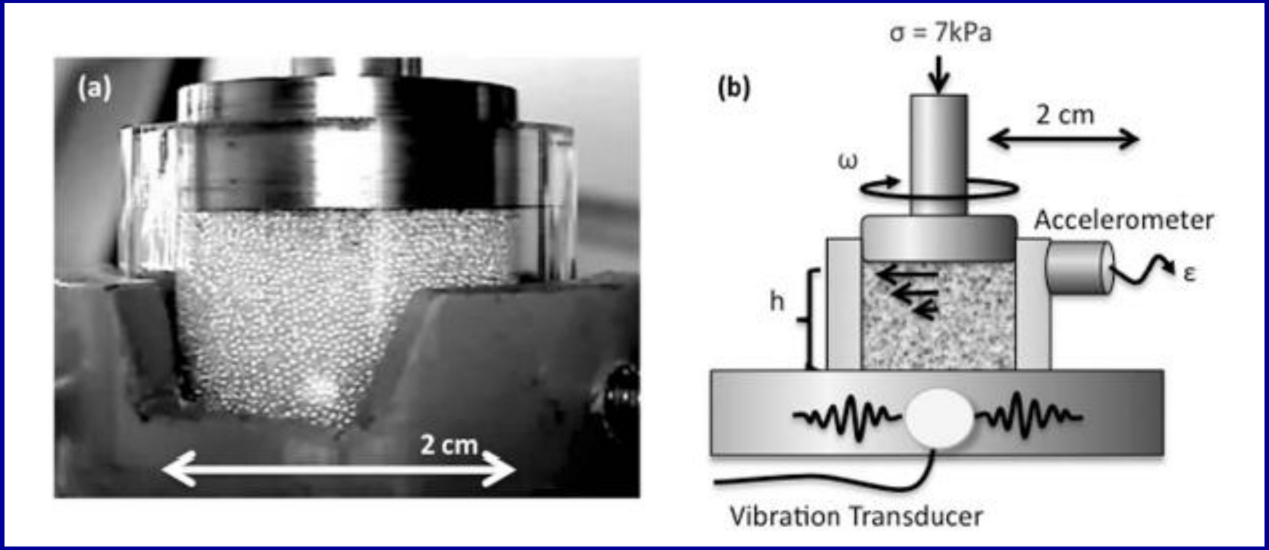
For example, shear banding: Larger χ means more STZ's; thus larger flow at fixed stress, or smaller stress at fixed flow. This slip-weakening instability can produce shear-banding. (Manning, JSL and Carlson, 2007).

Other examples, including dislocation-mediated plasticity (JSL, Bouchbinder, Lookman, Acta Mat. 2010) and fracture (Rycroft and Bouchbinder, PRL 2012).

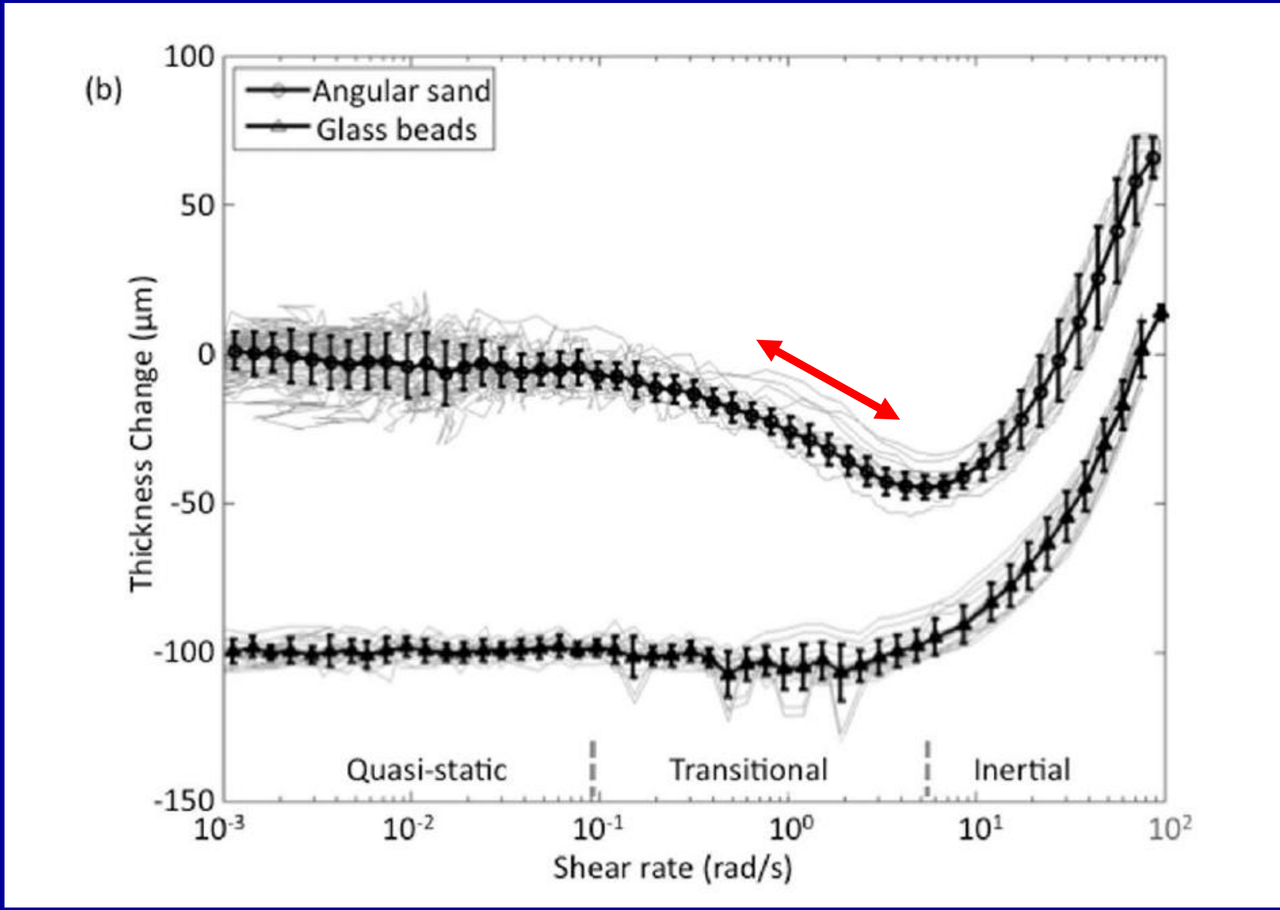
Focus here on recent work, primarily by Charles Lieou, on dense, flowing granular materials, e.g. fault gouge.

van der Elst, Brodsky, Le Bas, Johnson, J Geophys. Res. (2012)

Auto-acoustic compaction in [granular] shear flows



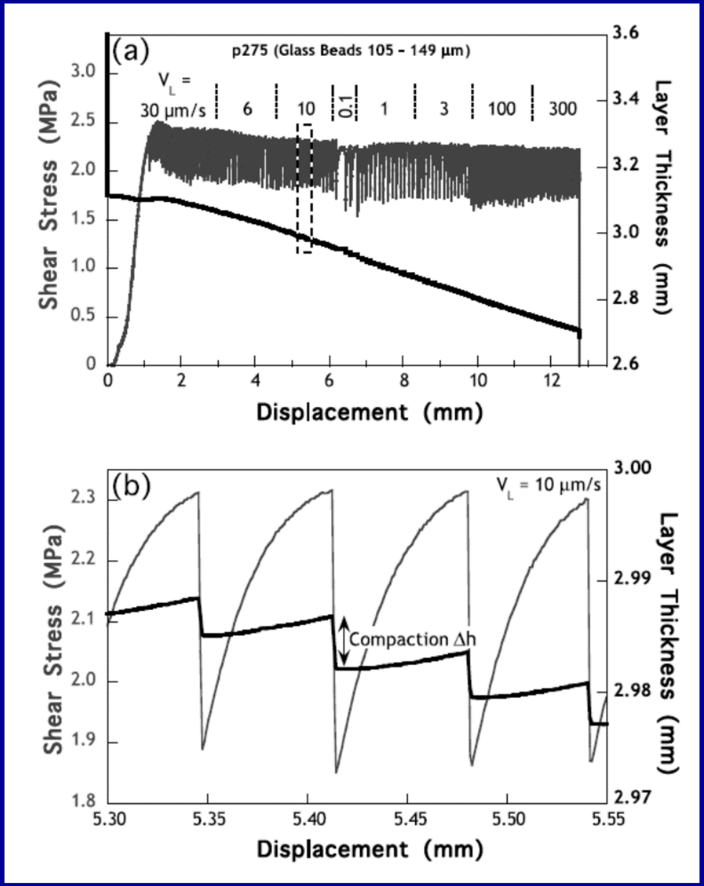
Reversible, non-monotonic behavior of the volume as a function of the strain rate. Also, sheared granular layers can undergo stick-slip instabilities. How can we understand these behaviors?



Van der Elst et al. Reversible variation of volume as a function of shear rate

Stick-slip in granular friction

Thin granular layers
between rock surfaces



JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 110, B08409, doi:10.1029/2004JB003399, 2005

Influence of particle characteristics on granular friction

Jennifer L. Anthony[1] and Chris Marone

Rock Mechanics Laboratory, Department of Geosciences, Pennsylvania State University, University Park, Pennsylvania, USA

Main idea: The plastic response, and the volume of the granular system are controlled by the effective temperature χ

The equation of motion for χ is a statement of the first law of thermodynamics.

$$\chi\,\dot{s} \cong C\,\dot{\chi} = \mathrm{V}\,\sigma\,\dot{\gamma^{pl}} - K(\chi - \theta)$$

= driving power – heat flow to thermal reservoir

The thermal conductivity K is determined by noisy fluctuations which govern the coupling between the configurational subsystem and the thermal reservoir. Thus

$$\mathrm{K} = a\,\Gamma + \text{other contributions}$$

where Γ is the noise generated by external driving.

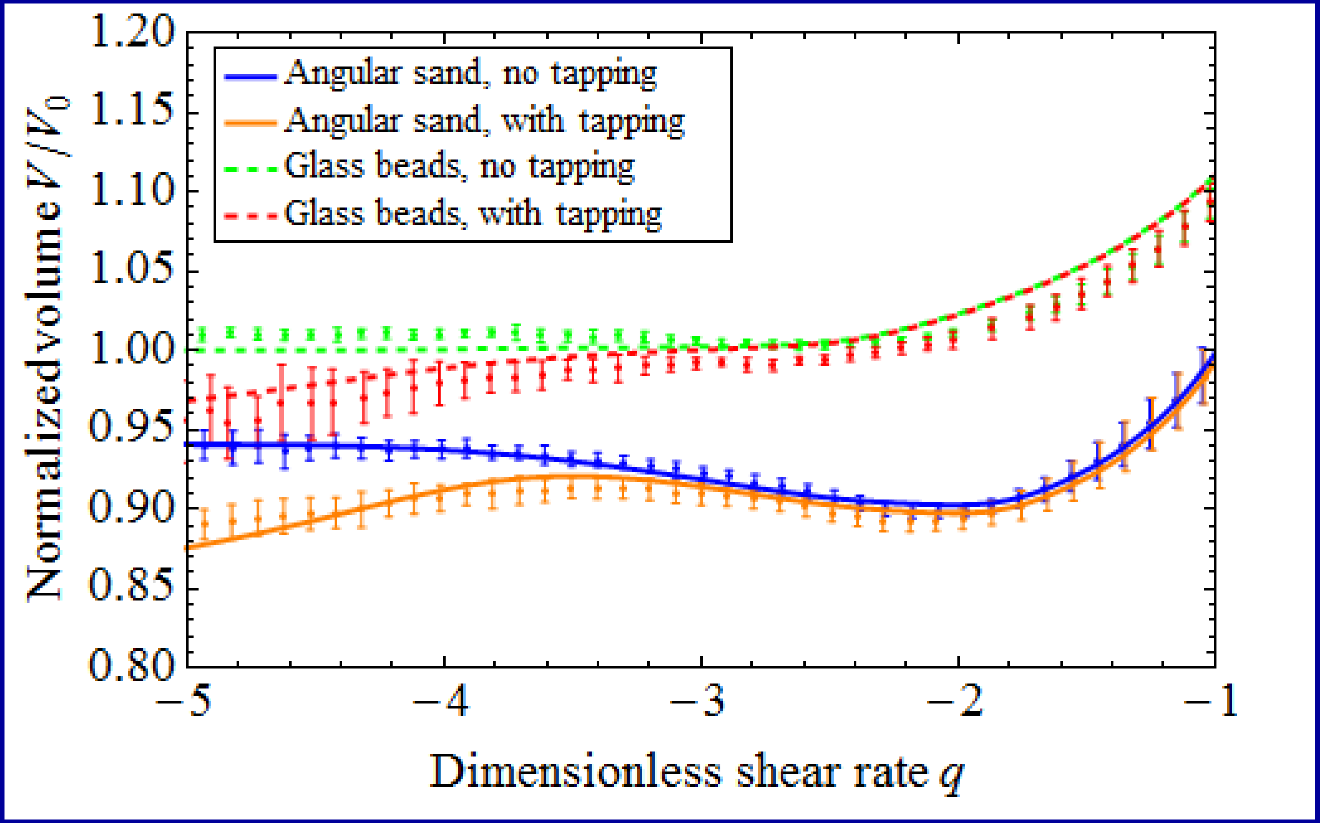
Volume effect

The volume V is (usually) an increasing function of χ.

For angular sand, i.e. for strongly frictional grains, Lieou adds a term depending on the square of the strain rate to the thermal conductivity K.

$$K \sim a\,\Gamma + K_{frict}\, tanh(b\,\dot{\gamma}^2) + K_{tap}$$

Thus, dissipative, frictional interactions between particles, and tapping, increase K and "cool" the configurational subsystem.



Lieou, Elbanna, JSL and Carlson, PRE 90, 032204 (2014)
Data from Van der Elst et al.

Mechanically generated noise

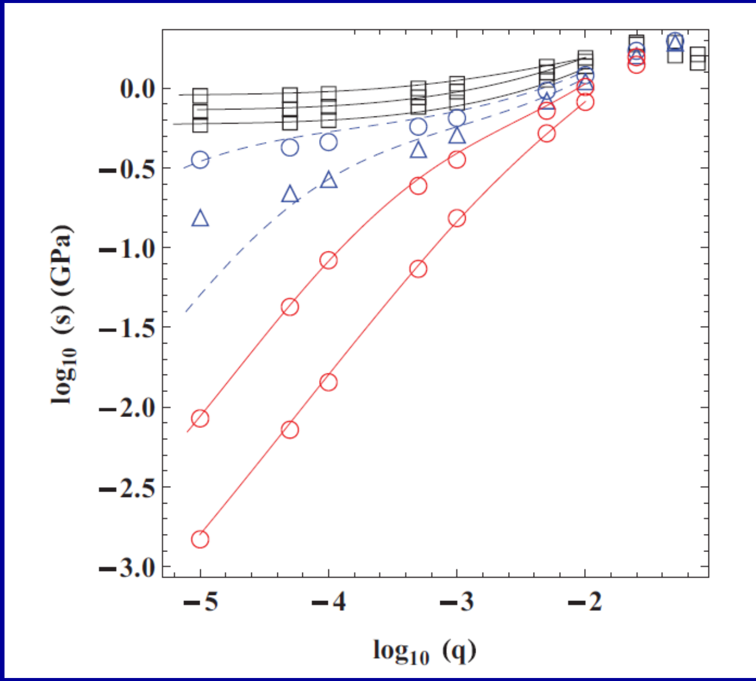
STZ creation rate $\sim \Gamma\, e^{-\,\epsilon/\chi}$

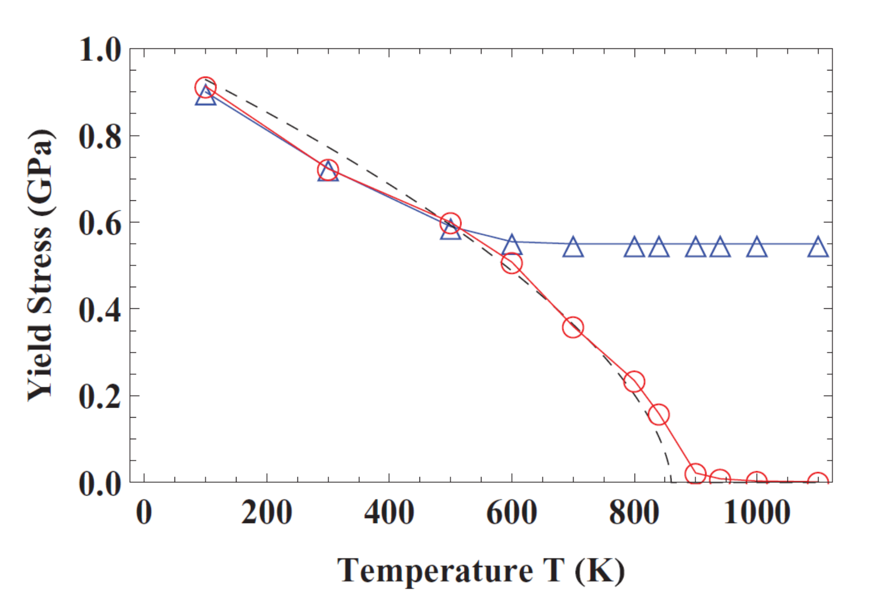
$\Gamma =$ noise (attempt) frequency;
ϵ = activation energy (or volume)

Pechenik relation: $\Gamma \sim \dfrac{\sigma\, \dot{\gamma}^{pl}}{\sigma_o\, \Lambda}$

$1/\Lambda$ = volume per STZ

The stress σ_o controls the conversion of driving power to noise. At low temperature, it turns out to be the yield stress, i.e. the minimum flow stress. It decreases with increasing temperature. Thus, the STZ creation rate increases, i.e. the material increasingly resembles a liquid at higher temperatures. This behavior enhances slip weakening.

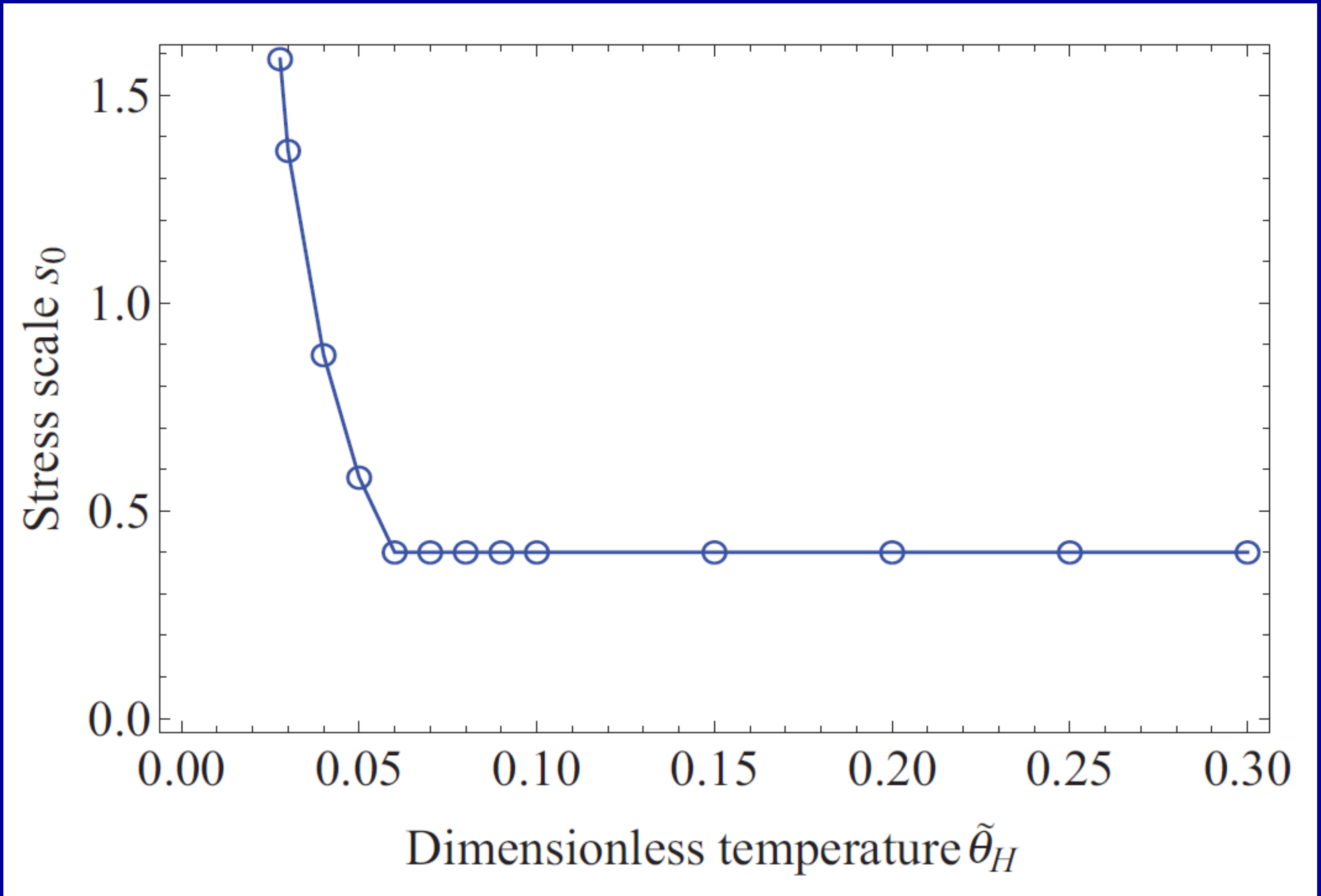




Stress vs. strain rate for a wide range of temperatures

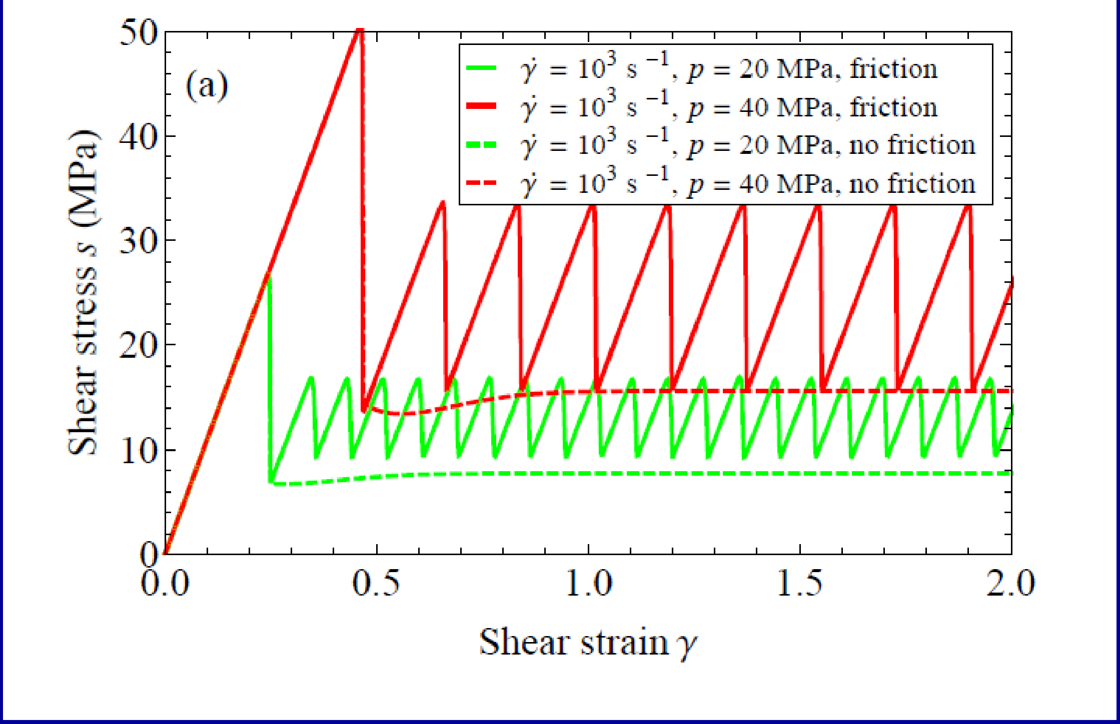
$\sigma_0(T)$ (blue triangles) Red circles are actual yield stresses.

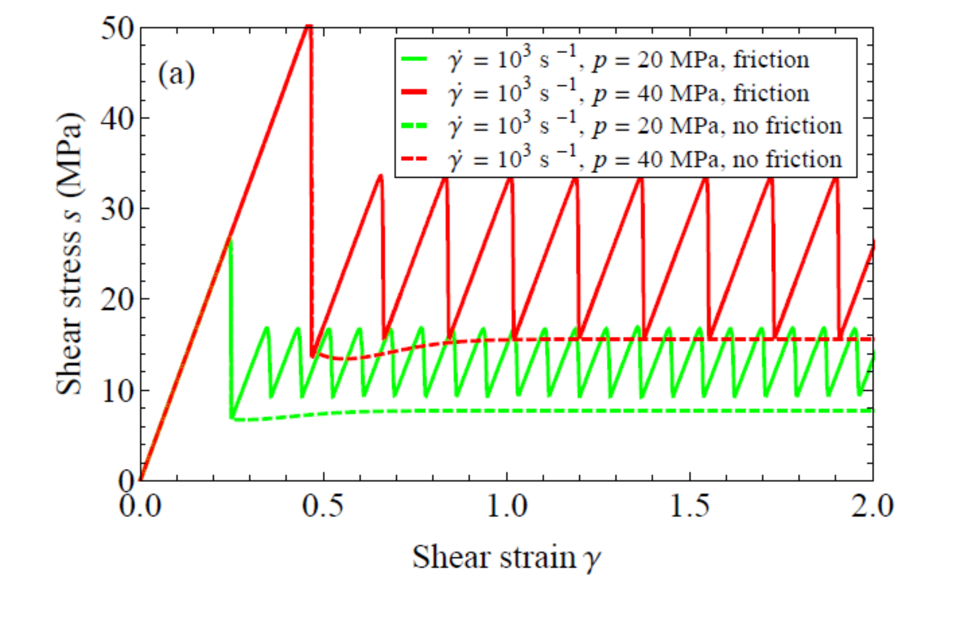
JSL and T. Egami, PRE 2012, Analysis of MD simulations of a BMG.

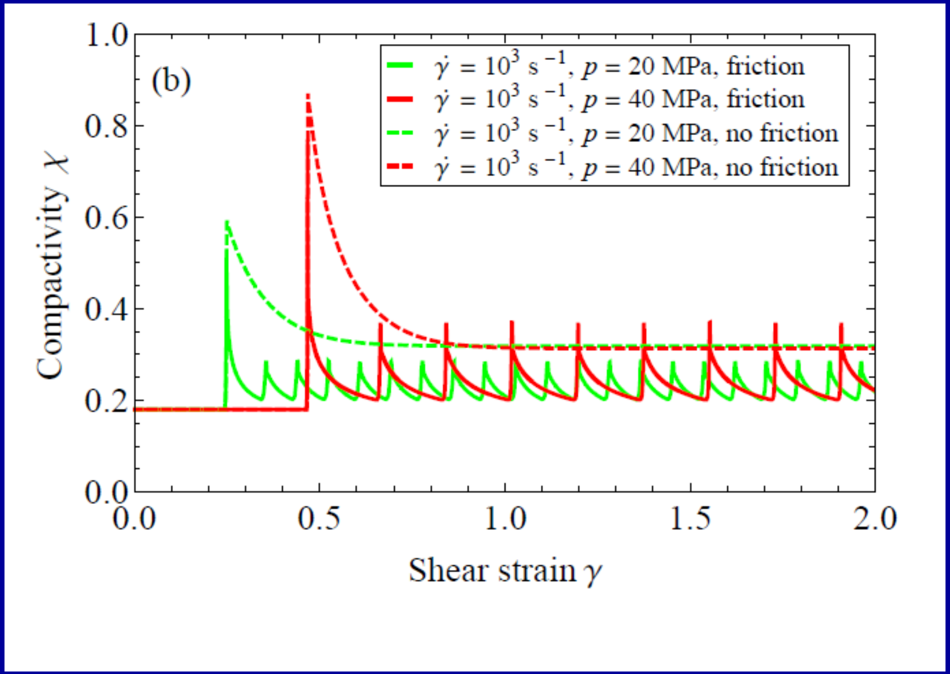


Lieou and JSL PRE 2012. Analysis of simulated sheared hard spheres by Haxton, Schmiedeberg and Liu. The graph shows σ_0 as a function of scaled ordinary temperature.

In his latest calculations, Lieou chooses σ_o to be a decreasing function of increasing χ (not T). To see stick-slip, he needs both this effect and friction.




(a)
Shear stress s (MPa)
Shear strain γ
0 10 20 30 40 50
0.0 0.5 1.0 1.5 2.0
γ̇ = 10^3 s^−1, p = 20 MPa, friction
γ̇ = 10^3 s^−1, p = 40 MPa, friction
γ̇ = 10^3 s^−1, p = 20 MPa, no friction
γ̇ = 10^3 s^−1, p = 40 MPa, no friction


(b)
Compactivity χ
Shear strain γ
0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.5 1.0 1.5 2.0
γ̇ = 10^3 s^−1, p = 20 MPa, friction
γ̇ = 10^3 s^−1, p = 40 MPa, friction
γ̇ = 10^3 s^−1, p = 20 MPa, no friction
γ̇ = 10^3 s^−1, p = 40 MPa, no friction

Concluding remarks:

The thermodynamic theory of driven systems opens possibilities for realistic, predictive descriptions of a wide variety of practically important materials phenomena.

An especially urgent outstanding problem is to understand the crossover between the regime in which thermodynamic STZ theory is valid, and the regime at low temperatures, small strain rates, in which large, correlated, avalanche-like events occur.