Out of equilibrium relaxation of a time-dependent effective temperature

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Structural glasses

- Amorphous materials
  - granular materials
  - foams
  - colloidal suspensions
  - short polymers (non-entangled)
- Questions
  - Flow equations for complex fluids
  - Plasticity and fracture (brittle or ductile)
  - Friction laws, earthquakes
- Response under shear deformation (rheology)
  - constant stress
  - constant strain rate
  - strain step

Outline

- Phenomenological models
  - Glass transition: Free-volume, Adam-Gibbs
  - Glassy solids
  - Rate-and-state equations
- A heuristic argument
  - Enthalpy relaxation
  - Response under shear
- Consequences
  - Stress relaxation
  - Rheology
  - Boundary lubrication

Glass transition

[Cohen, Turnbull (1959)]

- Vogel-Fulcher expression for viscosity
- Free-volume activated processes (not thermal)

$$\dot{\gamma} \sim \frac{1}{\tau} \propto \exp\left[-\frac{v_0}{v_f}\right]$$

[Adam, Gibbs (1965)]

- Cooperative motion
- Size of zones: $z \sim 1/S_c$
- Activation factors:

$$\dot{\gamma} \sim \frac{1}{\tau} \propto \exp\left[-\frac{\Delta E}{T S_c(T)}\right]$$

Rate-and-state

[Dietrich (1979), Ruina (1983)]

- Rock on rock friction
- State variable:

$$\begin{aligned} \sigma &= f(V, \phi) \\ \dot{\phi} &= \cdots \end{aligned}$$

Rate-and-state

[Dietrich (1979), Ruina (1983)]

- Rock on rock friction
- More physically:

$$\begin{aligned}\dot{\sigma} &= 2\mu\left(\dot{\epsilon}(t) - \dot{\gamma}\right)\\ \dot{\gamma} &= f(\sigma, \Phi, P, V, \ldots)\\ \dot{\Phi} &= \cdots\end{aligned}$$

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[Caroli, Baumberger (1994)] Dry friction
[Carlson, Batista (1996)] Boundary lubrication
[Aranson, Tsimring (2001)] Granular materials
[Derec, Ajdari, Lequeux (2001)] Soft glassy materials

Shear Transformation Zones

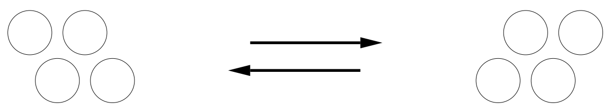
[Spaepen(1977), Argon (1979)]

- Shear deformation occurs in localized zones

$$\dot{\gamma} \propto (\text{density of zone}) \times (\text{net number of forward jumps})$$

[Falk and Langer, (1998)]

- Two types of zones: $\dot{\gamma} \propto R_+ n_+ - R_- n_-$



- Populations dynamics:

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \sigma \dot{\gamma} \left(\mathcal{A}_c - \mathcal{A}_a \, n_\pm \right)$$

- Free-volume activation factors $R_\pm \sim \exp\left[- \left(\frac{V_0(\sigma)}{v_f} \right) \right]$

Adiabatic ensemble

- Fluctuation of enthalpy: $h_i = Pv_i$
- Mechanical contact between zones:

$$\rho(h) = \frac{1}{Z} \exp\left[-\lambda h\right]$$

- Partition function:

$$Z = \int_{Pv_0}^{\infty} \exp\left[-\lambda h\right] = \frac{1}{\lambda} \exp\left[-\lambda\, h_0\right]$$

- Lagrange multiplier fixed by H: $\lambda \equiv \frac{1}{k\Theta}$

$$k\Theta = H(t) - Pv_0$$

Transformation rates

- Local reconformation of zones:

$$k\dot{\Theta} = \dot{H}(t) = \int \mathrm{dhdh'p(h \to h')}\rho(\mathrm{h})(\mathrm{h'} - \mathrm{h}) + \mathrm{W^{ext}}$$

- Barrier height: $h_b(v)$ non-increasing
  $\Rightarrow$ define $Pv_a = h_b(v_a) = h_a$
- Two types of pathways:
  - $h, h' < h_a$: activated rearrangements,
    $p(h \to h') \propto \exp(-(h_b - h)/(kT))$
  - otherwise: *non*-activated rearrangements,
    $p(h \to h') \propto \min\left[1, \exp(-(h' - h)/(kT))\right]$

Enthalpy relaxation

Dominant terms:

$$k\dot{\Theta} = E_1 \, \exp\left[-\frac{\Delta h}{k\,\Theta}\right] \, \left(\exp\left(\frac{\delta q}{k\Theta} - \frac{\delta q}{kT}\right) - 1\right) + \sigma \, \dot{\gamma}$$

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- $\sigma = 0$
- Fixed-point:
  equilibrium $\Theta = T$
- Slowing down

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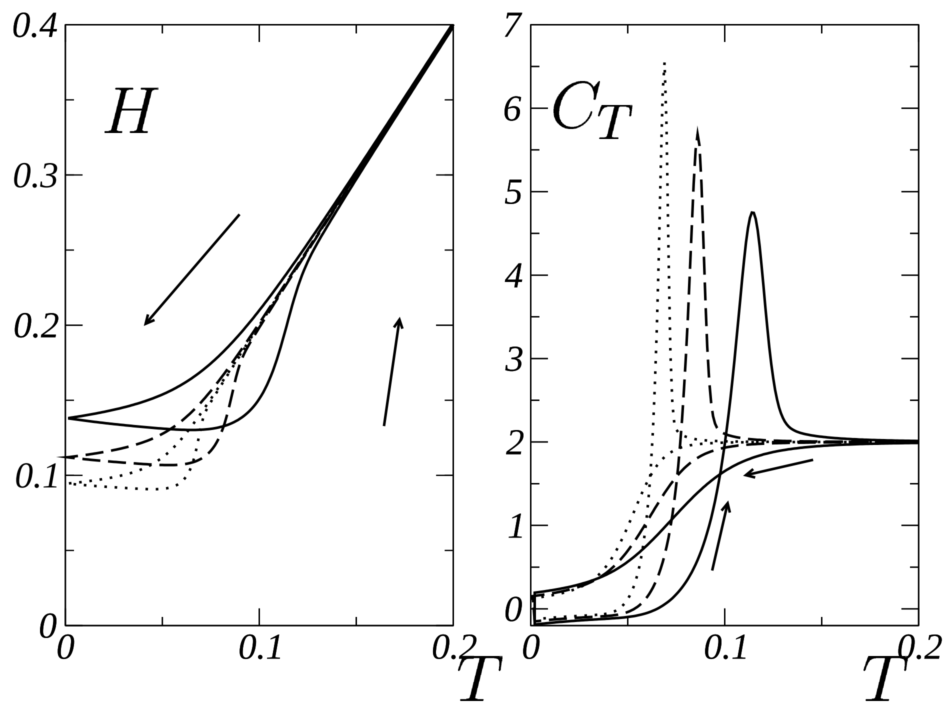


Zero-temperature dynamics

For $\Theta >> T$:

$$k\,\dot{\Theta} = -E_1\,\exp\left[-\frac{\Delta h}{k\,\Theta}\right] + \sigma\,\dot{\gamma}$$

$\sigma = 0$: logarithmic relaxation:

$$k\,\Theta(t) \simeq \frac{\Delta h}{\log\left(E_1\,t/\Delta h\right)}$$

Shear transformations

- Similar calculation:

$$\dot{\gamma} = E_0 \exp\left[-\frac{\Delta h'}{k\,\Theta}\right]\sigma$$

- Different reactional pathways: $h \neq h'$
- Consequences of this coupling?

Shear transformations

- Similar calculation:

$$\dot{\gamma} = E_0 \exp\left[-\frac{\Delta h'}{k\,\Theta}\right]\,\sigma$$

- Different reactional pathways: $h \neq h'$
- Consequences of this coupling?
- Coupled with STZ theory:

$$\begin{aligned}
\dot{\gamma} &= E_0 \exp\left[-\frac{\Delta h'}{k\,\Theta}\right]\,(\sigma - \Delta) \\
\dot{\Delta} &= \frac{\dot{\gamma}}{\epsilon_0}\,(1 - \sigma\Delta)
\end{aligned}$$

with $\Delta \propto n_- - n_+$

Relaxation modulus

- Step strains at t_w
- Stress relaxation:

$$\dot{\sigma} = -2\mu\,\dot{\gamma}$$

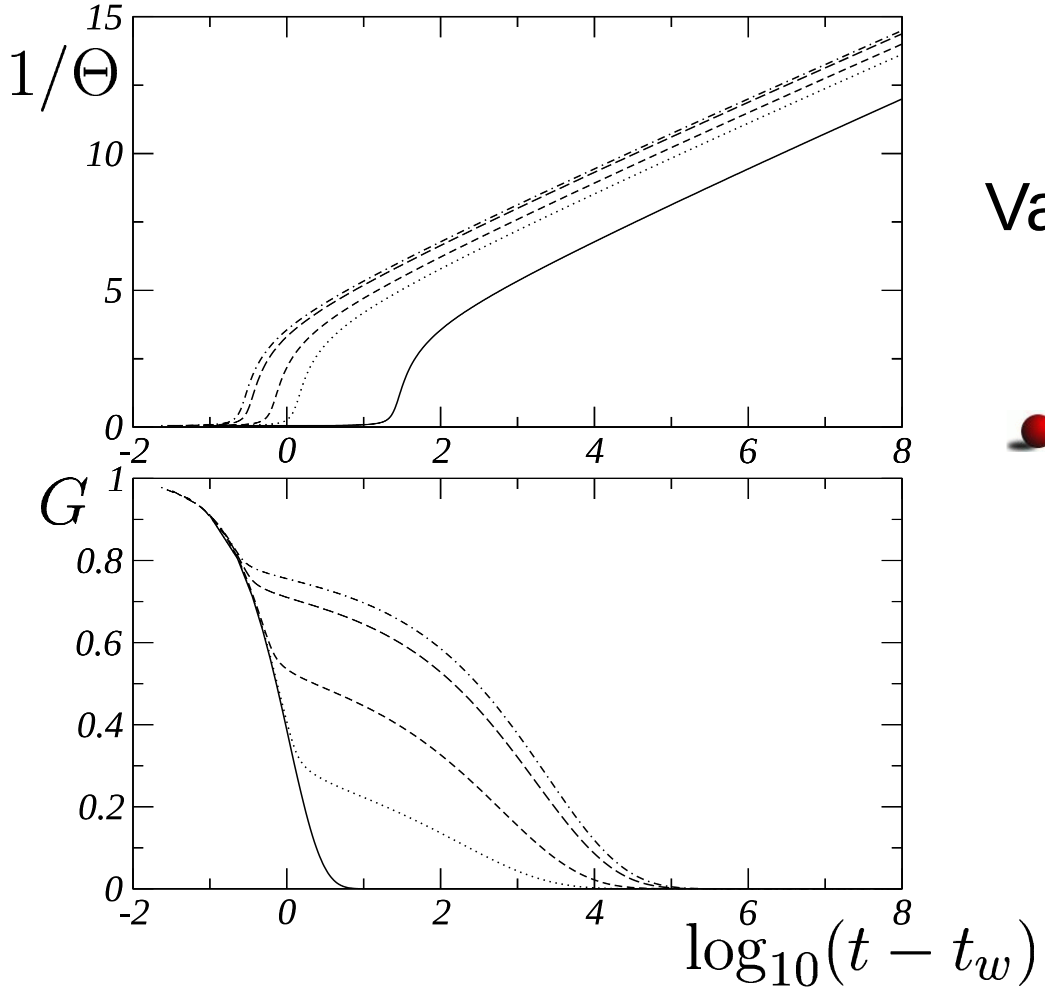
- Modulus:

$$G(t) = \sigma(t)/\sigma(t_w) \simeq \exp\left[A\left(t_w^{\beta} - t^{\beta}\right)\right]$$

with

$$\beta = 1 - \frac{1}{\kappa} \quad , \kappa = \frac{\Delta h}{\Delta h'} \quad , \quad \text{and} \quad A = \frac{2\mu\,E_0}{\beta}\left(\frac{E_1}{\kappa}\right)^{-1/\kappa} \quad .$$

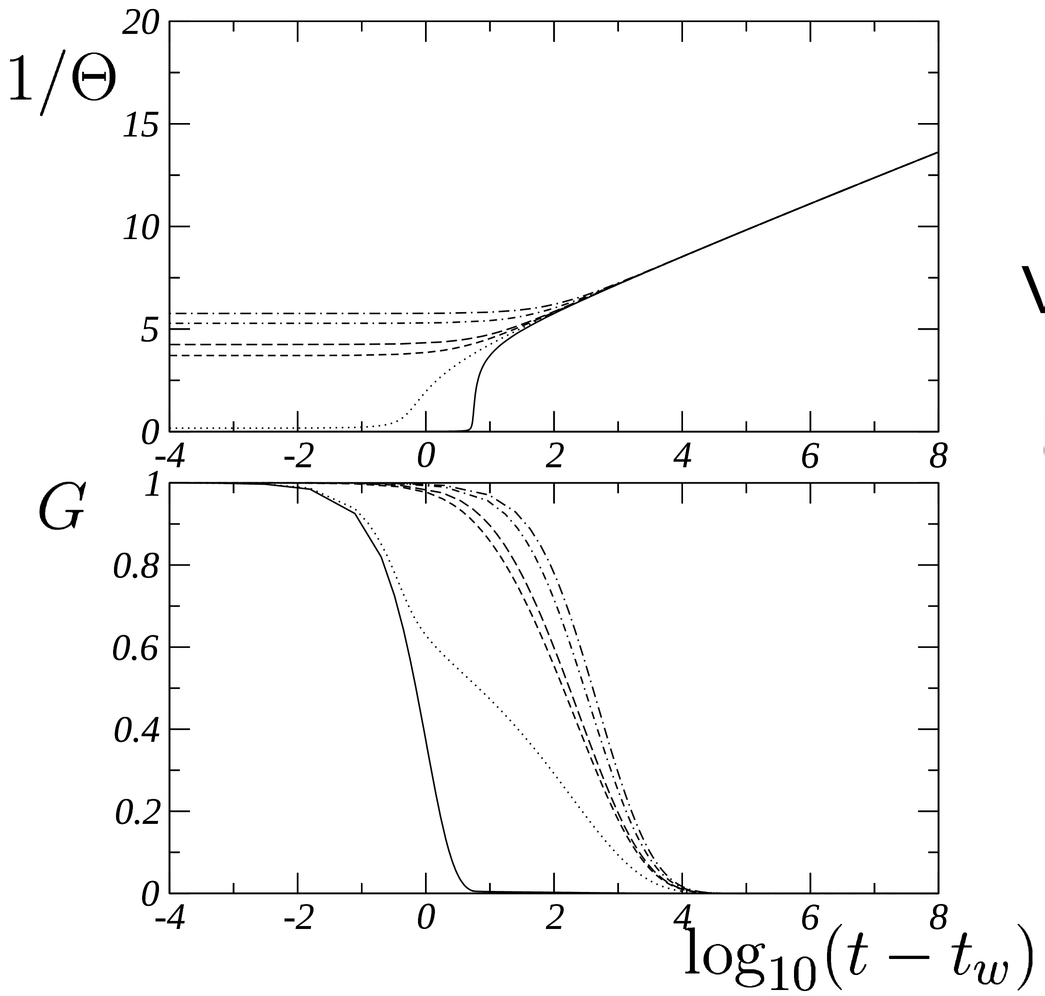
Stress relaxation



Varying E_0/E_1

- Crossover to KWW relaxation

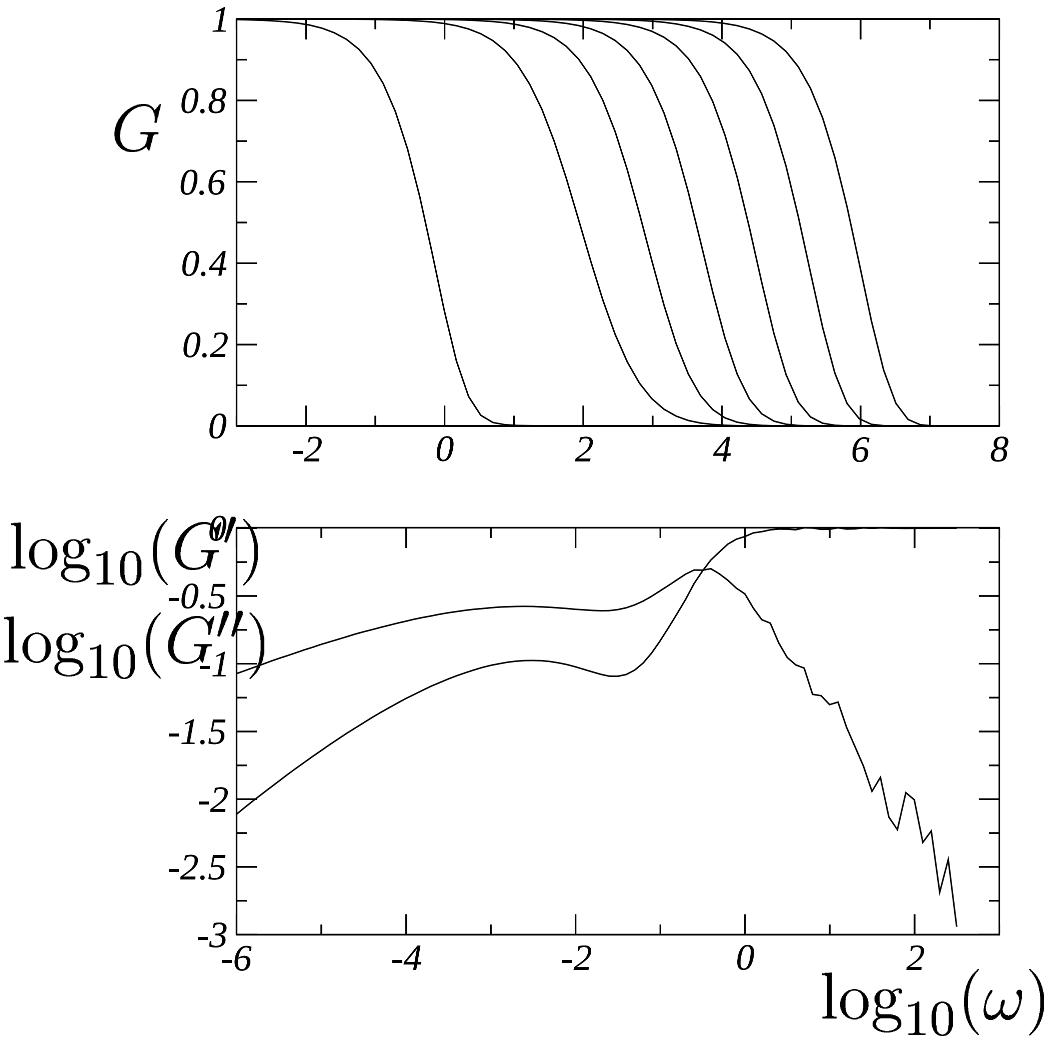
Stress relaxation



Varying t_w

- Crossover to KWW relaxation

Stress relaxation



- Crossover to KWW relaxation
- Aging exponent $\alpha = 1 - \beta$

Steady state

- High temperature: viscous liquid (Arrhenius)
- Low temperature:

$$\sigma = \frac{\dot{\gamma}^n}{E_0} \left(\frac{1}{E_0 E_1} \right)^{\frac{n-1}{2}}$$

with, $n = \frac{\kappa - 1}{\kappa + 1}$

- with STZ theory:

$$\dot{\gamma} = E_1 \left(\frac{E_0}{E_1} \right)^{\frac{\kappa}{\kappa - 1}} \frac{1}{\sigma} \left(\sigma^2 - 1 \right)^{\frac{\kappa}{\kappa - 1}} \quad .$$

Illustration: SFA

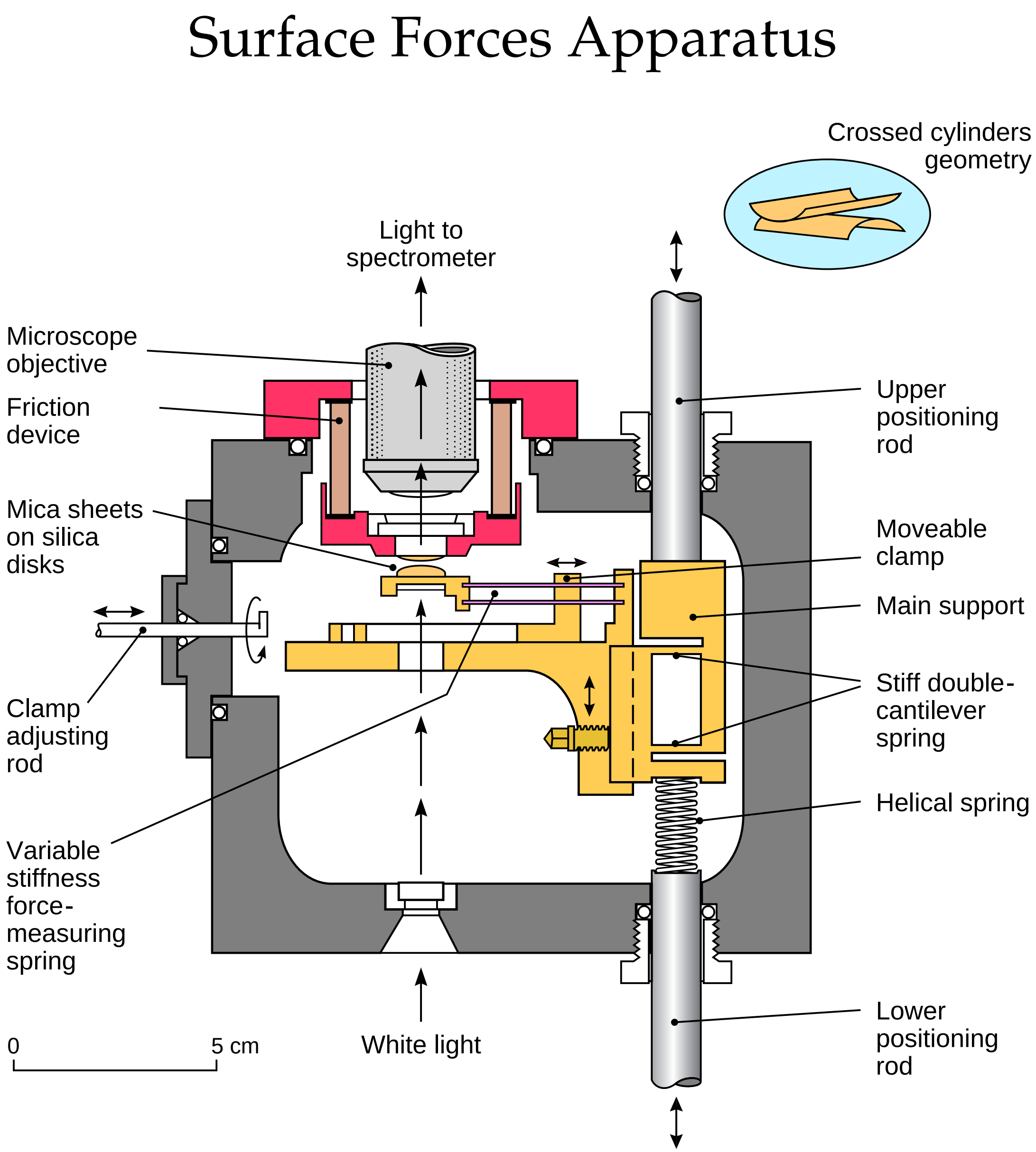
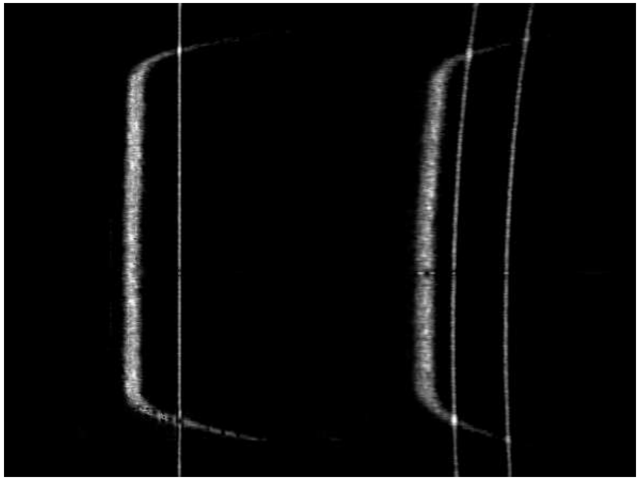
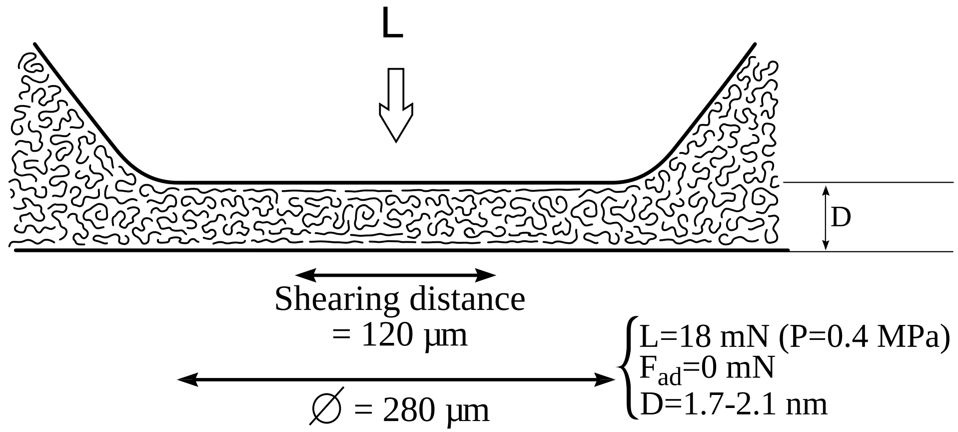
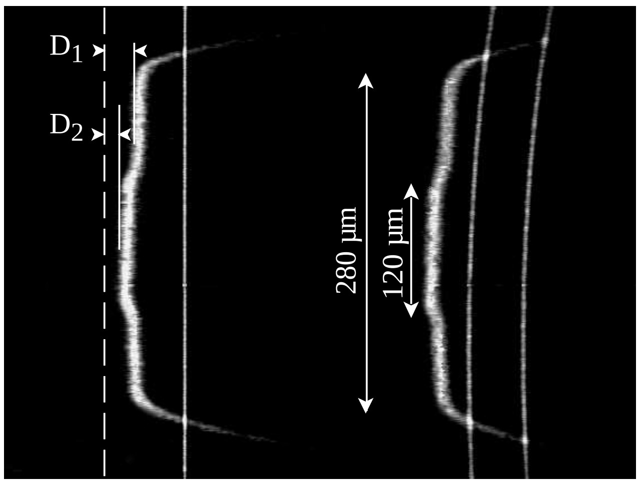


Illustration: SFA

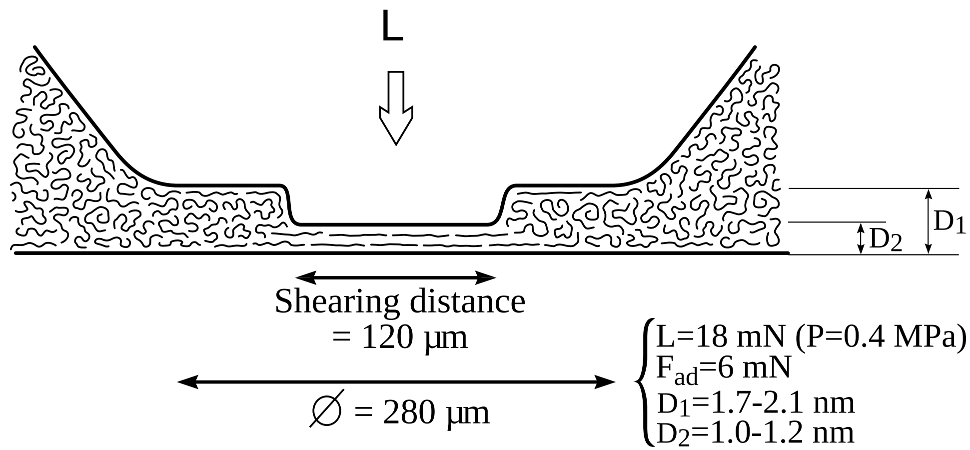


T ≃ 26 °C

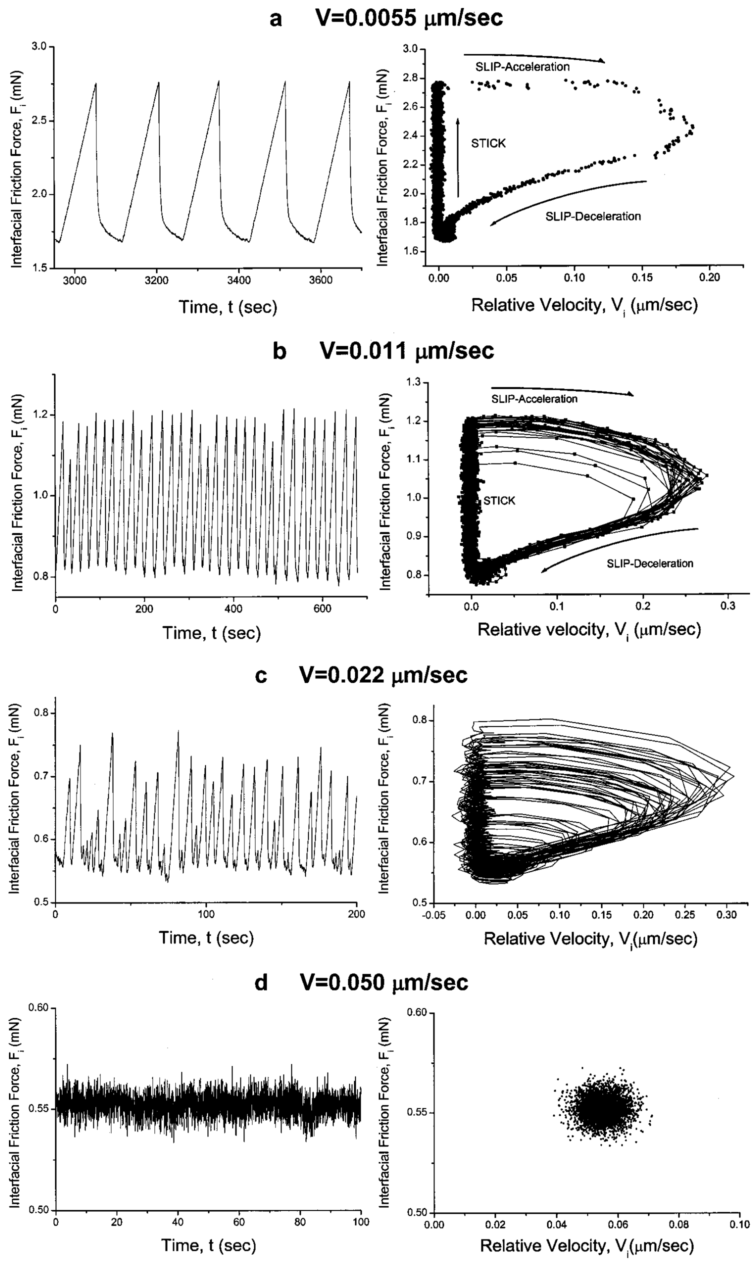




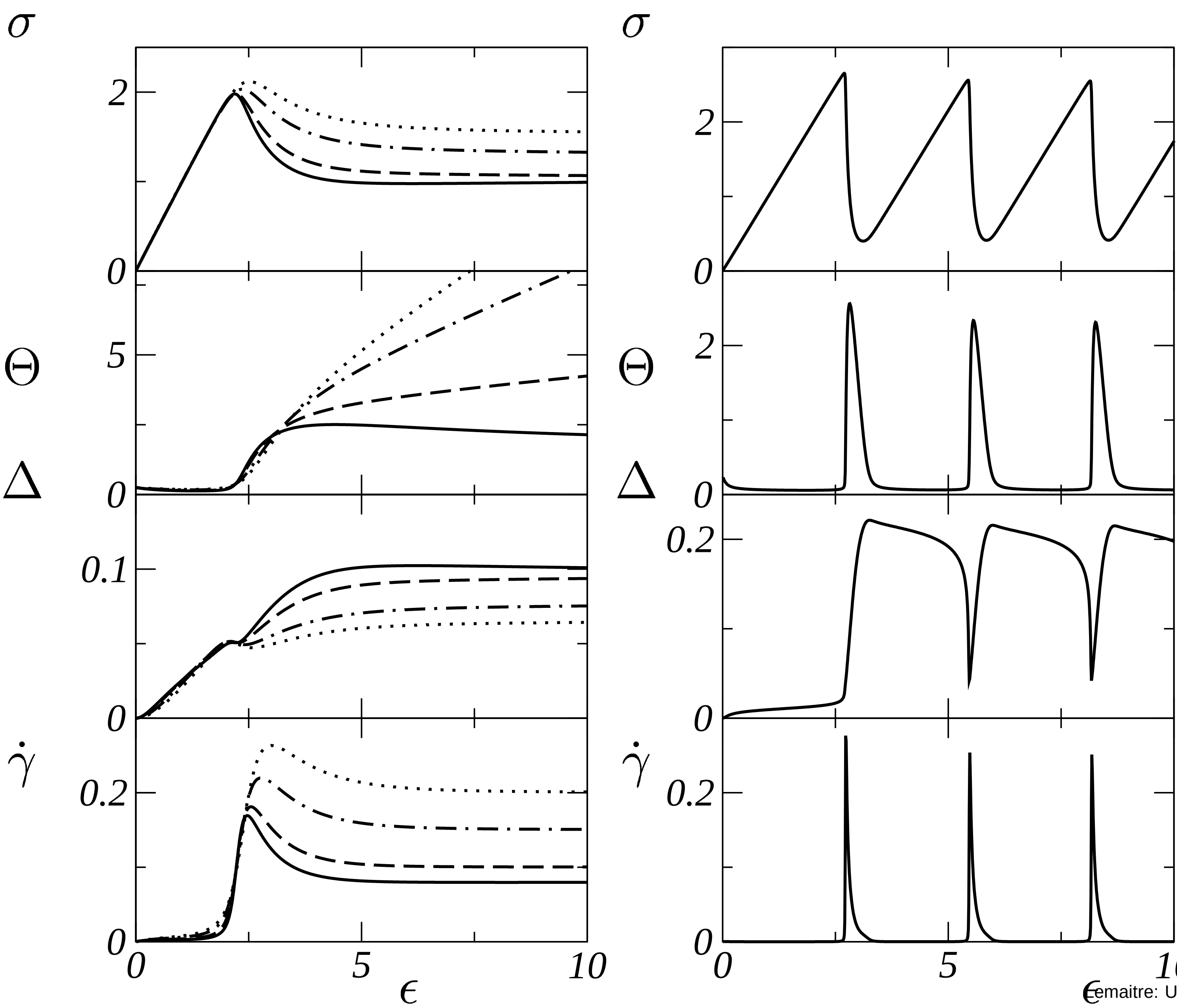
T = 15 °C



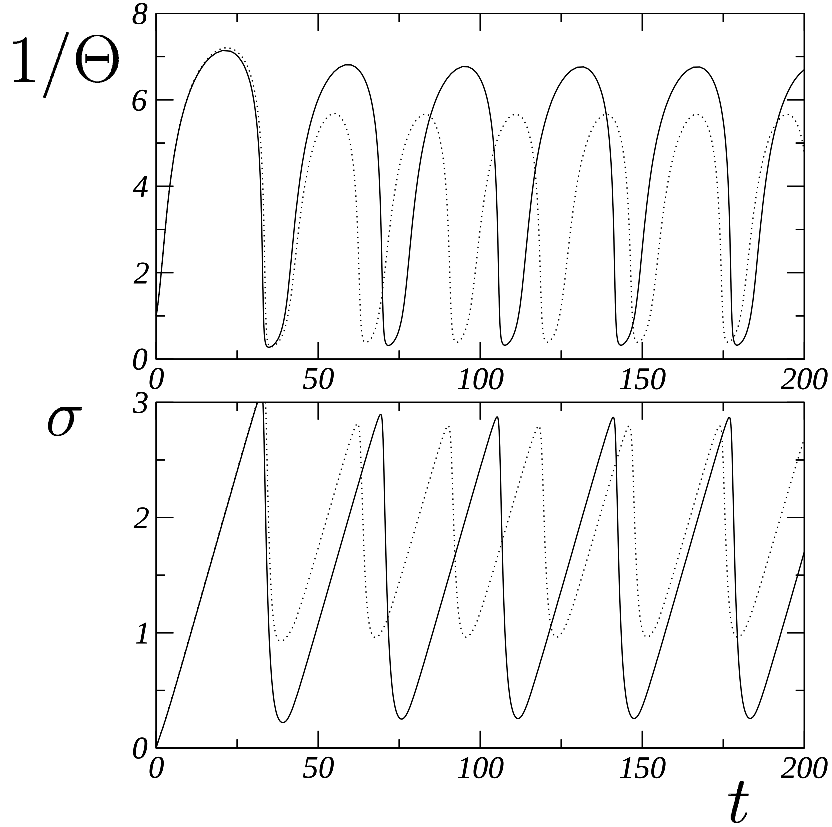
Stick-slip transition



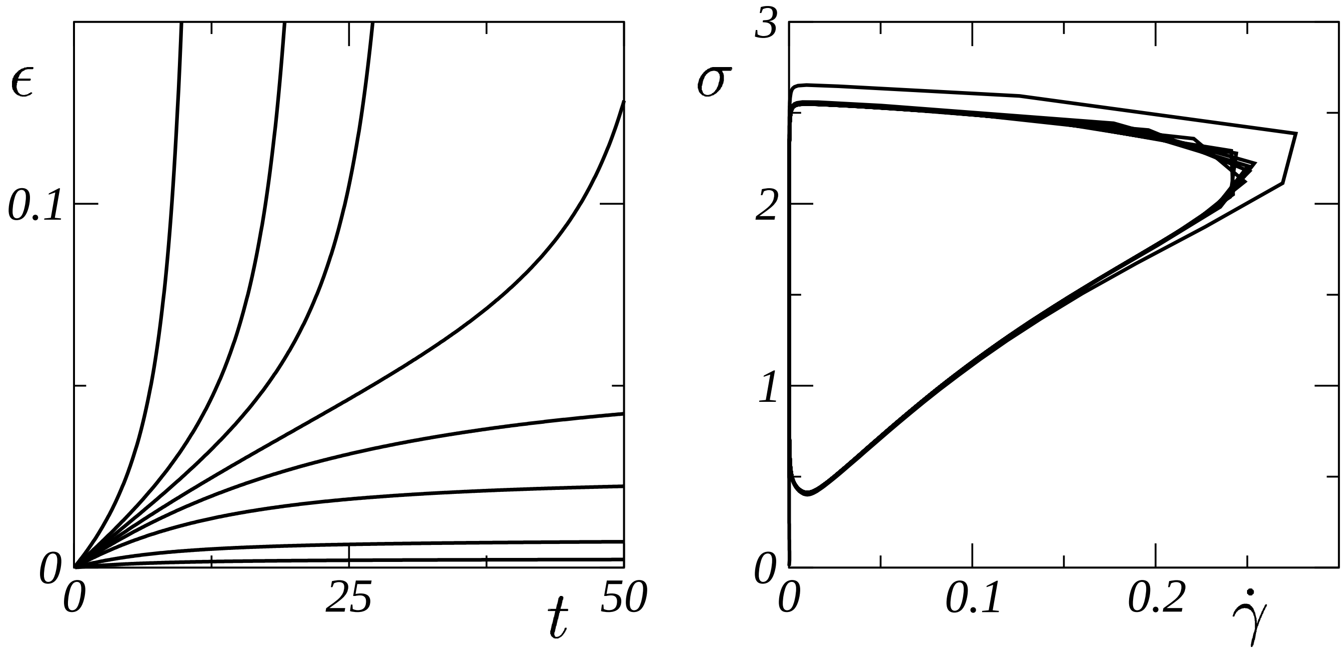
Transient dynamics



Stickslip



Creep test



Conclusion

Summary:

- Crossover between viscous liquid and glassy material
- KWV relaxation of stress β, aging α
- Power law rheology n
- all exponent related to κ

Questions:

- Boundary lubrication: Stick-slip instability
- Dilatancy in granular materials
- Relation to rate-and-state laws and relevance in earthquake dynamics
- Dynamical nature of the glass transition?