Poorly connected soft solids: dynamical processes, shear localization and yielding in colloidal gels

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Outline

- Colloidal gels and model gels
- Dynamical processes for restructuring at rest.
- Athermal deformation and yielding.
A colloidal gel *in silico*

- Molecular Dynamics
- $\sim 10^6$ particles
- $\Phi = 0.1$
- periodic boundaries

3-coordinated particle (cross-link)

2-coordinated particle (chain)

short-range attraction

+ chains with bending stiffness


Jader Colombo, Asaph Widmer-Cooper and EDG, *PRL* 2013

Lindström et al., *Soft Matter* 8, 3657 (2012)
Local density of nodes

J. Colombo, A. Widmer-Cooper and EDG, PRL 2013
Cooperative dynamics

$$\Phi_s(q, t + t_0) = \frac{1}{N} \sum_{j=1}^{N} e^{i \mathbf{q} \cdot [\mathbf{r}_j(t + t_0) - \mathbf{r}_j(t_0)]}$$

$$F_s(q, t) = \langle \Phi_s(q, t + t_0) \rangle_{t_0}$$

\[
\chi_4(t) = N \left[ \langle |\Phi_s(q, t + t_0)|^2 \rangle_{t_0} - \langle \Phi_s(q, t + t_0) \rangle_{t_0}^2 \right]
\]

J. Colombo, A. Widmer-Cooper and EDG, PRL 2013
J. Colombo and EDG, Soft Matter 2014
Iso-configurational analysis for gels

For the same initial configuration, draw momenta from Maxwell-Boltzmann and evolve for a prescribed $\tau^*$

Filter vibrations: constrain bonds and compute average position of every particle during a sufficiently long run

$p_i = \langle (r_i' - r_i)^2 \rangle_{\mathcal{C}'}$

propensity for displacement

$b_i = \langle n_i \rangle_{\mathcal{C}'}$

propensity for breaking
Bond-breaking events

J. Colombo, A. Widmer-Cooper and EDG, PRL 2013
Consequences of bond-breaking

J. Colombo, A. Widmer-Cooper and EDG, PRL 2013
Athermal, incremental strain

\[ r_i' = \Gamma \delta \gamma r_i \]
\[ \delta \gamma = 10^{-2} \]

\[ m \frac{d^2 r_i}{dt^2} = -\xi \frac{dr_i}{dt} - \nabla_{r_i} U \]

\[ \tau_0 = \xi \sigma^2 / \epsilon \]
\[ \dot{\gamma}_1 = 2 \cdot 10^{-5} \tau_0^{-1} \]
\[ \dot{\gamma}_2 = 10^{-4} \tau_0^{-1} \]
\[ \dot{\gamma}_3 = 10^{-3} \tau_0^{-1} \]

Aqueous colloidal suspension:

\[ \sigma \approx 100 \text{ nm} \]
\[ \epsilon \approx 10 k_B T \]
\[ \tau_0 \approx 10^{-4} \text{ s} \]

\[ n = 100 \]

\[ \dot{\gamma}_1 \approx 0.2 \text{s}^{-1} \]
\[ \dot{\gamma}_2 \approx 1.0 \text{s}^{-1} \]
\[ \dot{\gamma}_3 \approx 10 \text{s}^{-1} \]
Load curves
Stretching of the chains

\[ \theta_k \]
Stress localization

- Stiffening due to pulling of the bonds of completely stretched chains
- Stress concentrates in specific parts of the structure
- Yielding results from bond breaking in overstressed chains

\[
\sigma^i_{\alpha\beta}
\]
Bonds breaking & new bonds

- **σ_{xy}**
- **γ**

- **stress**
- **broken bonds**
- **newly formed bonds**

Graph showing the relationship between stress and bond breaking and formation.
Density fluctuations

- Formation of excess bonds under shear favors a densification in certain regions
- A region from which particles are depleted starts to develop
Shear localization

\[ d_n(y) = \frac{1}{M} \sum_{|y_{i,n} - y| < \Delta/2} (x_{i,n} - x_{i,n-1}) \]
Shear localization

See Divoux, Gibaud and Manneville experiments
Summary

Yielding due to breaking of a small fraction of bonds

Fewer new bonds & more homogeneous deformation

Pulling on the bonds of fully stretched chains & Stress Localization

Excess bonds enhance density fluctuations and favour shear localization

Bending rigidity of the chains & floppy modes

\[ \gamma_1 \]

\[ \gamma_2 \]
References

J. Colombo and EDG
Journal of Rheology 2014
Soft Matter 2014
J. Colombo, A. Widmer-Cooper and EDG, PRL 2013