

Soft glasses, rheology, and trap models

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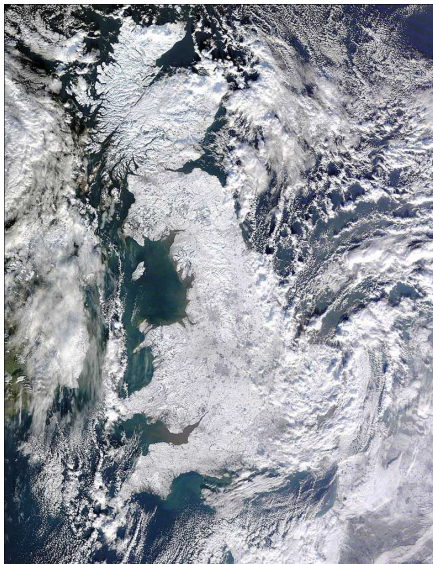
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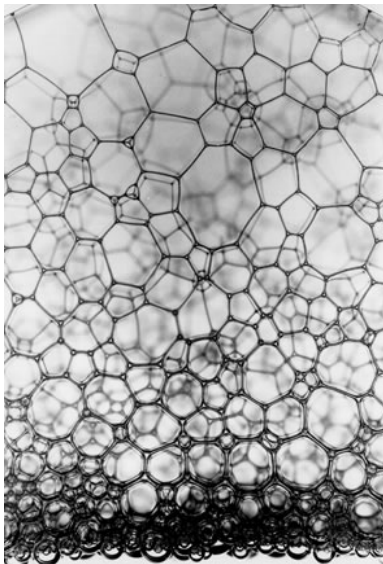
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Ask me questions before dinner

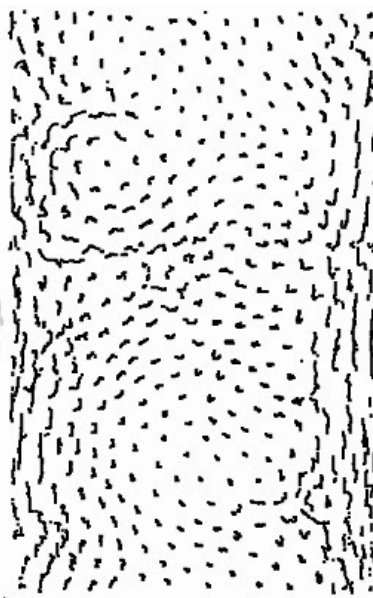
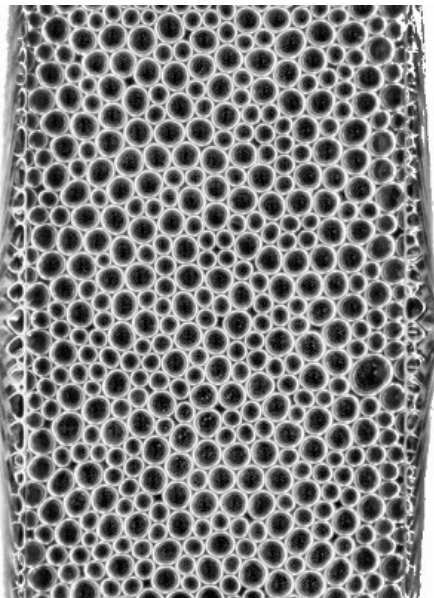
Though I'd rather stay here...



What's glassy about foam?



What's glassy about foam?



Complex fluids/soft matter

- **Foams** (shaving foam, mousse au chocolat)
- **Emulsions** (mayonnaise)
- Dense **colloidal suspensions** (yogurt, paint)
- Most **soft things you can eat** (cream cheese, ketchup)
- Clays, pastes, surfactant phases (“onions”)

Other important examples (not discussed here):

- Polymers (except star polymers \approx soft colloids)
- Gels

Rheology



- Science of **flow and mechanical deformation**
- Everything flows (Heraclitus $\pi\alpha\nu\tau\alpha\ \rho\epsilon\iota$, Dali see above)
- Important for e.g. industrial processing
- Usefulness of materials (“mouth-feel” for foods, spreading of paint/printing ink)

Complex fluids vs simple fluids

- **Simple fluids** (water):
only one lengthscale (atomic/molecular),
beyond this continuum theory (Navier-Stokes)
- **Complex fluids**: Hierarchy of scales, e.g. in foam =
air bubbles surrounded by fluid films stabilized by soap:
 - Water/soap molecules
 - Film thickness, size of channels where films meet
 - Bubble diameter
- Often intermediate behaviour between **fluid** and **solid**:
Shaving foam flows out of a spray can,
but doesn't drip off face

Soft glasses

- Emulsions, dense colloidal suspensions, foams, microgels
- **Structural similarities**: made up of squishy “particles”
- Oil droplets [ignore coalescence], colloidal particles, air bubbles [ignore coarsening]
- Typical particle scale μm , larger for foams, smaller for colloids
- Particles have different shapes and sizes (polydisperse)
- Particle packing is **amorphous** (disordered)
- **Metastable**: $k_B T$ too small to make system ergodic & reach optimal packing (crystalline, if polydispersity not too strong)
- So **glassy** (repulsive glass) – but soft, can easily be made to flow

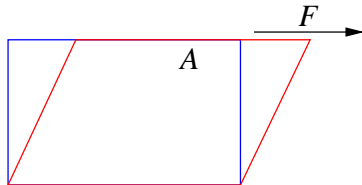
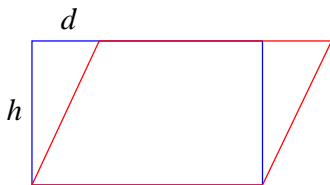
Outline

- 1 Rheology: A reminder
- 2 Soft glasses: Phenomenology and SGR model
- 3 Intermezzo: Trap models
- 4 SGR predictions and model limitations
- 5 Comparison with simulations: Virtual strain analysis
- 6 Effective temperature dynamics, shear banding
- 7 Outlook

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Shear stress and strain



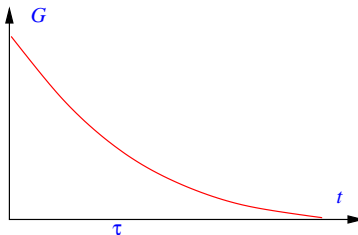
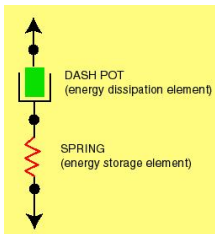
- Shear strain: $\gamma = d/h$, shear stress $\sigma = F/A$ (really tensors)
- Elastic solid: $\sigma = G\gamma$, elastic (shear) modulus G
- Newtonian fluid: $\sigma = \eta\dot{\gamma}$, viscosity η

Linear rheology & viscoelasticity

- Small strain increment (step) $\Delta\gamma$ at $t = 0$ causes stress $\sigma(t) = G(t)\Delta\gamma$
- $G(t) =$ **stress relaxation function**
Constant for solid, spike $\eta\delta(t)$ for fluid
- Most materials are in between: **viscoelastic**
- For short t , $G(t)$ nearly constant (solid), but eventually $\rightarrow 0$ (fluid)
- Linear superposition of many small strain steps $\Delta\gamma = \dot{\gamma}\Delta t$:

$$\sigma(t) = \int_0^t G(t-t')\dot{\gamma}(t') dt'$$

Maxwell model



- Elastic solid and viscous fluid “in series” (spring & damper)
- **Common stress** σ , **elastic strain** obeys $\sigma = G_0 \gamma_{\text{el}}$,
viscous strain $\sigma = \eta \dot{\gamma}_{\text{visc}}$
- Total strain rate $\dot{\gamma} = \dot{\gamma}_{\text{el}} + \dot{\gamma}_{\text{visc}} = \dot{\sigma}/G_0 + \sigma/\eta$
- Solve for small strain step ($\dot{\gamma}(t) = \Delta\gamma \delta(t)$):

$$G(t) = G_0 \exp(-t/\tau), \quad \tau = \eta/G_0$$

- Note $\eta = \int_0^\infty G(t) dt$, generally true if(!) flow with constant strain rate is a linear perturbation

Another Maxwell model



Complex modulus

- Experimentally, **oscillatory measurements** often easier
- If $\gamma(t) = \gamma_0 \cos(\omega t) = \gamma_0 \operatorname{Re} e^{i\omega t}$, then

$$\sigma(t) = \operatorname{Re} \int_0^t G(t-t') i\omega \gamma_0 e^{i\omega t'} dt' = \operatorname{Re} G^*(\omega) \gamma(t)$$

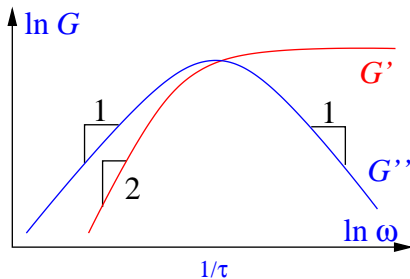
$$G^*(\omega) = i\omega \int_0^\infty G(t'') e^{-i\omega t''} dt'' \quad \text{for large } t$$

- Write **complex modulus** $G^*(\omega) = G'(\omega) + iG''(\omega)$, then

$$\sigma(t) = G'(\omega) \gamma_0 \cos(\omega t) - G''(\omega) \gamma_0 \sin(\omega t)$$

- Elastic modulus** $G'(\omega)$: in-phase part of stress
- Viscous or loss modulus** $G''(\omega)$: out-of-phase (ahead by $\pi/2$)

Complex modulus of Maxwell model



- $G^*(\omega) = i\omega \times \text{Fourier transform of } G_0 \exp(-t/\tau) = G_0 \frac{i\omega\tau}{1+i\omega\tau}$

$$G'(\omega) = G_0 \frac{\omega^2 \tau^2}{1 + \omega^2 \tau^2}, \quad G''(\omega) = G_0 \frac{\omega \tau}{1 + \omega^2 \tau^2}$$

- Single relaxation time gives **peak** in $G''(\omega)$ at $\omega = 1/\tau$

Creep

- Similar setup can be used when **imposing stress** and **measuring strain**
- Step stress: **creep compliance** $J(t)$

$$\gamma(t) = \int_0^t J(t-t') \dot{\sigma}(t') dt'$$

- Oscillatory stress: $\gamma(t) = \text{Re } J^*(\omega) \sigma(t)$
- Consistency with oscillatory strain requires $G^*(\omega) J^*(\omega) = 1$
- **Maxwell model**: $J^*(\omega) = (1 + i\omega\tau)/G_0$, $J(t) = 1/G_0 + t/\eta$

Nonlinear rheology

- For most complex fluids, steady flow (rate $\dot{\gamma}$) is **not** a small perturbation, don't get $\sigma = \eta\dot{\gamma}$
- **Flow curve** $\sigma(\dot{\gamma})$: stress in steady state
- Often shear-thinning: downward curvature
- Many other nonlinear perturbations:
 - large step stress or strain
 - large amplitude oscillatory stress or strain
 - startup/cessation of steady shear etc
- Most general description: **constitutive equation**

$$\sigma(t) = \text{some function(al) of strain history } [\gamma(t'), t' = 0 \dots t]$$

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Soft glasses: Linear rheology

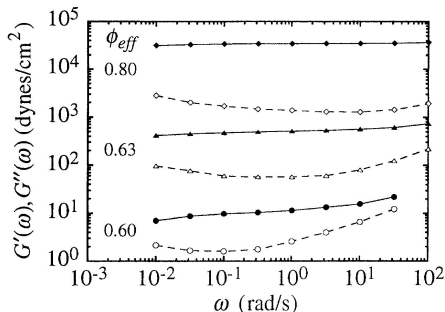
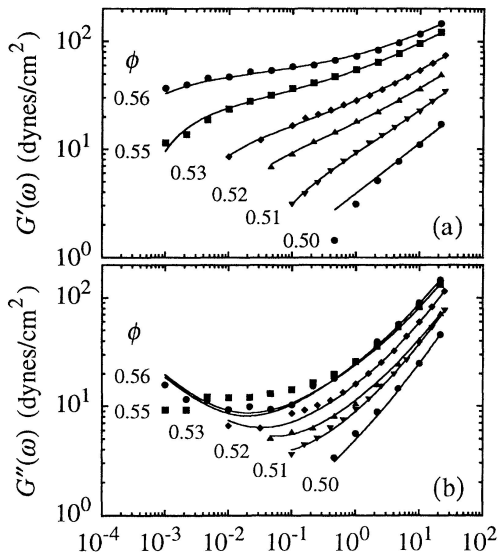


FIG. 2. The frequency dependence of the storage G' (solid points) and loss G'' (open points) moduli of a monodisperse emulsion with $r \approx 0.53 \mu\text{m}$ for $\phi_{eff} = 0.80$ (diamonds), 0.63 (triangles), and 0.60 (circles). The results for the two larger

- 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

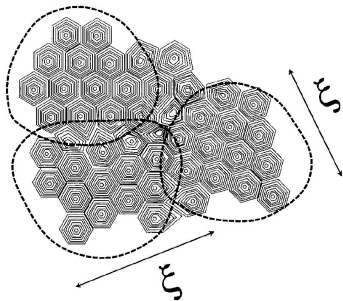
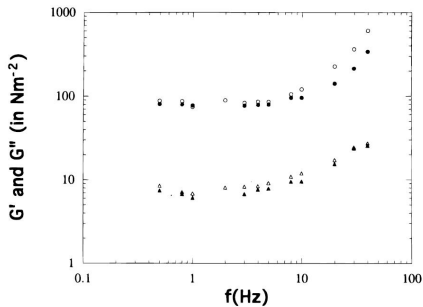


Figure 3. Schematic representation of an onion phase. ξ is the characteristic length of monodomains. Each monodomain is



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

Microgel particles

Purnomo van den Ende Vanapalli Mugele 2008

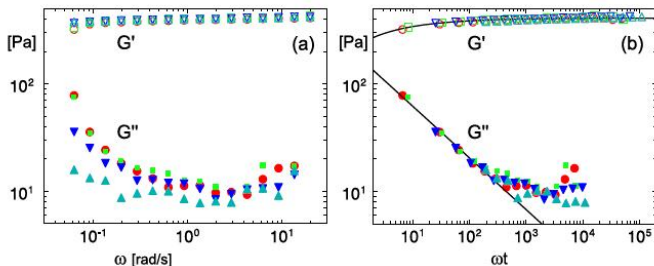
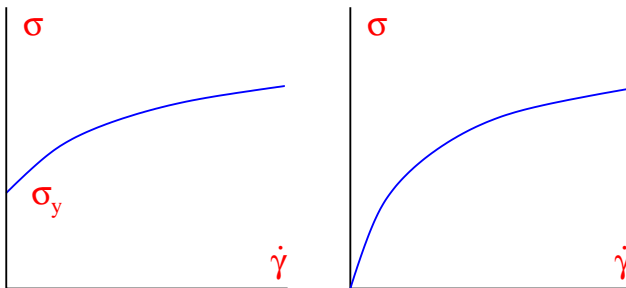


FIG. 1 (color online). G' (open symbols) and G'' (solid symbols) of a 7% w/w suspension at 25 °C plotted versus ω (a) or ωt (b) for $t_w = 3$ (○), 30 (□), 300 (▽), and 3000 s (△). Lines represent the SGR model ($x = 0.55$, $G_p = 410$ Pa).

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

Nonlinear rheology: Flow curves

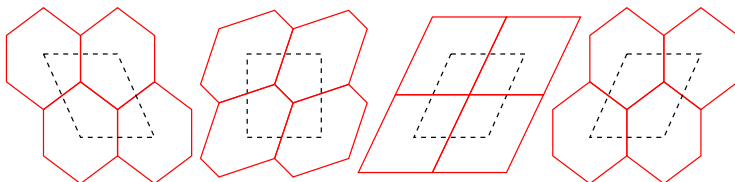


- Flow curves typically well fitted by $\sigma(\dot{\gamma}) - \sigma_y \sim \dot{\gamma}^p$ ($0 < p < 1$)
- **Herschel-Bulkley** if **yield stress** $\sigma_y \neq 0$,
unsheared state = “glass”
- Otherwise **power law** flow curve,
unsheared state = “fluid” (but $\eta = \sigma/\dot{\gamma} \rightarrow \infty$ for $\dot{\gamma} \rightarrow 0$)
- Shear thinning: $\sigma/\dot{\gamma}$ decreases with $\dot{\gamma}$

A non-glassy model for foam rheology

Princen 1968

- **Ideal 2d foam** (identical hexagonal cells), $T = 0$
- Apply shear: initially perfectly reversible response, stress increases
- Eventually interfaces rearrange, bubbles “slide”: global yield
- Process repeats under steady shear
- **We get**: yield stress
- **We don't get**: broad relaxation time spectrum (Buzza Lu Cates 1995), aging



SGR model

PS Lequeux Hébraud Cates 1997, PS 1998

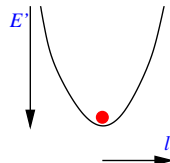
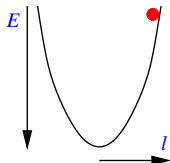
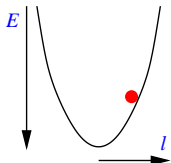
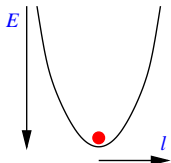
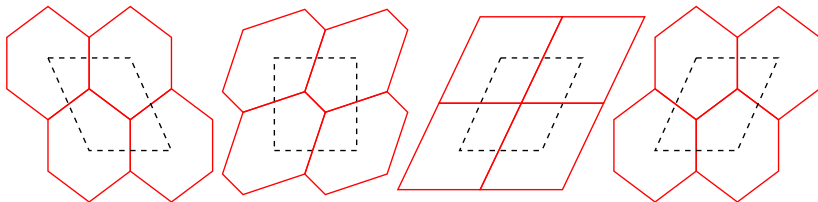
- How do we incorporate structural disorder?
- Divide sample conceptually into mesoscopic **elements**
- Each has **local shear strain l** , which increments with macroscopic shear γ
- Assumes **strain rate $\dot{\gamma}$** uniform throughout system, but allows for variation in local strain and stress (see Barrat & Falk talks)
- When **strain energy $\frac{1}{2}kl^2$** reaches **yield energy E** , element can **yield** and so reset to $l = 0$
- **$k = \text{local shear modulus}$**
- If all elements have same E and k , this would essentially give back the Princen model

SGR model

PS Lequeux Hébraud Cates 1997, PS 1998

- **New ingredient 1:** disorder \Rightarrow every element has **its own E**
- Initial distribution of E across elements depends on preparation
- When an element yields, it rearranges into new local equilibrium structure \Rightarrow acquires new E from some distribution $\rho(E) \propto e^{-E/\bar{E}}$ (assume no memory of previous E)
- **New ingredient 2:** Yielding is **activated by an effective temperature x** , to model interactions between elements
- x should be of order \bar{E} , $\gg k_B T$ (negligible)
- Model implicitly assumes low frequency/slow shear: yields are assumed instantaneous, no solvent dissipation

Sketch



Dynamical equation for SGR

- $P(E, l, t)$: probability of an element having yield energy E and local strain l at time t
- Master equation (Γ_0 = attempt rate for yields)

$$\begin{aligned} \dot{P}(E, l, t) = & -\dot{\gamma} \frac{\partial P}{\partial l} && \text{convection of } l \\ & - \Gamma_0 e^{-(E-kl^2/2)/x} P && \text{elements yield} \\ & + \Gamma(t) \rho(E) \delta(l) && \text{elements reborn after yield} \end{aligned}$$

where $\Gamma(t) = \Gamma_0 \langle e^{-(E-kl^2/2)/x} \rangle$ = average yielding rate

- Macroscopic **stress** $\sigma(t) = k \langle l \rangle$
- Given initial condition $P(E, l, 0)$ and **strain history** (input) can in principle calculate **stress** (output)
- We'll rescale E, t, l so that $\bar{E} = \Gamma_0 = k = 1$; this means also typical yield strains are 1

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Trap model

Bouchaud 1992, also Dean, Monthus ...

- Without shear ($\dot{\gamma} = 0$), can ignore local strains (all $l \rightarrow 0$ eventually)
- Master equation for $P(E, t)$

$$\dot{P}(E, t) = -e^{-E/x} P + \Gamma(t) \rho(E)$$

where $\Gamma(t) = \langle e^{-E/x} \rangle$

- Physical (re-)interpretation: “particle hopping” by activation, in landscape of **traps** of depth E
- Landscape has golfcourse shape: all traps hang off same energy level
- No geometry: every trap connected to every other

Equilibrium & glass transition in the trap model

- Master equation for $P(E, t)$

$$\dot{P}(E, t) = -e^{-E/x} P + \Gamma(t) \rho(E)$$

- $P(E, t)$ approaches equilibrium $P_{\text{eq}}(E) \propto \exp(E/x) \rho(E)$ for long t (Boltzmann distribution; E is measured downwards)
- Get **glass transition** if $\rho(E)$ has exponential tail (possible justification from extreme value statistics)
- Reason: for low enough x , $P_{\text{eq}}(E)$ cannot be normalized
- For $\rho(E) = e^{-E}$ this transition happens at $x = 1$
- For $x < 1$, system is in glass phase; never equilibrates
- **Aging**: evolution into ever deeper traps

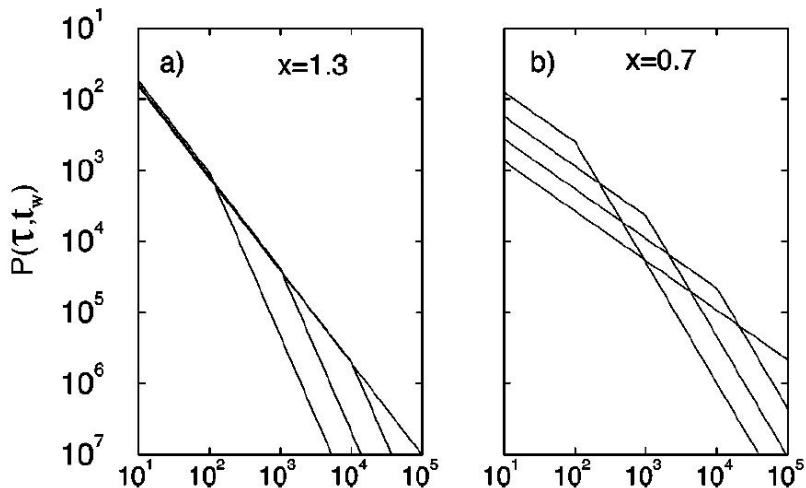
Aging in the trap model

- Easier in terms of lifetimes $\tau = \exp(E/x)$
- Then $\rho(\tau) \sim \tau^{-x-1}$, $P_{\text{eq}}(\tau) \sim \rho(\tau)\tau \sim \tau^{-x}$
- Assume initial condition $P(\tau, 0) = \rho(\tau)$
- At age t_w , particle hasn't hopped if initial $\tau \gg t_w$; traps with $\tau \ll t_w$ have become equilibrated:

$$P(\tau, t_w) \propto \begin{cases} \tau^{-x} & \text{for } \tau \ll t_w \\ t_w \tau^{-x-1} & \text{for } \tau \gg t_w \end{cases}$$

- Normalization: for $x > 1$, most “mass” for $\tau = O(1)$, $P(\tau, t_w) \rightarrow \text{const} \times \tau^{-x}$ for large t_w
- For $x < 1$, in **glass phase**, most mass for $\tau = O(t_w)$
- Then get scaling form $P(\tau, t_w) = (1/t_w)f(\tau/t_w)$:
typical relaxation times $\sim t_w$, simple aging

Aging in the trap model: Sketch



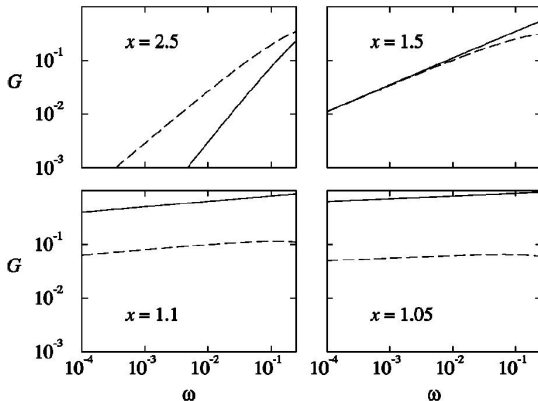
Trap model: Interpretations and uses

- Originally proposed by Bouchaud as model for motion in phase space (spin glasses)
- Simple(st?) aging mechanism, controlled by **energy barriers and activation**
- Distinct from mean-field spin glasses, aging controlled by **entropy barriers** (rare downhill directions), T not crucial
- Connection with **real-space dynamics?**
Small subsystems \approx independent trap models (Heuer et al)
- Intriguing fluctuation-dissipation behaviour (see my webpage)

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Linear response in the fluid phase



- Calculation yields average of Maxwell models:

$$G^*(\omega) = \left\langle \frac{i\omega\tau}{1+i\omega\tau} \right\rangle, \text{ average is over } P_{\text{eq}}(\tau)$$

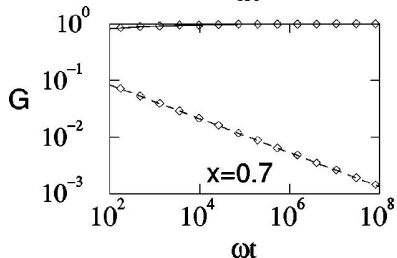
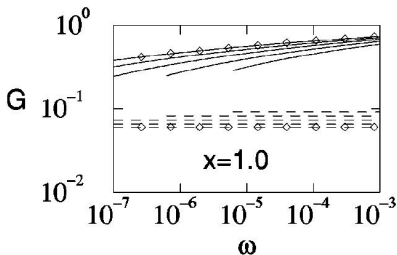
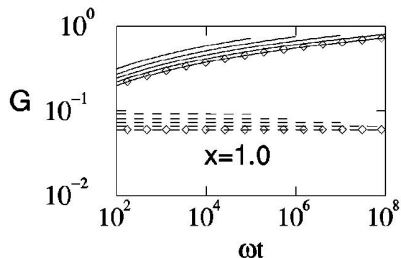
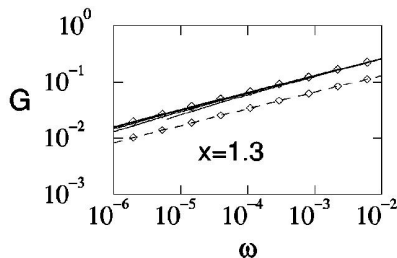
- For large x , get usual power-law dependences for small ω
- But near $x = 1$ get $G' \sim G'' \sim \omega^{x-1}$: both become **flat**

Linear response: Aging

Sollich PS Cates 2000

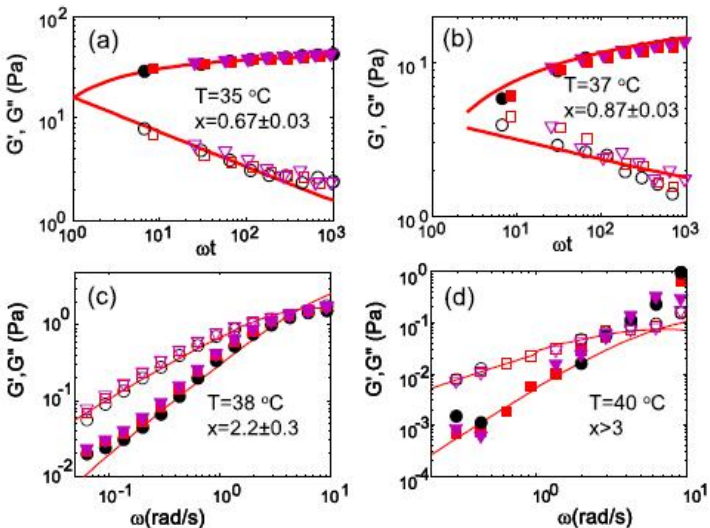
- Conceptual issue: with aging, $G^*(\omega) \rightarrow G^*(\omega, t, t_w)$
- $G^*(\omega, t, t_w)$ could depend on final time t
and start time t_w of shear
- Luckily, dependence on t_w is weak: $G^*(\omega, t)$
- “Inherits” simple aging $1/\omega \sim t$: $G^*(\omega, t) \sim 1 - (i\omega t)^{x-1}$

Linear response: Aging

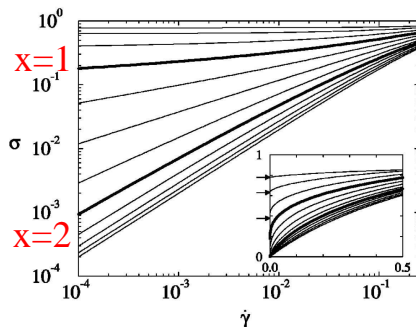


Comparison with experiments on microgel particles

Purnomo van den Ende Vanapalli Mugele 2008



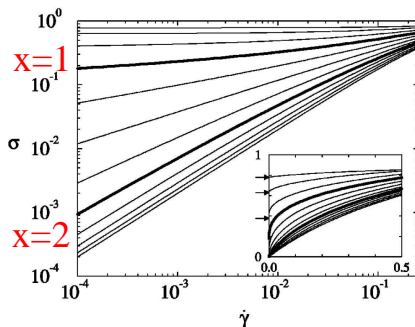
Flow curve



- Calculation: steady state, so set $\dot{P} = 0$ in master equation, integrate differential eqⁿ for l ; Γ from normalization (try it)
- Three regimes for small $\dot{\gamma}$:

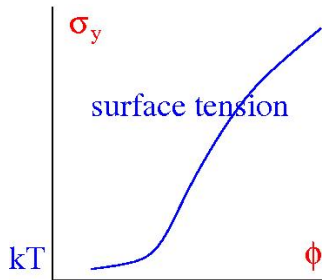
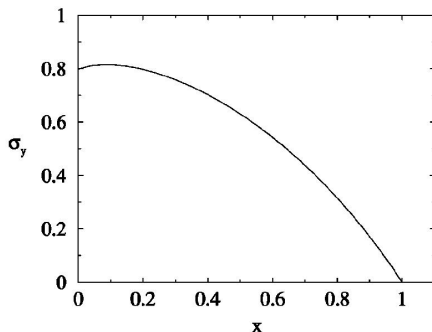
$$\sigma \sim \begin{cases} \dot{\gamma} & \text{for } 2 < x : & \text{Newtonian} \\ \dot{\gamma}^{x-1} & \text{for } 1 < x < 2 : & \text{power law} \\ \sigma_y(x) + \dot{\gamma}^{1-x} & \text{for } x < 1 : & \text{Herschel-Bulkley} \end{cases}$$

Relation between flow and aging



- **No** aging in steady flow
- Driving by shear restores ergodicity
- **Flow interrupts aging** (Kurchan)

Yield stress



- Yield stress increases **continuously** at glass transition
- Compare MCT prediction: **discontinuous** onset of yield stress
- Physics?
 - Elastic networks/stress chains** vs **caging?**
 - Jamming transition** vs **glass transition?**
- Could e.g. emulsions exhibit both transitions?

General nonlinear rheology: Constitutive equation

PS 1998

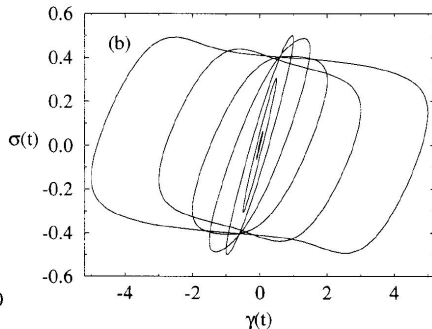
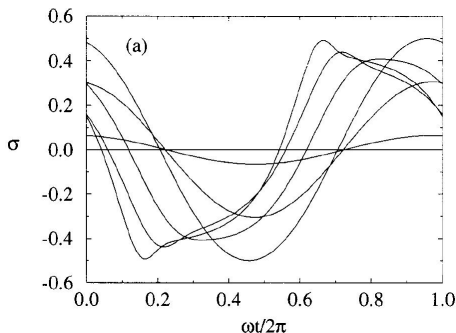
- SGR model can be solved: switch variable $l \rightarrow l - \gamma(t)$ to eliminate $\partial P / \partial l$ term, then integrate (try it)
- For simplest initial condition $P(E, l, 0) = \rho(E)\delta(l)$ get **constitutive equation** (2nd equation determines $\Gamma(t)$)

$$\sigma(t) = \gamma(t)G_\rho(Z(t, 0)) + \int_0^t \Gamma(t')[\gamma(t) - \gamma(t')]G_\rho(Z(t, t')) dt'$$

$$1 = G_\rho(Z(t, 0)) + \int_0^t \Gamma(t')G_\rho(Z(t, t')) dt'$$

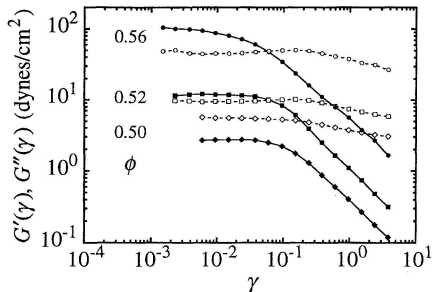
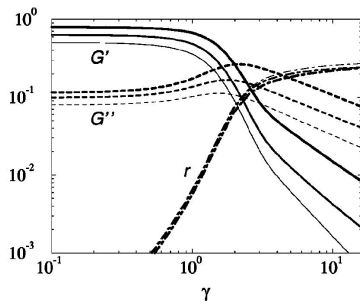
- $G_\rho(t) = \int \rho(E) \exp(-te^{-E/x}) dE$ **survival probability**
- $Z(t, t') = \int_{t'}^t \exp([\gamma(t'') - \gamma(t')]^2 / 2x) dt''$ **effective time**,
 $Z(t, t') = t - t'$ for small strains
- Overall interpretation as **birth-death process**

Example: Large amplitude oscillatory strain



- Close to but above glass transition ($x = 1.1$, $\omega = 0.01$)
- Increasing strain amplitude gives stronger **nonlinearities**
- Hysteresis-like loops

Large oscillatory strain: Complex modulus



- G'' first increases with amplitude, becomes larger than G'
- Large strain **fluidizes** an initially predominantly elastic system
- Compare experiments on colloidal hard spheres (right)
- Quantitative comparison for foam
(Rouyer Cohen-Addad Höhler PS Fielding 2008)

SGR predictions: Summary

- **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
- Large amplitude G' and G'' show **fluidization behaviour** similar to experiments
- Stress overshoots in shear startup, linear and nonlinear creep, rejuvenation and overaging (Lequeux, Viasnoff, McKenna, Cloître, Roettler ...)

Limitations of SGR model

- **Scalar model** with ideal local elasticity up to yield – both can be fixed (Cates PS 2004)
- No spatial information: geometry of stress redistribution might be important, also non-affine flow (Barrat talk)
- **Length scale** of elements: needs to be large enough to allow local strain and stress to be defined, but otherwise unspecified
- Interpretation of **effective temperature x** ?
Link to material parameters?
Should have own dynamics? (see later)
- What sets fundamental **time scale** (attempt rate for yielding)?

Outline

- 1 Rheology: A reminder
- 2 Soft glasses: Phenomenology and SGR model
- 3 Intermezzo: Trap models
- 4 SGR predictions and model limitations
- 5 Comparison with simulations: Virtual strain analysis**
- 6 Effective temperature dynamics, shear banding
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Simulations to the rescue?

- Can we use **simulation data** to:
- See how far the SGR model represents physical reality?
- Get better understanding of model parameters?
- Tell us where we should improve the model?
- Need to develop **method for explicit coarse-graining** of simulation data

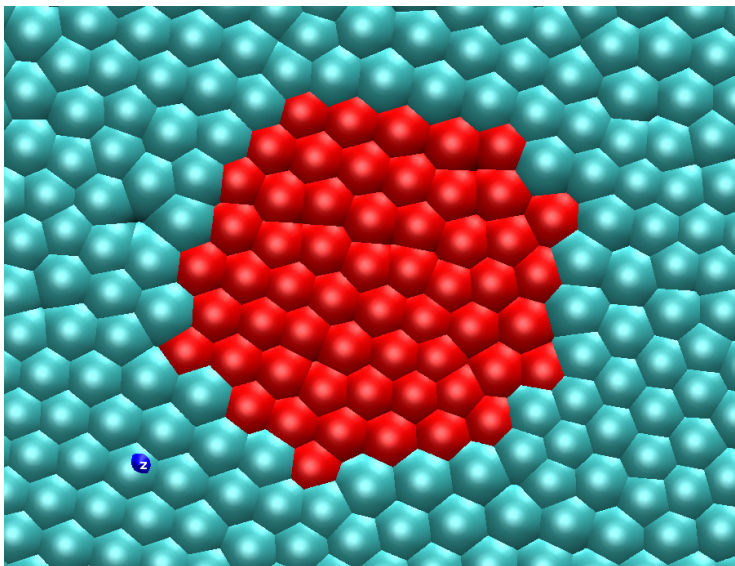
Defining elements

- 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
- 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?

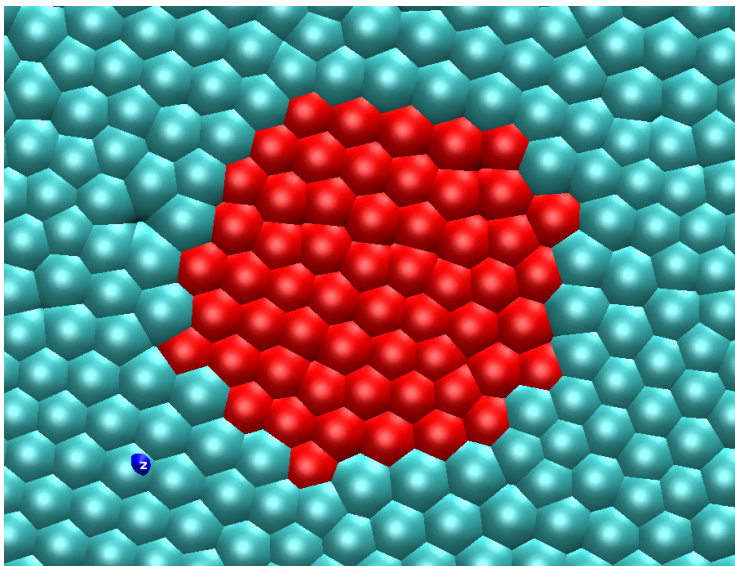
Virtual strain analysis

- Deliberately want **local** yield points etc: interaction between elements is accounted for separately within model
- 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)

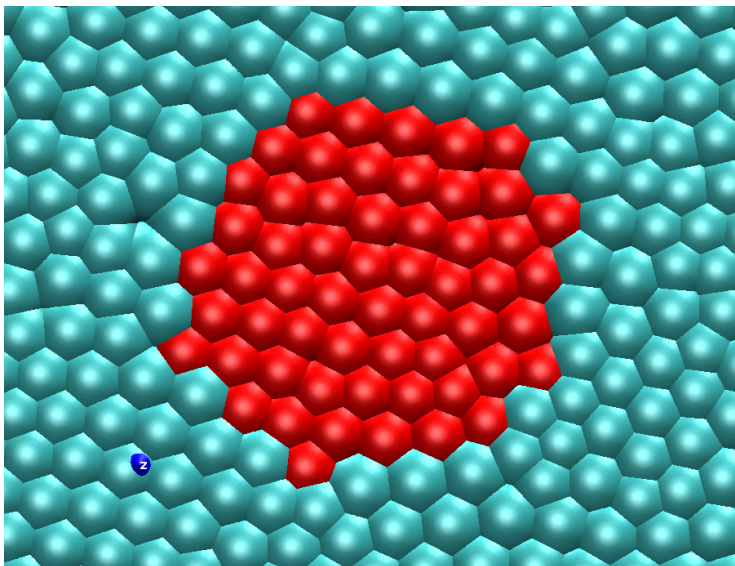
Example: Virtual strain sequence 1



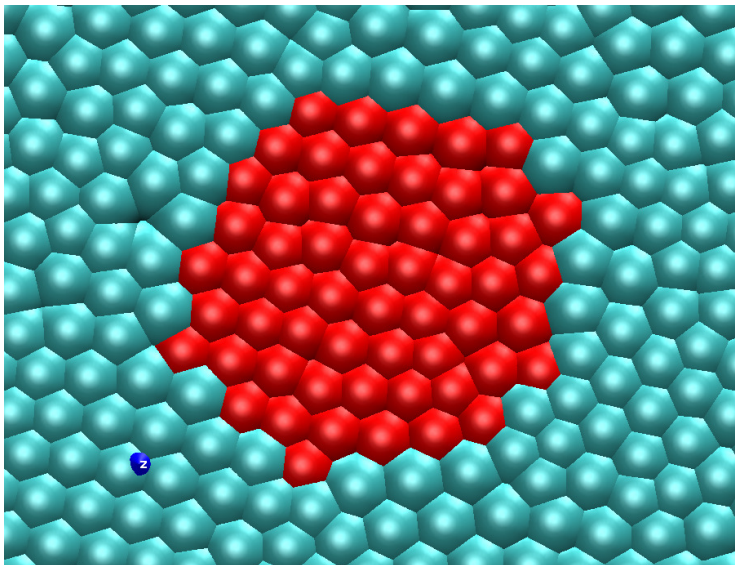
Example: Virtual strain sequence 2



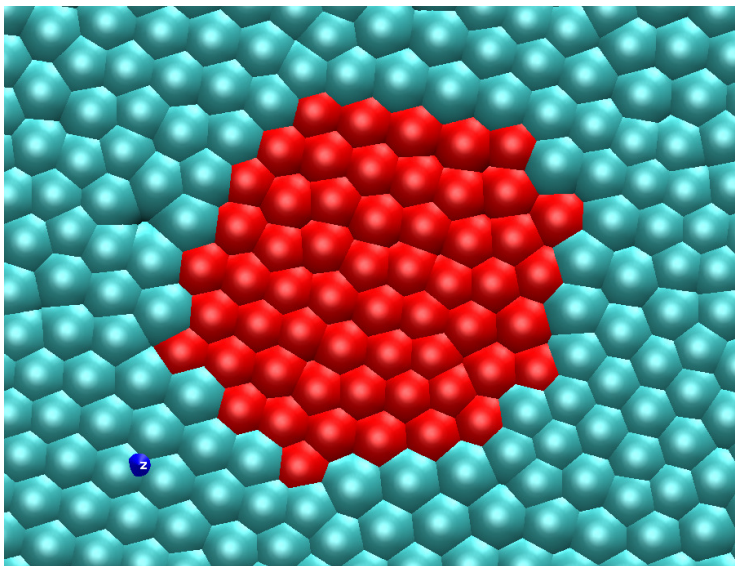
Example: Virtual strain sequence 3



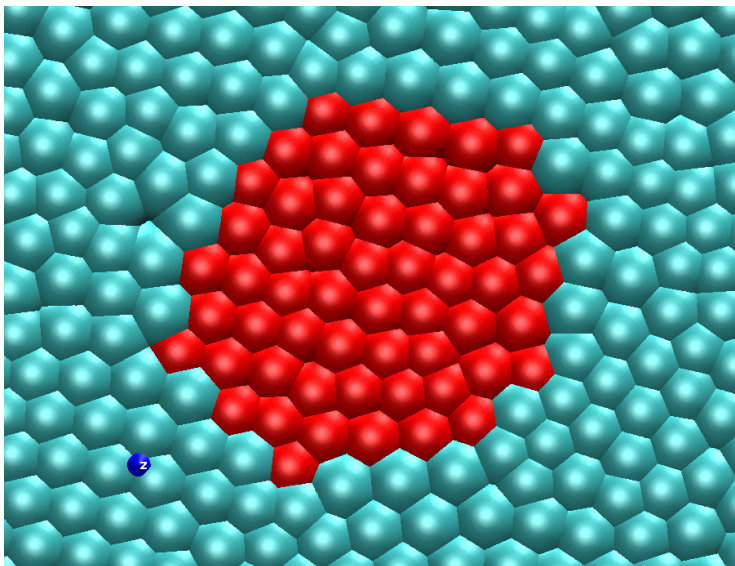
Example: Virtual strain sequence 4



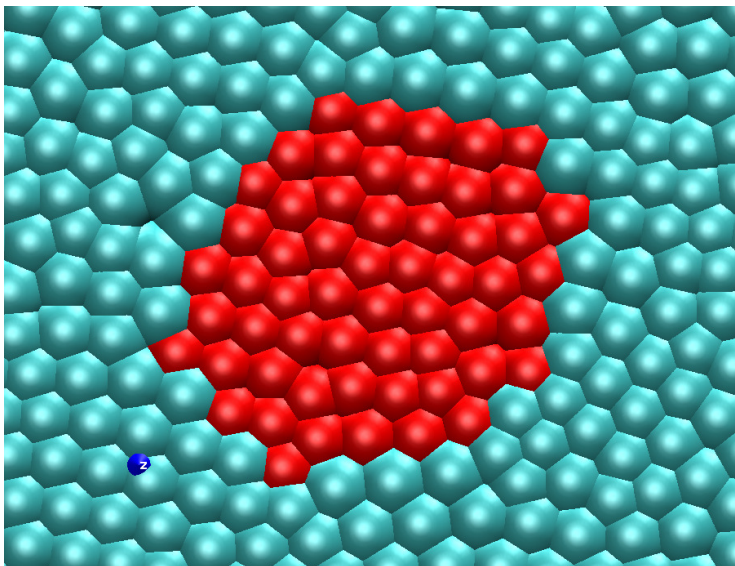
Example: Virtual strain sequence 5



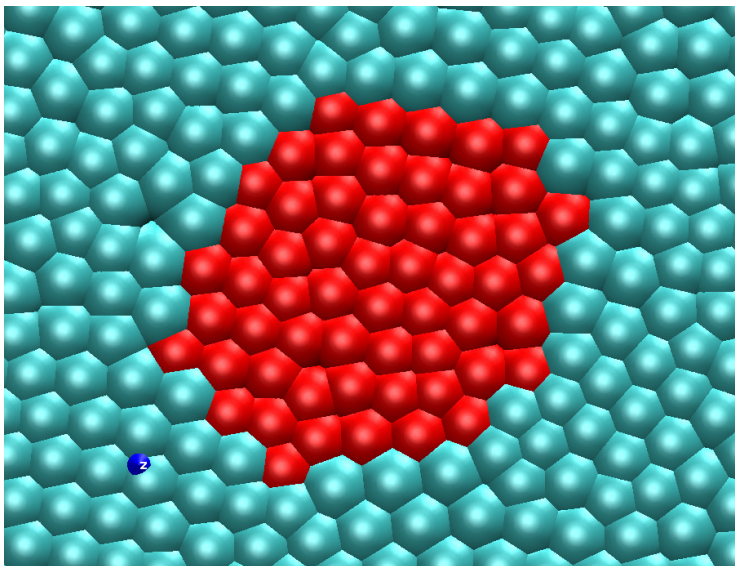
Example: Virtual strain sequence 6



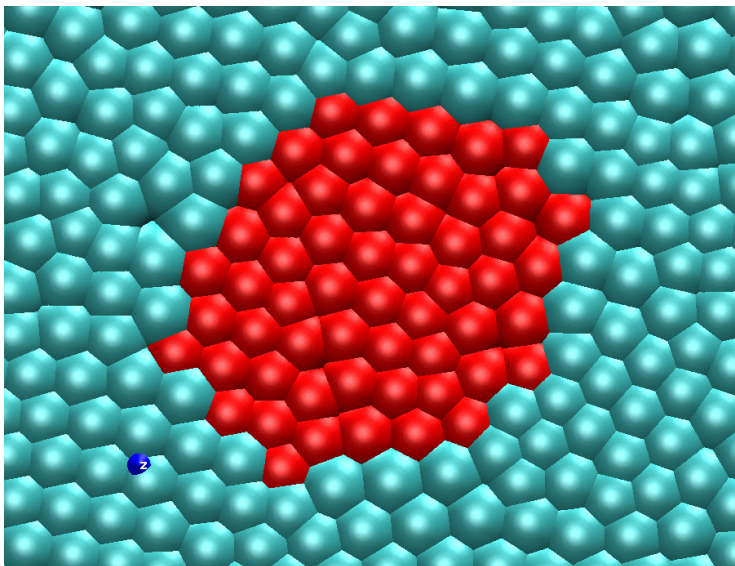
Example: Virtual strain sequence 7



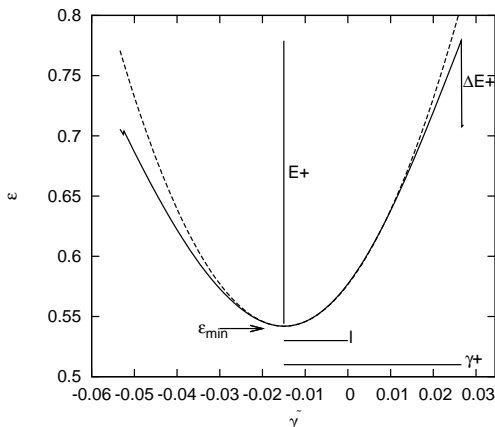
Example: Virtual strain sequence 8



Example: Virtual strain sequence 9



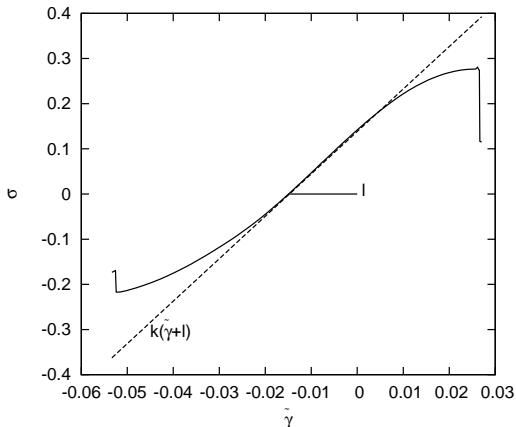
Element energy landscape



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

Local modulus

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



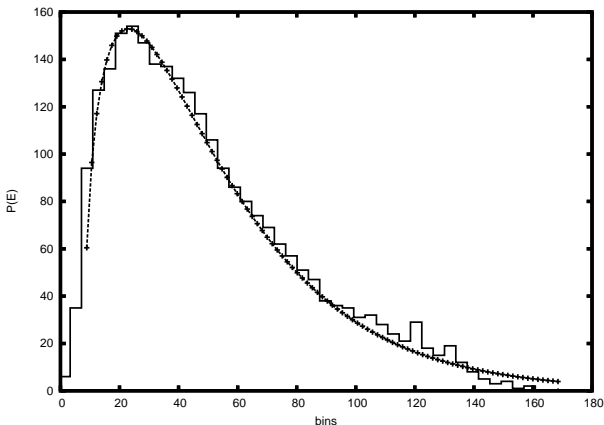
Systems studied

- Polydisperse Lennard-Jones mixtures (Tanguy et al), quenched to low temperatures ($T = 0.005 \ll T_g$)
- Low shear rates $\dot{\gamma} \sim 10^{-3}$; $N = 10^4$ particles at $\rho = 0.95$
- 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 ≈ 40 particles (diameter = 7): large enough to have near-parabolic energy landscape, small enough to avoid multiple local yield events inside one element

Simulation demo

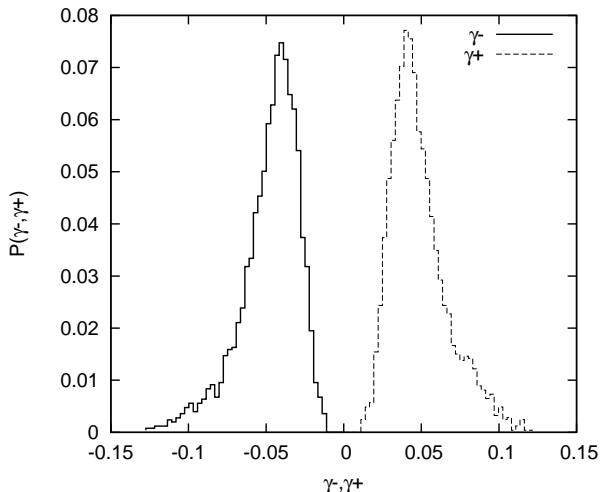
Close-up

Results: Yield energy distribution



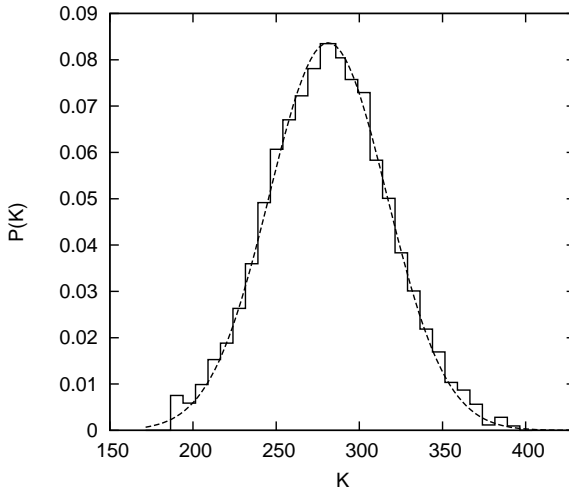
Exponential tail; detailed form can be fitted by SGR model

Yield strain distributions



Symmetric as assumed in SGR; gap around 0 or maybe power-law approach (exponent ≈ 4)

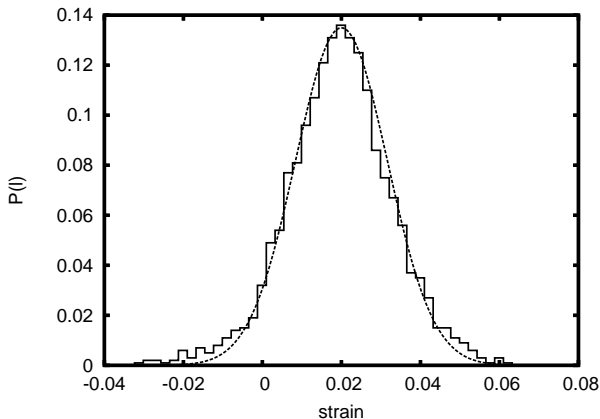
Modulus distribution



Clear spread; not constant as assumed in model.

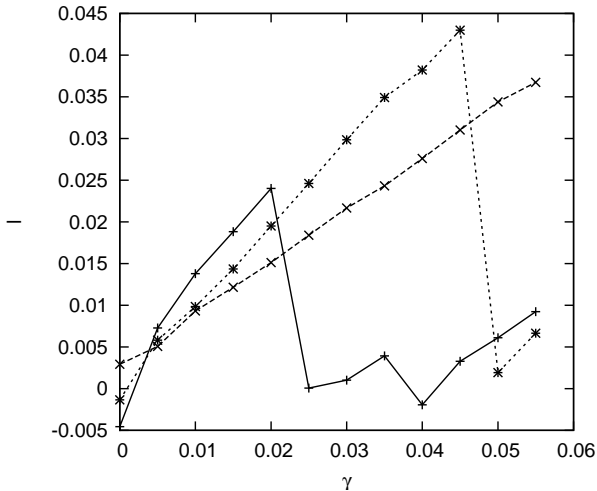
But yield strains γ_{\pm} still controlled by E_{\pm} ; no correlation with k

Local strain distribution



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

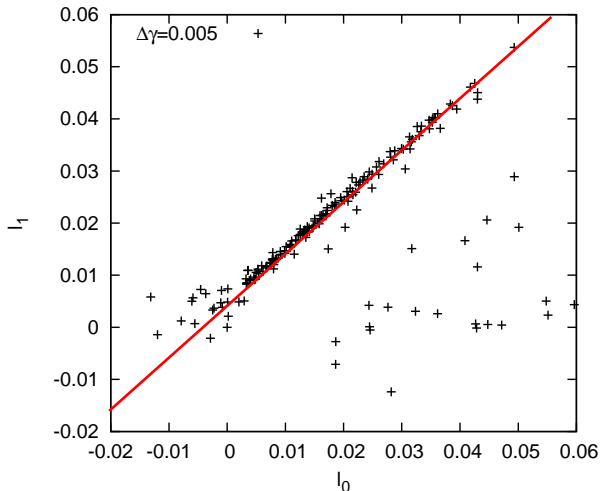
Dynamics: Evolution of local strain with time



Typical sawtooth shape assumed by SGR

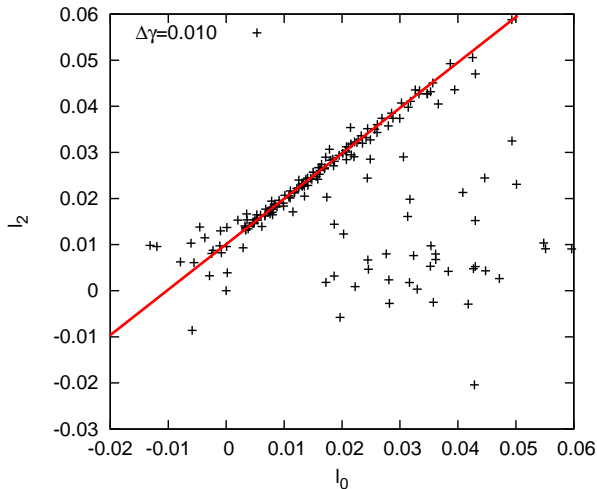
Population picture of l -dynamics

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

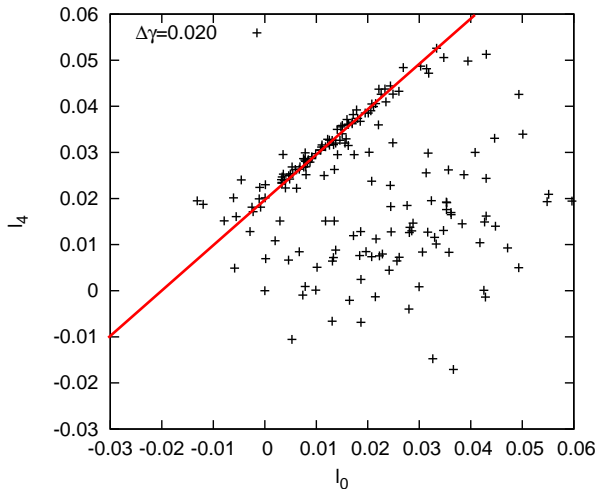


Separation into strain convection and yield events

Same for larger $\Delta\gamma$

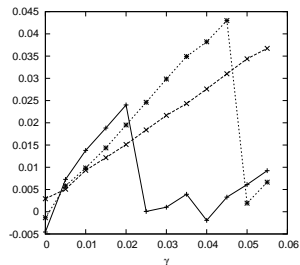
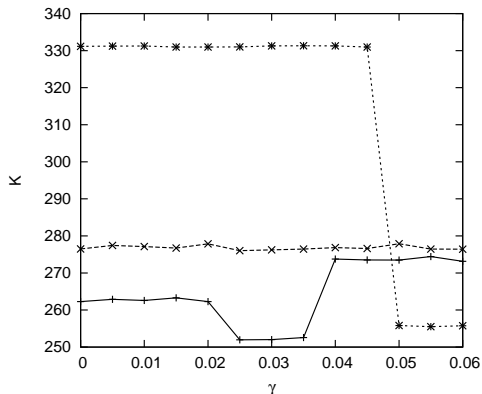


...and yet larger



Change in other landscape properties

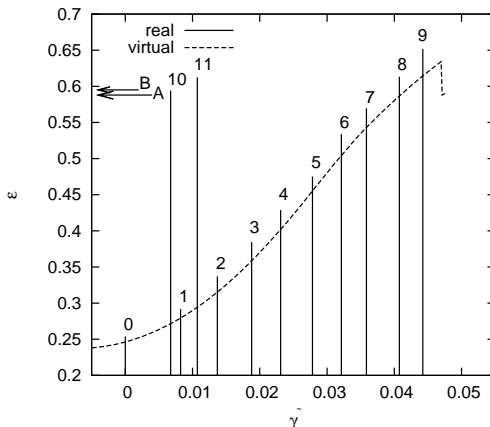
Example of modulus



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

Comparing real and virtual deformations

Primary yield



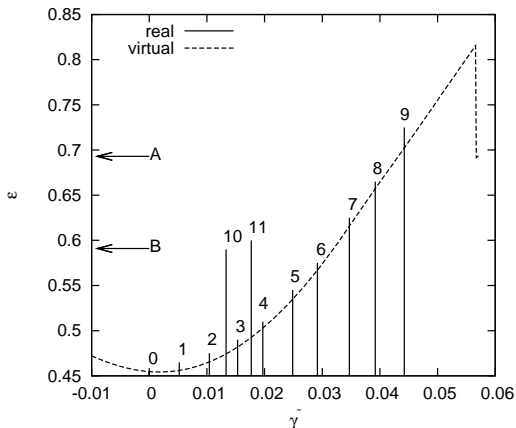
Curve: virtual energy landscape.

Vertical lines: Real ϵ versus $l - l_0$ for uniform steps $\Delta\gamma$

Good match, even for energy drop after yield

Comparing real and virtual deformations (cont)

Induced yield



Curve: virtual energy landscape.

Vertical lines: Real ϵ versus $l - l_0$ for uniform steps $\Delta\gamma$

Summary for virtual strain analysis

- **Virtual strain method** for assigning local strains, yield energies
- **Generic**: can be used on configurations produced by any (low- T) simulation
- Steady state distributions in shear flow seem in line with SGR (detailed fits in progress), 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
- Energy landscapes for real and virtual deformations match (but not purely quadratic)
- To do: analysis of induced yield events – well modelled by effective temperature?

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Effective temperature dynamics

Fielding Cates PS 2008

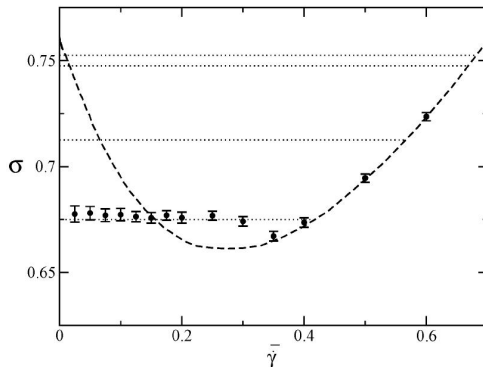
- Shouldn't effective temperature x be determined self-consistently by dynamics?
- To allow for potential **shear banding**, split sample in y (shear gradient)-direction
- Separate SGR model for each y , with $x(y)$
- Relaxation-diffusion dynamics:

$$\tau_x \dot{x}(y) = -x(y) + x_0 + S(y) + \lambda^2 \frac{\partial^2 x}{\partial y^2}$$

- x is “driven” by **energy dissipation rate**:
 $S = a \langle l^2 \exp(-[(E - l^2/2)/x]) \rangle$
- Assume that x equilibrates (locally) quickly: $\tau_x \rightarrow 0$

Flow curve

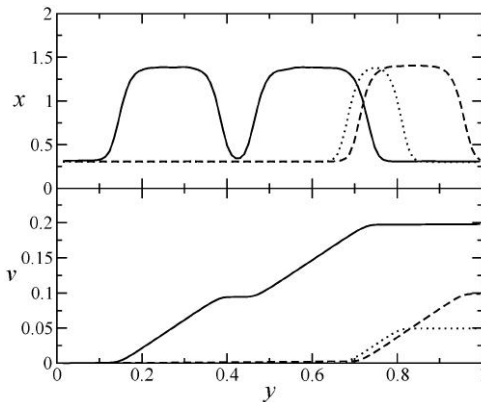
$$a = 2, x_0 = 0.3$$



- Steady state: $x = x_0 + 2a\sigma(x, \dot{\gamma})\dot{\gamma}$
- Shear startup with imposed mean $\dot{\gamma}$ across sample:
shear banding

Nature of banded state

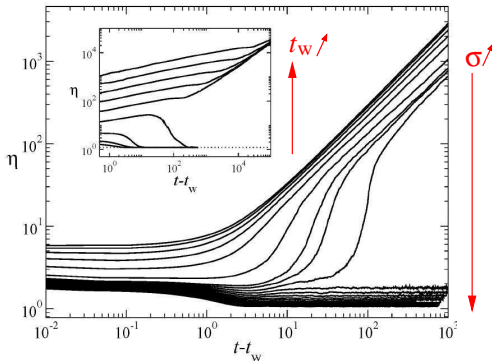
$a = 2$, $x_0 = 0.3$, $\dot{\gamma} = 0.05, 0.1, 0.2$



- “Hot” band: $\dot{\gamma} > 0$, ergodic
- “Cold” band: $\dot{\gamma} = 0$, aging

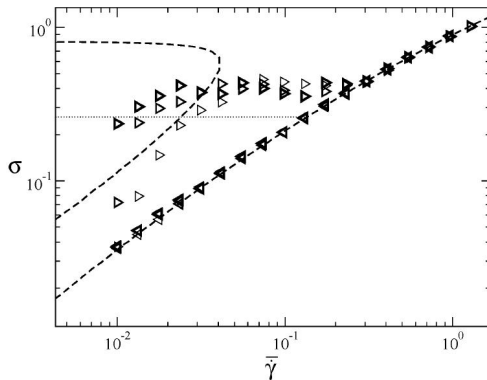
Viscosity bifurcation at imposed stress

Coussot, Bonn, ...



- Plot instantaneous viscosity $\eta = \sigma / \dot{\gamma}$
- Sample only reaches steady flow when σ is large enough
- Depends on age t_w when stress is applied

Variation of driving term for x



- x now driven by yield rate, $S \propto \langle \exp(-[(E - l^2/2)/x]) \rangle$
- **Hysteresis** in shear rate sweep: banding on way up, stay on fluid branch on way down
- Resembles data for multi-arm polymers (Holmes Callaghan Vlassopoulos Roovers 2004)

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Summary & Outlook

- **Trap models** for aging dynamics in glasses, focus on activation
- **SGR model** adds strain to this & re-interprets trap depths as yield energies
- Reproduces much (not all) of **rheological behaviour** of soft glasses
- ...and some cytoskeletal rheology(?)
- **Virtual strain** method allows detailed comparison with simulations: some encouraging agreement, but also suggests modifications
- **Dynamics of x** : phenomenological models useful, but too much choice?
- **To do**: linking to other approaches (STZ, Picard et al); coarse-graining from “microscopic” models?