Long-ranged elastic stresses and their consequences for the mechanical response of amorphous solids

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Overview

- I) Elasticity
 - a) The Eshelby problem
 - b) Affinity and non-affinity
 - Strains and stresses
 - Homogeneous response Born-Huang
 - Non-affine contribution to elasticity
- II) Plasticity
 - a) The onset of failure
 - b) Predictors for plasticity
 - c) Avalanches

The Eshelby problem





Eshelby (1957): the effect of the transformation can be modeled by forces lying at the boundary

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Picard et al, EPJE, 15, 371 (2004)

$$\mu \Delta \vec{u} - \nabla p = \sum_{i} \vec{f}_{i} \delta \left(\vec{r} - \vec{r}_{i} \right)$$



Dipolar strength: $f a = \mu a^2 \Delta \epsilon_0$

The Eshelby problem



Eshelby (1957): the effect of the transformation can be modeled by forces lying at the boundary

Picard et al, EPJE, 15, 371 (2004)

$$\mu \Delta \vec{u} - \nabla p = \sum_{i} \vec{f}_{i} \delta \left(\vec{r} - \vec{r}_{i} \right)$$





A transforming zone is embedded in an elastic medium

Size-dependence of Lamé constants





Tanguy et al, PRB 66, 174205 (2002)

Example: simple shear



Example: simple shear



The Green-Saint-Venant strain tensor

Barron and Klein, Proc. Phys. Soc, 85, 523 (1965)

Stress tensors

Lagrangian

2nd Piola-Kirchhoff stress tensor



Cauchy stress

Homogeneous deformation



 ${oldsymbol{\mathcal{Y}}_0}$ $\underline{r_i}({oldsymbol{\mathcal{Y}}_0})$

Homogeneous deformation



 $\underline{\underline{F.}} \underline{\underline{r}}_i(\boldsymbol{\gamma}_0)$









Non-affine displacements

Lemaître *et al*, J. Stat. Phys. **123**, 415 (2006)

$$\Xi_{j} = -\frac{\partial^{2} U}{\partial \gamma \partial r_{j}} = \frac{\partial F_{j}}{\partial \gamma}$$



Non-affine displacements

Lemaître *et al*, J. Stat. Phys. **123**, 415 (2006)

$$\frac{\mathrm{d} r}{\mathrm{d} \gamma} = H^{-1} \cdot \Xi$$

$$\Xi_{j} = -\frac{\partial^{2} U}{\partial \gamma \partial r_{j}} = \frac{\partial F_{j}}{\partial \gamma}$$





Amorphous materials are, well... amorphous

In crystals

defects = dislocations (Volterra, 1930; SEM, 1960)



Interaction and motion understoon (Peierls, Nabarro, Friedel, 1950's)

Dislocation dynamics in computer codes since the 1980's

In disordered materials

No topological order => defects?



What are the elementary mechanisms of deformation?

How can we up-scale the dynamics?

Glassy solids



Plasticity

We are in the world of hard glasses, characterized by flow curves



Fig. 2. Constant true strain rate tests on quenched PMMA at 296 and 323 K.

PMMA, uniaxial tension (Hasan & Boyce, 1997)



(Johnson, Caltech)

Depending on loading conditions:

- Fracture
- Localization
- Homogeneous flow

Shear Localization in metallic glasses







Localization in soft glasses

Bubble Rafts (Dennin *et al.*, 2004)

Chocolate

0.004

(Coussot et al.)

Granular pastes

(Barentin et al., 2003)







velocity





Rheology

Find the odd one...



particles (Ballauff *et al*, 2005) We u

We use the language of soft matter

Deformation map for a metallic glass



Mechanisms of localization?



$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) \boldsymbol{\sigma} - (\nabla \mathbf{v}^{\dagger} \cdot \boldsymbol{\sigma} + \boldsymbol{\sigma} \cdot \nabla \mathbf{v}) = G(\rho) \left(\nabla \mathbf{v}^{\dagger} + \nabla \mathbf{v}\right) - \frac{1}{\tau(\rho)} \boldsymbol{\sigma}$$

Kawasaki, Tanaka (2009)

Shear transformations

Ali Argon (1979): Deformation due to local "shear transformations"





Michael Dennin





$$\propto 2\Delta\epsilon_0\omega_0 \exp\left(-\frac{\Delta G_m}{kT}\right) \left(\frac{\sigma\Omega_0}{kT}\right)$$
 for small σ

but no yield stress....

Mean-field theories

Free-volume theory (Spaepen, 1977)

 $\dot{y} = \Delta \epsilon_0 e^{-v_0 / v_f} (R_+ - R_-)$ $v_f =$ free-volume, varies with time

STZ theory (Falk & Langer, 1998)

 $\dot{y} = \Delta \epsilon_0 (R_+ n_+ - R_n)$ $n_{\pm} =$ "zone" densities, varies with time density of defects $\propto e^{-1/\chi}$ with χ a dynamical "effective temperature"

SGR theory (Sollich, 1998)

$$\frac{\partial P}{\partial t} = -\dot{y}\frac{\partial P}{\partial l} - \Gamma_0 e^{-(E - \frac{1}{2}kl^2)/x} P + \Gamma(t)\rho(E)\delta(l)$$

P = distribution of barrier energies (from Bouchaud's trap model)

x = effective temperature, fixed, interpreted as due to "noise" $\sigma = k \langle l \rangle_P$

What are the mechanisms of plastic deformation?

- Plasticity results from the accumulation of local flips, yet:
 - what triggers them?
 - where do they occur?
- Some areas of space should be more susceptible to shearing:
 - what are they? zones? defects? fertile sites?
- Mean-field theories
 - treat flow-events (flips) as independent
 - activation process?
 - how to explain that \exists plastic activity at low T? => effective T

Elastic models

Bulatov & Argon J. Non Cryst. Sol. 172-174, 876 (1994)





Baret *et al* PRL 89, 195506 (2002) Picard *et al* PRE 71, 010501 (2005)

Numerics are cool, specifically at T=0



The typical LJ time unit: $\tau_{LJ} \sim 10^{-13} \, \mathrm{s}$

Simulations can access: $10^5 \tau_{LJ} \sim 10^{-8} \, \mathrm{s}$ To reach 100% strain: $\dot{\chi} \sim 10^8 \, \mathrm{s}^{-1}$

Low temperature glass:

• As soon as $T < T_g$ a glass usually lies near local minima (inherent structures):



• Strain biases landscape (Malandro and Lacks 98):



Elastic segment: system follows an energy minimum; reversible.

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Elastic segment: system follows an Plastic event: local minimum energy minimum; reversible. annhilates; irreversible.
Potential Energy Perspective

• Strain biases landscape (Malandro and Lacks 98):

Elastic segment: system follows an Plastic event: local minimum energy minimum; reversible. Plastic event: local minimum annhilates; irreversible.

Plastic Step

Brillouin 1904:

Finite yield stress \Rightarrow finite dissipation for vanishing γ As $\gamma \nearrow$, periods of adiabatic adaption (shifted equilibrium) interspeded with fast instability events

Yield stress = signature of multistability

Events occur at spinodals in stress-biased landscape

What is the nature of elementary events?

AQS simulations

$$\dot{\epsilon}_{aging}^{-1} \ll \dot{\epsilon} \ll \tau_{relax}^{-1}$$

Athermal, quasi-static protocol:
$$T = 0$$
 $\dot{y} \rightarrow 0$

- Minimize energy
- Apply a small increment of strain (homogeneously)

Τ

- Repeat

 $\langle \sigma \rangle$

 σ

<σ>



Focus on steady state

C. Maloney and AL, PRL 93, 016001 (2004); PRE 74, 016118 (2006)

Onset of a plastic event



C. Maloney et al, PRL 93, 195501 (2004)

 $\sigma \sim \mu_{\infty}(\gamma - \gamma_0) - A \sqrt{\gamma_c} - \gamma$

$$\mu \sim -A/\sqrt{\gamma_c - \gamma}$$

 $\frac{\mathrm{d} r}{\mathrm{d} \gamma} \!\rightarrow\! \infty$

Dynamics of eigenvalues

Demkowicz and Argon, PRB 72, 255206 (2005)



Exact expression for non-affine field PRL 93, 195501 (2004); JSP 123, 415 (2006)

$$\frac{\mathrm{d}r}{\mathrm{d}\gamma} = H^{-1} \cdot E \qquad H_{ij} = \frac{\partial^2 U}{\partial r_i \partial r_j} \qquad E_j = \frac{\partial^2 U}{\partial \gamma \partial r_j} = \frac{\partial F_j}{\partial \gamma}$$

2

Near threshold, the non-affine field ~ the lowest mode

Are flips actually analogous to Eshelby transformations? Near threshold, the non-affine field ~ the lowest mode



PRE 74, 016118 (2006)



$$\vec{u} = \frac{2 a^2 \Delta \epsilon_0}{\pi} \frac{x y}{r^4} \vec{r}$$
$$\sigma_{xy} = \frac{2 \mu a^2 \Delta \epsilon_0}{\pi} \frac{\cos(4\theta)}{r^2}$$

Predicting plastic events



A typical plastic event











































During a plastic event



A plastic event is an avalanche







Distribution of event sizes in 2D



E. Lerner and I. Procaccia, PRE 79, 066109 (2009)

 $\Delta E \sim L^{\beta}$, $\beta = 0.74$

C. Maloney and AL, PRL 93, 016001 (2004); PRE 74, 016118 (2006) $\Delta E \sim L$

Scaled stress drop distribution

Expect: $\Delta \sigma \sim \mu a/L$



Distribution of event sizes in 3D



Simulations of $Mg_{0.85}Cu_{0.15}$ with LE boundary conditions

Collect data on: - stress drop - energy drop



Partial conclusion

- Elementary quadrupolar transformations can be observed at the onset of a plastic event...
- ...but they are difficult to isolate at later stages
- A plastic event is a complex process: an avalanche
 - power-law distribution of avalanche sizes
 - size of largest events determined by system size
- Questions:
 - What are the mechanisms of avalanche dynamics?
 - What determines the scalings observed?

A short detour along elastic branches



Elastic response occurs when the system reversibly follows a local minimum in potential energy landscape.

Langer, Liu (1997); Tanguy *et al*, PRB **66**, 174205 (2002): small-strain elastic response involves non-affine displacement fields, which alter the elastic moduli.

Dynamics of soft zones


Can we actually speak of interacting zones?

A.L. and Ch. Caroli, PRE 76, 036104 (2007)

 $\gamma = 5.56 \& 5.58 \%$



Can we actually speak of interacting zones? A.L. and Ch. Caroli, PRE 76, 036104 (2007)

 $\gamma = 2.69 \& 2.70 \%$



What is the avalanche mechanism?

- Zones advected towards their thresholds
- progressively softening near threshold
- each flip produces a measurable Eshelby field
- this alters the internal strain of nearby zones and may trigger secondary events



Remark:

Real life is not AQS!

Conclusion & remarks

- Focus here on the elementary, small scale, mechanisms of plastic deformation: valid for homogeneous materials
- Should we expect to see the same phenomenology at finite \dot{Y} ? finite T ?
 - Does this give rise to avalanche behavior?
 - With which correlation length?
- If so, how can we evidence it?
 - Stress fluctuations?
 - Something else?
- Relevance to e.g. localization? What is the appropriate scale of description?





Schall, Spaepen & Weitz (2007)

Finite strain-rate simulations



$$L = 160$$

 $\dot{y} = 5.10^{-5}$

The stress field



Stress noise



Decomposing the plastic response in terms of flips

Each flips releases on average:

a strain $\Delta \epsilon_0$

in a region of size a^2

In steady state, over a large strain interval:

$$N_{f}(\Delta \gamma) \Delta \epsilon_{0} a^{2} = \Delta \gamma L^{2}$$

Average number of flips

Each Eshelby flip induces:

$$\vec{u} = \frac{2a^2 \Delta \epsilon_0}{\pi} \frac{x y}{r^4} \vec{r}$$

$$\sigma_{xy} = \frac{2\mu a^2 \Delta \epsilon_0}{\pi} \frac{\cos(4\theta)}{r^2}$$

$$\Delta \overline{\sigma_{xy}} = \frac{2\mu a^2 \Delta \epsilon_0}{L^2}$$

$$N_f(\Delta \gamma) = \frac{L^2 \Delta \gamma}{a^2 \Delta \epsilon_0}$$

$$\Delta \gamma = \dot{\gamma} \Delta t$$

$$N_f(\Delta t) = \frac{L^2 \dot{y} \Delta t}{a^2 \Delta \epsilon_0}$$



• If events = independent flips

Event duration = flip duration (acoustic radiative damping) $\tau_{flip} \sim a/c_s$

QS regime $\dot{y} \ll \dot{y}_c \approx \Delta \epsilon_0 a c_s / L^2$ Atomic glass: $a \sim 1 \text{ nm}$ $L \sim 1 \text{ mm} \rightarrow \dot{y}_c \sim 4.10^{-2} \text{ s}^{-1}$

• If events = avalanches of n flips duration ~ travel delay of acoustic signals Most pessimistic: travel n times across L $\Rightarrow \tau_{av} \approx n L/c_s$

$$\langle \Delta t_{av} \rangle^{-1}$$
 = avalanche rate = flip rate / n = $\langle \Delta t_{flip} \rangle^{-1} / n$
QS regime $\dot{y} \ll \dot{y}_c a / L$ Extremely small??

Stress and stress fluctuations

20201.2 σ 18 18 16 16 14 12 •--• L = 10 14 - L = 20→ L = 40 10 0.8 -1L = 800.0011e-05 0.00010.01⊲ L = 160 12 10 0.6^{L}_{0} 0.005 0.01 0.002 0.004 0.006 0.008 0.01 Herschel-Bulkley rheology The stress fluctuations: $\sigma = \sigma_y + A\sqrt{\dot{y}}$ - converge to QS values when $\dot{\gamma}
ightarrow 0$ - present normal statistics when $\dot{y} > 10^{-3}$

PRL 103, 065501 (2009)

Plastic events at finite strain-rate?

Quasi-static simulations:

Plastic events = discontinuous drops = avalanches

At finite strain rates:

Flips and avalanches have a finite duration



Remark about: Hentschel *et al*, PRL (2010)

The strain field

From the dynamics of non-affine velocity field, we saw: Flips retain same nature Acoustic propagation of long range signals observable

So, the Eshelby picture seems valid

But:

- Are flips correlated?
- Are there avalanches?

Deformation maps

$$\epsilon_{xy}(\vec{r})$$



Transverse diffusion in AQS

Avalanches are directional and:

 $l_{\rm av} \sim L$ (2D) $\sim L^{3/2}$ (3D Bailey et al)







σ

Particle displacement distribution in AQS



 $\omega = \partial_y u_x - \partial_x u_y$

Maloney & Robbins, J. Phys. Cond. Mat. 20, 244128 (2008)

Transverse diffusion at finite strain rate

Track the transverse motion of particles:



Assume flips independent

Over a large strain interval:

$$\Delta y_i = \sum_f u_y(\vec{r}_i - \vec{r}_f)$$

 $\Rightarrow \langle \Delta y^2 \rangle = N_f(\Delta \gamma) \langle u_y^2 \rangle$

$$N_f(\Delta \gamma) = \frac{L^2 \Delta \gamma}{a^2 \Delta \epsilon_0}$$

One Eshelby flip induces:

$$\vec{u} = \frac{2a^2 \Delta \epsilon_0}{\pi} \frac{x y}{r^4} \vec{r}$$

$$\sigma_{xy} = \frac{2\mu a^2 \Delta \epsilon_0}{\pi} \frac{\cos(4\theta)}{r^2}$$

$$\Delta \overline{\sigma_{xy}} = \frac{2\mu a^2 \Delta \epsilon_0}{L^2}$$

$$\langle u_y^2 \rangle = \frac{1}{L^2} \int_a^L u_y^2 \mathrm{d} \vec{r} = \frac{a^4 \Delta \epsilon_0^2}{4 \pi} \ln (L/a) \checkmark$$

$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} = \frac{a^2 \Delta \epsilon_0}{4\pi} \ln(L/a)$$

Transverse diffusion at finite strain rate

$$\frac{\langle \Delta y^2 \rangle}{\Delta y} = \frac{a^2 \Delta \epsilon_0}{4\pi} \ln(L/a)$$

$$\Rightarrow a^2 \Delta \epsilon_0 \sim 1 \quad \begin{cases} \Delta \epsilon_0 \sim 4\% \\ a \sim 5 \end{cases}$$

 \hat{D} 3 2 50 100 150 100 10

Very high strain rates $(\dot{\gamma} = 10^{-2})$

~ no flip correlations

Decreasing \dot{y} : growing departure from ln*L* = growing correlation length (avalanche size)?

Assume events = correlated flips = linear avalanches



Deformation maps

 $\epsilon_{xy}(\vec{r})$

Assume events = correlated flips = linear avalanches

Avalanches:

- linear extension: l (= flip correlation length)
- density of flips in an avalanche, $\boldsymbol{\nu}$ constant

 $N_{\rm av}(\Delta \gamma) = N_f(\Delta \gamma)/\nu l$



$$\begin{split} \langle \Delta y^2 \rangle_{\text{av}} &= v^2 \int_0^l \int_0^l \mathrm{d} s \, \mathrm{d} s \, ' \langle u_y(\vec{r} - \vec{r}_s) u_y(\vec{r} - \vec{r}_{s'}) \rangle \\ &= \frac{a^4 \Delta \epsilon_0^2 v^2}{2\pi} \left(\frac{l}{L}\right)^2 \ln(L/l) \\ &\equiv \langle u_y^2 \rangle_A \end{split}$$

Particles diffusion $\Delta y_i = \sum_A u_y^A (\vec{r}_i - \vec{r}_A)$ Assuming avalanches independent: $\langle \Delta y^2 \rangle = N_A (\Delta \gamma) \langle u_y^2 \rangle_A$

$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} = \frac{a^2 \Delta \epsilon_0}{4\pi} v l \ln(L/l)$$

Transverse diffusion at finite strain rate

$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} = \frac{a^2 \Delta \epsilon_0}{4\pi} v l \ln(L/l)$$



Large $\dot{y} \Rightarrow l \sim a$ $\widehat{D} \sim \ln L$ $\dot{y} \rightarrow 0 \Rightarrow l \sim L$ $\widehat{D} \sim L$ QS regime

In between, evaluate $l(\dot{y})$?

What determines the avalanche size?

Each zone receives noise = elastic signals

Rate
$$R_{\text{flip}} = \frac{L^2 \dot{y}}{a^2 \Delta \epsilon_0}$$

Autocorrelation time $\tau_{\text{flip}} = \frac{a}{c_s}$

Decompose noise into:

- near-field signals from sources r < l

rate $R_l = R_{\text{flip}} l^2 / L^2$, strain amplitude $\Delta \gamma_{\text{near}} \ge a^2 \Delta \epsilon_0 / l^2$

- all others (r > l) = background

rate $R'_l = R_{\text{flip}} - R_l \simeq R_{\text{flip}}$ $(l \ll L)$

- **Ansatz:** *l* = correlation length iff near-field signals = shot noise standing out of incoherent background
 - \Rightarrow (i) no overlap of near signals \Rightarrow $R_l < \tau_{flip}^{-1}$

(ii) $\Delta \gamma_{\text{near}} \ge \beta$ background fluctuation accumulated over τ_{flip} :

$$\overline{\Delta \gamma^2} \sim \dot{\gamma} \tau_{\rm flip} (a^2 \Delta \epsilon_0 / l^2)$$

(i) & (ii)
$$\Rightarrow l \sim \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$$

$$\widehat{D} = \frac{a^2 \Delta \epsilon_0^2}{2\pi} v l \ln (L/l)$$
$$l \sim \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{flip}}$$
$$\widehat{D} / L \sim f(L \sqrt{\dot{\gamma}})$$





Crossover from dynamically controlled correlation length $l \sim \dot{y}^{-1/2}$ to QS regime $l \sim L$

For

$$\dot{y} \sim \dot{y}_{co} \approx a^2 \Delta \epsilon_0 / \tau_{flip} L^2$$

Inferences

• Extension to 3D $l(\dot{y}) \sim a (\Delta \epsilon_0 / \dot{y} \tau_{flip})^{1/3}$ \Rightarrow For atomic glass, with $\tau_{LJ} \sim 10^{-13} \sec$, $a \sim 1 \text{ nm}$, $\Delta \epsilon_0 \sim 5\%$

For
$$\dot{y} \leq 1 \sec^{-1}$$
 , $l \geq 10 \,\mu\,\mathrm{m}$

• 2D flow curve $\sigma(\dot{y})$

guess:
$$\sigma - \sigma_y \approx \mu \dot{\gamma} \tau_{av}$$

event duration: $\tau_{av} \sim l/c_s$ (domino-like avalanches)

$$\Rightarrow \sigma = \sigma_y + C \sqrt{\dot{y}}$$
$$C = \frac{\mu}{c_s} a^2 \frac{\Delta \epsilon_0}{\tau} \approx 13$$



Conclusion

Question was:

Is QS phenomenology (long-range couplings \rightarrow avalanches) relevant to finite \dot{y} ?

Our answer is:

YES.

As
$$\dot{\gamma}$$
 : crossover from $l \sim L$ to $l \sim \dot{\gamma}^{-1/2}$

(increasing flip rate destroys coherence of elastic signals)

Flow curve controlled by avalanche dynamics

Next: - finite temperature

- 3D...