# Soft glassy rheology: modelling & measuring strains in amorphous flows

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# Outline

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# Soft glasses: phenomenology

- Foams, dense emulsions, onion phases, colloidal glasses, clays, pastes, ...
- Common rheological features:
  - flow curves $\sigma(\dot\gamma) - \sigma_Y \sim \dot\gamma^p$ $(0 < p < 1)$, Herschel-Bulkley (if yield stress $\sigma_Y \neq 0$) or power-law
  - Nearly 'flat' viscoelastic spectra $G'(\omega)$, $G''(\omega)$ for low frequencies $\omega$ (also in cytoskeleton?)
  - Rheological aging
- Suggests common underlying features: arrangements of particles/droplets etc are disordered and metastable
- Analogy with glasses
- Soft glassy rheology approach exploits this; minimal model (based on Bouchaud's trap model)

# Soft glasses: Linear rheology

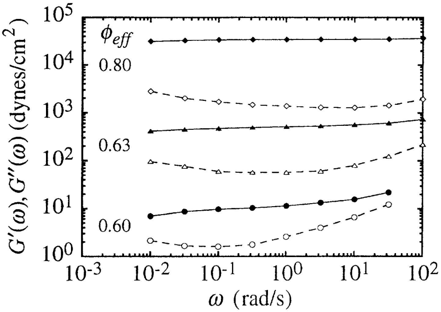
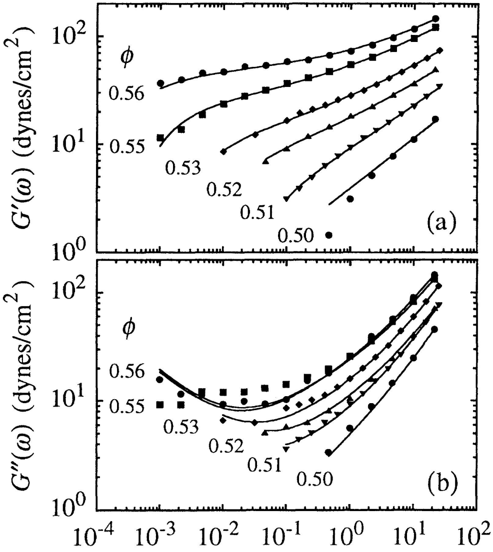



FIG. 2. The frequency dependence of the storage $G'$ (solid points) and loss $G''$ (open points) moduli of a monodisperse emulsion with $r \approx 0.53$ $\mu$m for $\phi_{\rm eff} = 0.80$ (diamonds), 0.63 (triangles), and 0.60 (circles). The results for the two larger

- Complex modulus for dense emulsions (Mason Bibette Weitz 1995)
- Almost flat $G''(\omega)$: broad relaxation time spectrum, glassy

# Colloidal hard sphere glasses
Mason Weitz 1995



# Onion phase
## Panizza et al 1996

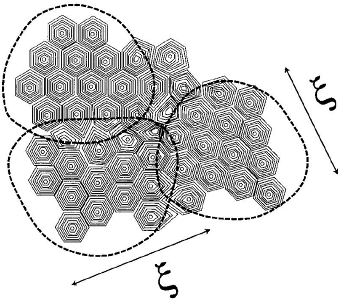
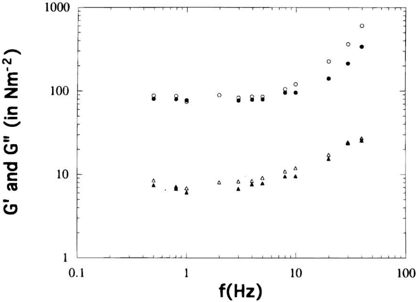



**Figure 3.** Schematic representation of an onion phase. ξ is the characteristic length of monodomains. Each monodomain is




- Vesicles formed out of lamellar surfactant phase
- Again nearly flat moduli

# Microgel particles

Purnomo van den Ende Vanapalli Mugele 2008

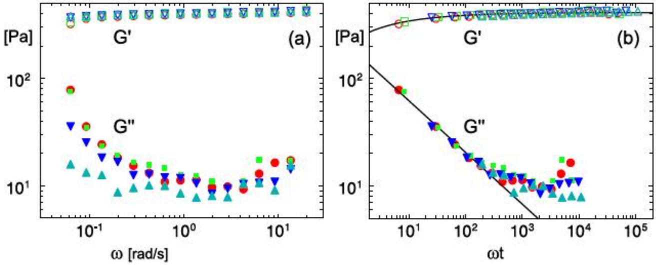
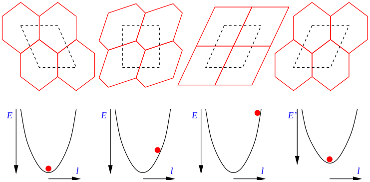



FIG. 1 (color online). $G'$ (open symbols) and $G''$ (solid symbols) of a 7% w/w suspension at 25 °C plotted versus $\omega$ (a) or $\omega t$ (b) for $t_w = 3$ (○), 30 (□), 300 (▽), and 3000 s (△). Lines represent the SGR model ($x = 0.55$, $G_p = 410$ Pa).

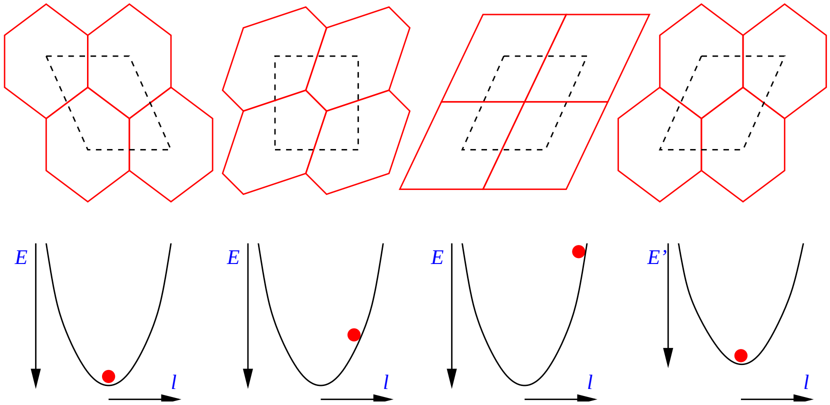
- $G''(\omega)$ flat but with upturn at low frequencies
- Aging: Results depend on time elapsed since preparation, typical of glasses

# SGR model

- Divide sample conceptually into mesoscopic elements
- Each has local shear strain $l$, which increments with macroscopic shear $\gamma$
- But when strain energy $\frac{1}{2}kl^2$ gets close to yield energy $E$, element can yield
- Yielding resets $l = 0$, and element acquires new $E$ from some distribution $\rho(E) \sim e^{-E}$
- Yielding is activated by an effective temperature $x$; models interactions between elements (also: thermodynamic interpretation)



# SGR model



# Equation of motion

- In dimensionless units (for time, energy)

$$\dot{P}(E,l,t) = -\dot{\gamma}\frac{\partial P}{\partial l} - e^{-(E-kl^2/2)/x}P + \Gamma(t)\rho(E)\delta(l)$$

  $\Gamma(t) = \langle e^{-(E-kl^2/2)/x}\rangle$ = average yielding rate
- Macroscopic stress $\sigma(t) = k\,\langle l\rangle$
- Without shear, $P(E,t)$ approaches equilibrium $P_{\rm eq}(E) \propto \exp(E/x)\rho(E)$ for long $t$
- Get glass transition if $\rho(E)$ has exponential tail; happens at $x = 1$ if $\rho(E) = e^{-E}$
  (possible justification from extreme value statistics)
- For $x < 1$, system is in glass phase; never equilibrates $\Rightarrow$ aging

# SGR predictions

- Flow curves: Find both Herschel-Bulkley ($x < 1$) and power-law ($1 < x < 2$)
- Viscoelastic spectra $G'$, $G'' \sim \omega^{x-1}$ are flat near $x = 1$
- In glass phase ($x < 1$) find rheological aging, loss modulus $G'' \sim (\omega t)^{x-1}$ decreases with age $t$
- Steady shear always 'interrupts' aging, restores stationary state
- Stress overshoots in shear startup, nonlinear $G'$ and $G''$, linear and nonlinear creep, normal stresses (in tensorial version). . .

# A broader issue: Defining local strains

- Model assigns local strain for any single configuration
- Harder than coarse graining change of strain between two successive configurations
- Problem: no reference configuration, as in a crystal

## Aim

Develop method for assigning local strains and yield energies to material elements, from single snapshots of simulation data

# Outline

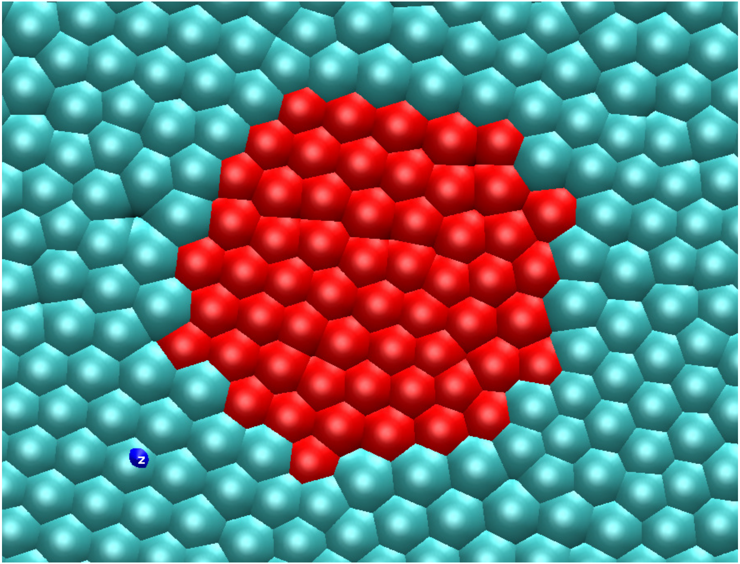
# Defining elements

- Focus on $d = 2$ ($d = 3$ can be done but more complicated)
- Make elements circular to minimize boundary effects
- Position circle centres on square lattice to cover all of the sample (with some overlap)
- Once defined, element is co-moving with strain: always contains same particles ("material element")
- Avoids sudden change of element properties when particles leave/enter, but makes sense only up to moderate $\Delta\gamma$
- Measuring average stress in an element is easy but how do we assign strain $l$, yield energy etc for a *given* snapshot?

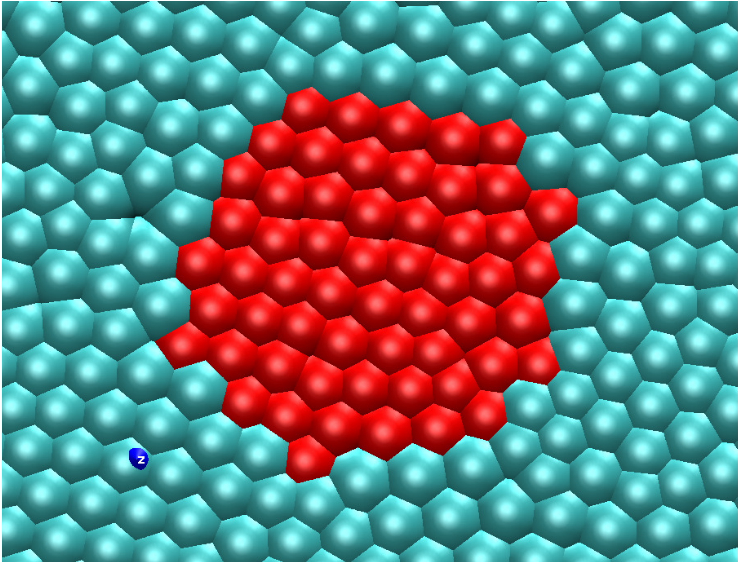
# Virtual strain analysis

- Cannot "cut" an element out of sample and then strain until yield – unrealistic boundary condition
- Idea: Use rest of sample as a frame
- Deform the frame affinely to impose a virtual strain $\tilde{\gamma}$
- Particles inside element relax non-affinely to minimize energy
- Gives energy landscape $\epsilon(\tilde{\gamma})$ of element
- Yield points are determined (for $\tilde{\gamma} > 0$ and $< 0$) by checking for reversibility for each small $\Delta\tilde{\gamma}$ (adaptive steps)
- Local analysis effectively at $T = 0$ to avoid stochastic effects; for consistency, do steepest descent to nearest global energy minimum of entire configuration first

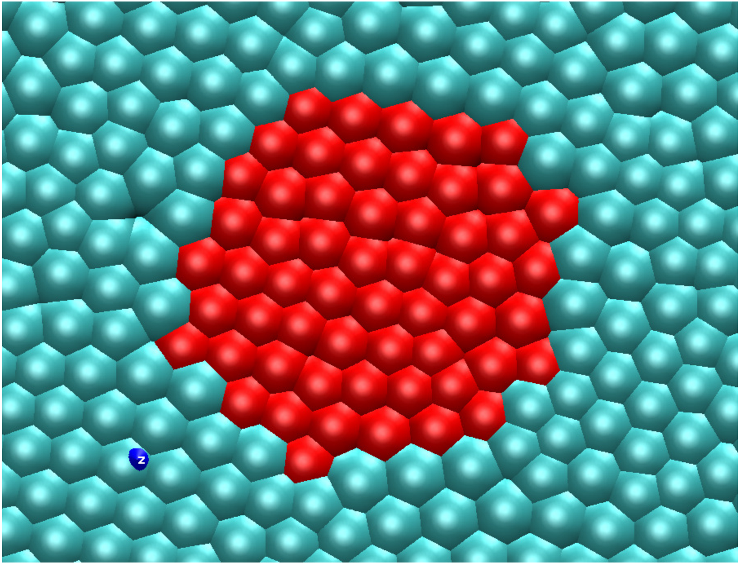
# Example: Virtual strain sequence 1



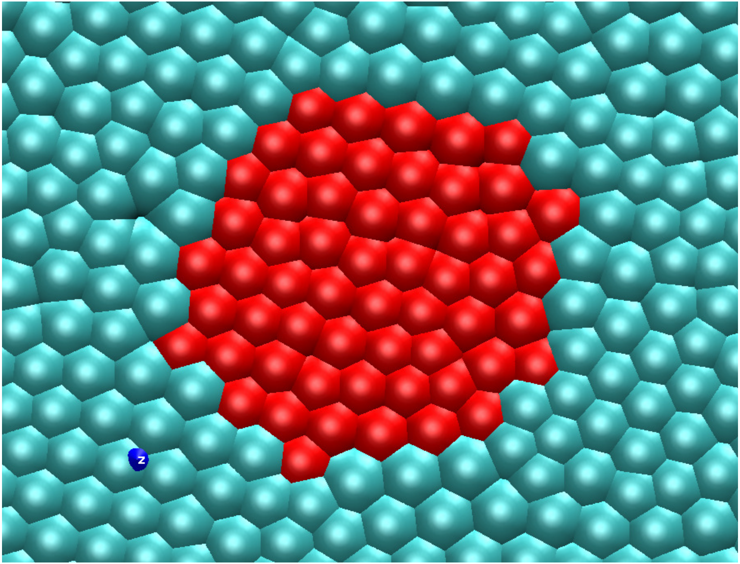
# Example: Virtual strain sequence 2



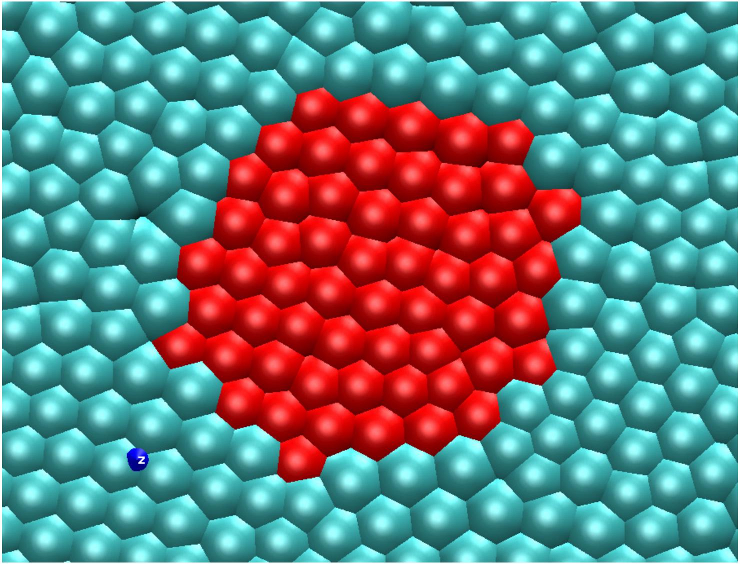
# Example: Virtual strain sequence 3



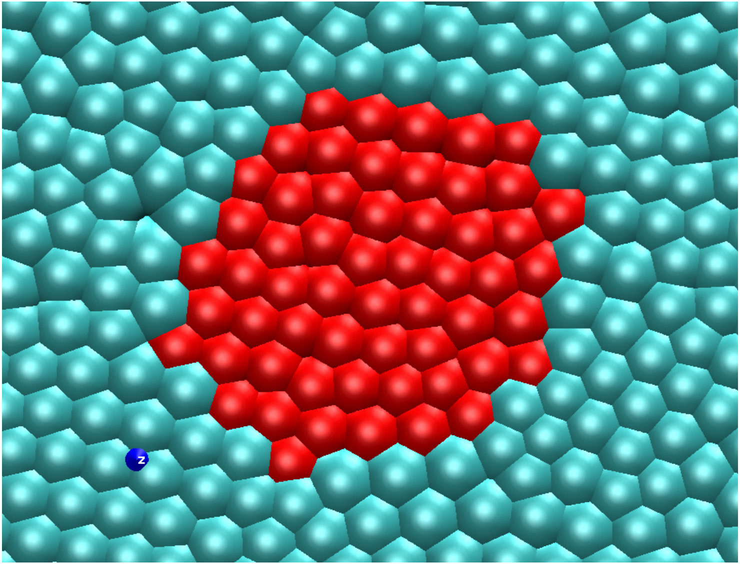
# Example: Virtual strain sequence 4



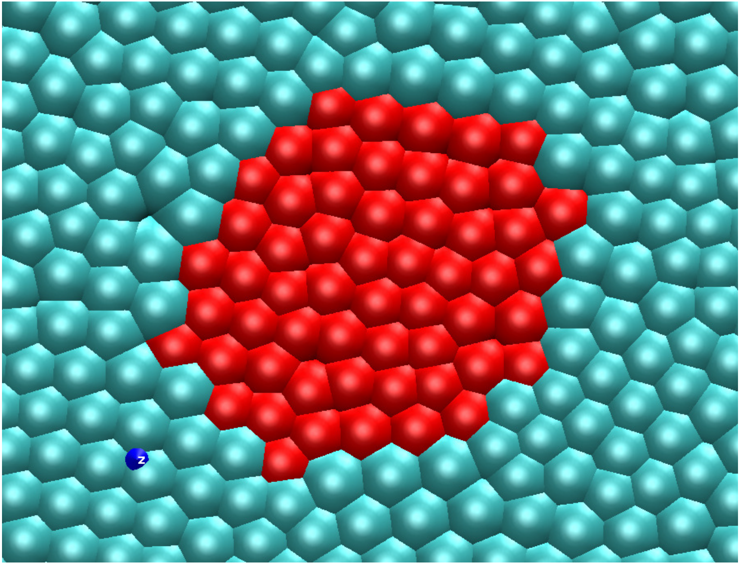
# Example: Virtual strain sequence 5



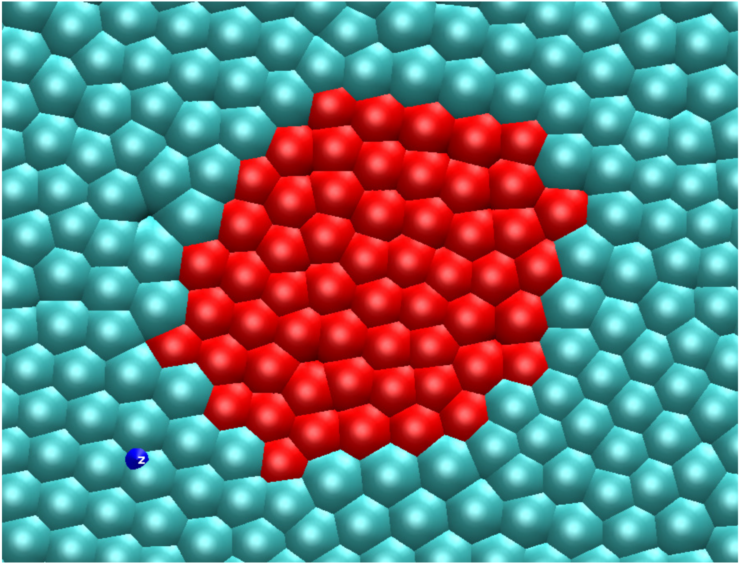
# Example: Virtual strain sequence 6



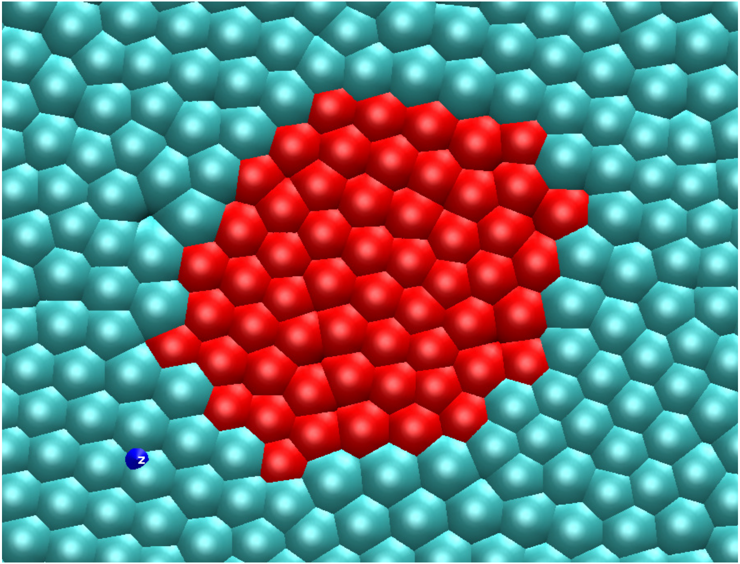
# Example: Virtual strain sequence 7



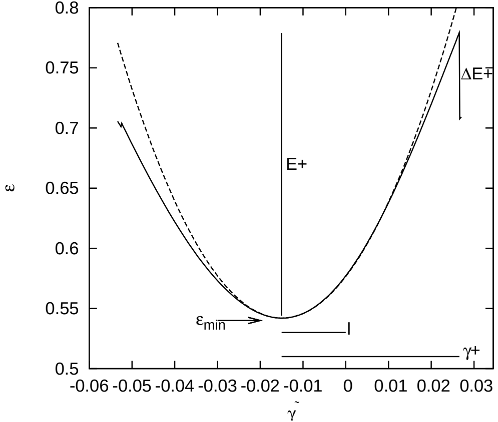
# Example: Virtual strain sequence 8



# Example: Virtual strain sequence 9



# Element energy landscape



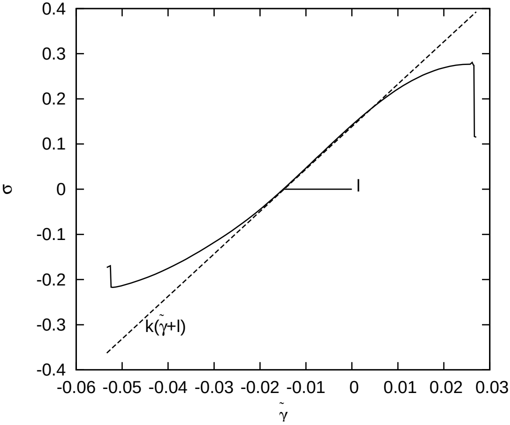

Extract: minimum energy $\epsilon_{\rm min}$, strain away from local minimum $l = -\tilde{\gamma}_{\rm min}$, yield strains $\gamma_{\pm}$, yield barriers $E_{\pm}$

# So what is the reference configuration?

- Locally determined
- Stress-free point on virtual energy landscape
- Local strain = virtual strain difference between original configuration and reference
- Doesn't presuppose specific structure for reference configuration (cf. Graner et al's texture tensor)

# Local modulus

Quadratic fit of energy near minimum, or linear fit of stress, gives local modulus $k$

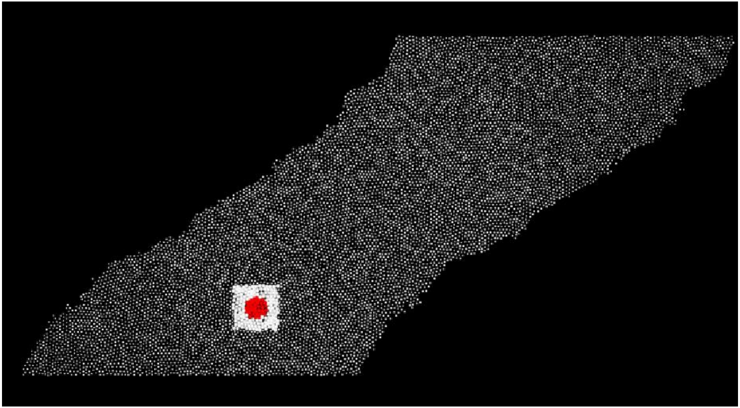


# Outline

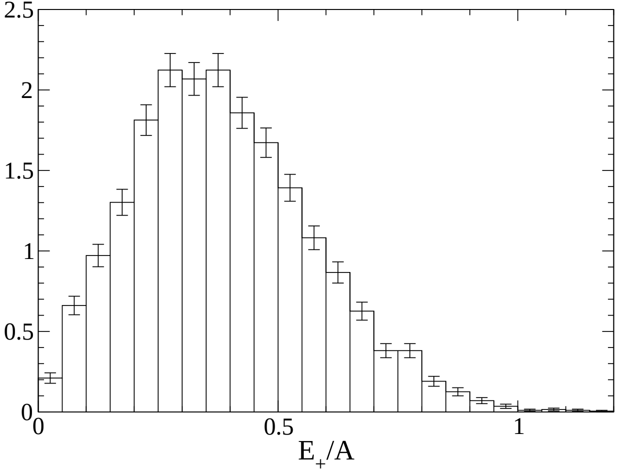
# Systems studied

- Polydisperse Lennard-Jones mixtures (Tanguy et al), quenched to low temperatures ($T = 10^{-4} \ll T_{\rm g}$)
- Low shear rates $\dot{\gamma} = 10^{-4}$; $N = 10^4$ particles at $\rho = 0.925$
- Steady shear driven from the walls (created by "freezing" particles in top/bottom 5% some time after quench)
- Check for stationarity & affine shape of velocity profile before taking data
- Each element contains $\approx 40$ particles (diameter $\approx 7$)
- Large enough to have near-parabolic energy landscape, small enough to avoid multiple local yield events inside one element (Tanguy, Tsamados et al)

# Simulation lengthscales



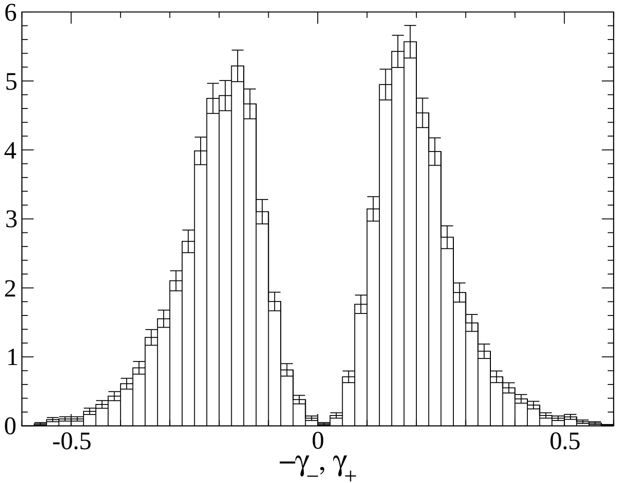
# Yield energy distribution




Roughly exponential tail as SGR model would postulate

Symmetric: $E_-/A$ has same distribution within error bars

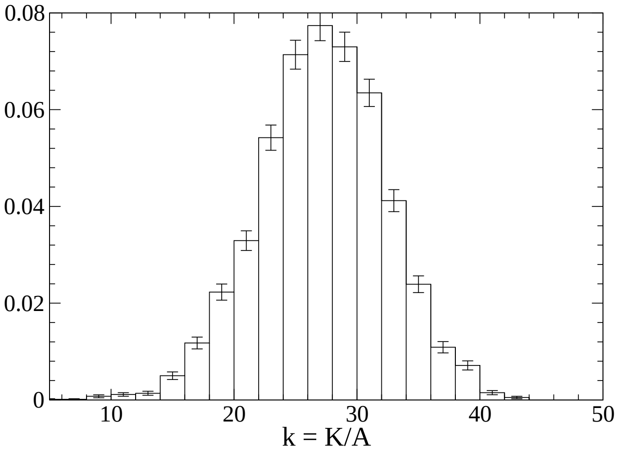
# Yield strain distributions




Symmetric as assumed in SGR

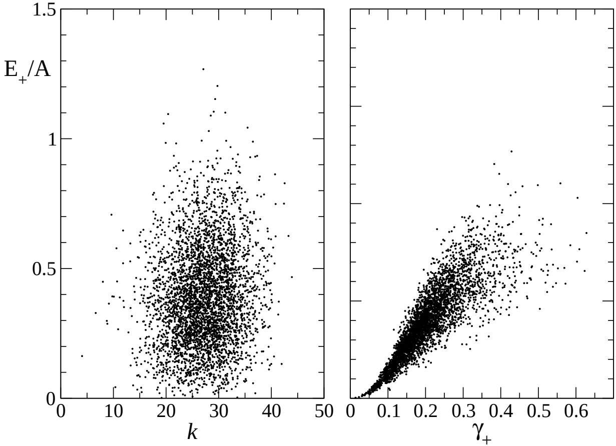
Power-law approach towards small yield strains?

# Modulus distribution



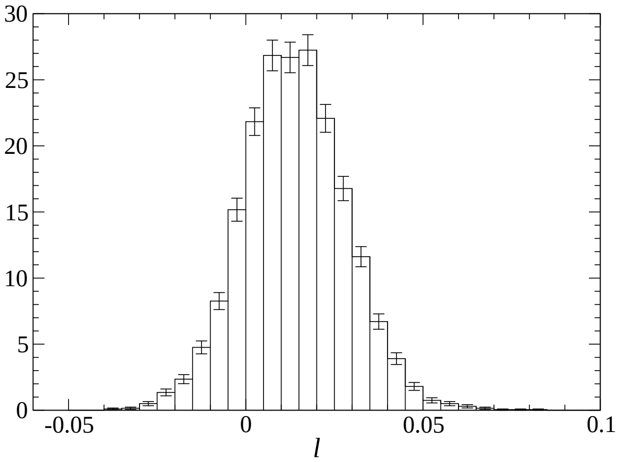

Clear spread; not constant as assumed in model

# Yield energies remain controlled by yield strains




Dominant effect on variation of $E_+$ is from yield strain $\gamma_+$, not from modulus $k$

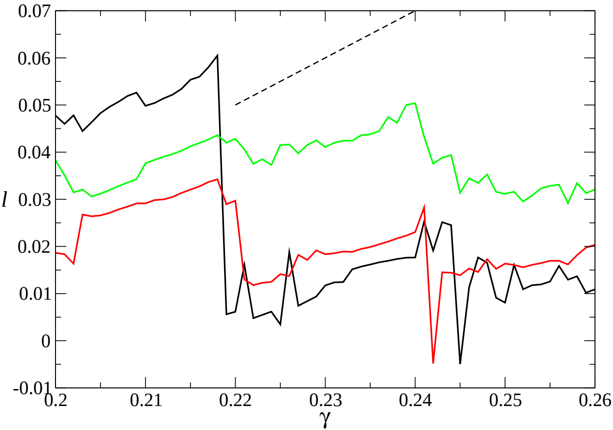
# Local strain distribution




Negative $l$, would need to extend SGR to allow frustration,
$l \neq 0$ after yield $(\delta(l) \to \rho(l|E) \propto (1 - kl^2/2E)^b)$

# Outline

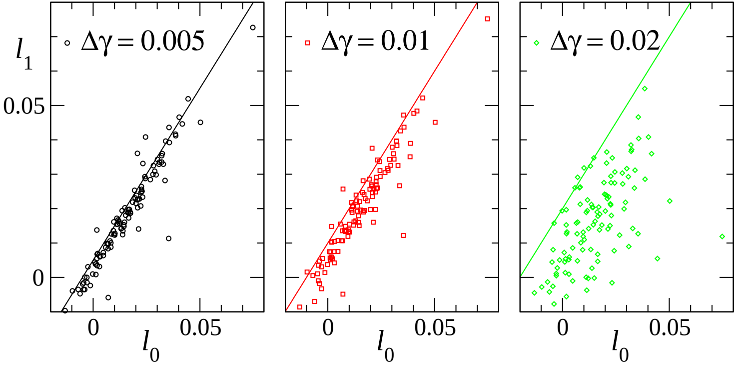
# Evolution of local strain with time




Some evidence for sawtooth shape assumed by SGR

Rearrangement events can perturb many elements at a time

# Population picture of $l$-dynamics

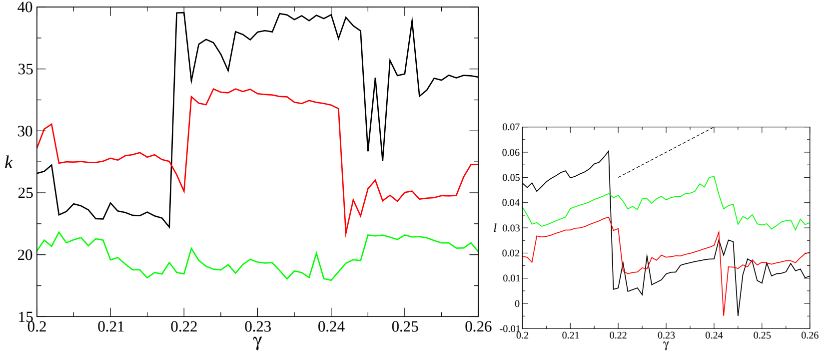



Scatter plot of $l_1 = l(\text{after } \Delta\gamma)$ vs $l_0 = l(\text{initial})$

Separation into strain convection and yield events?

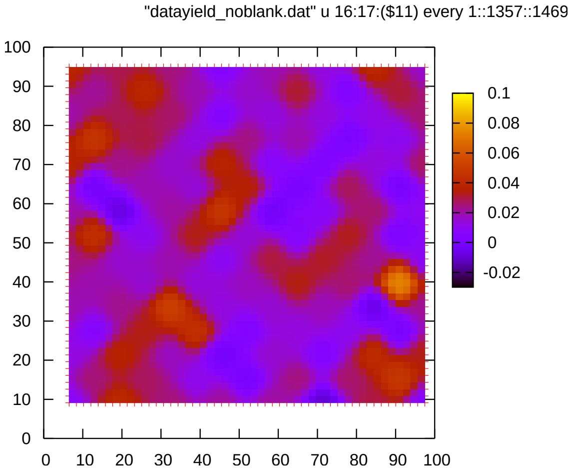
# Change in other landscape properties

## Example of modulus




Stays largely constant between yields as expected;
same for yield barriers etc

# Strain maps




Significant correlations along principal strain axes $\pm 45^{\mathrm{o}}$

# Outline

# Summary and outlook

- Virtual strain method for assigning local strains, yield energies
- Generic: can be used on configurations produced by any (low-$T$) simulation
- Also for experimental particle positions, given model of interaction?
- Steady state distributions in shear flow broadly in line with SGR though e.g. local modulus $\neq$ const
- Dynamics of local strain has typical sawtooth shape; local strain rate is of same order as global one but not identical
- To be done: effect of varying $\dot{\gamma}$, $T$, $\rho$
- Also: analysis of induced yield events – well modelled by effective temperature?

# Yield events

- Reversibility check: increment virtual strain, minimize energy, reduce virtual strain again, minimize energy
- Compare original and final configuration via largest particle displacement $\Delta$
- $\Delta = 0$: reversible, $\Delta > 0$: irreversible
- Surprisingly, find no obvious lower limit on $\Delta > 0$
- In practice ignore irreversibility if $\Delta < 0.01$
- Robust: using $\Delta < 0.1$ gives qualitatively same results