Elasticity, Facilitation and Dynamic Heterogeneity in Glass Forming Liquids

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Ozawa and Biroli, arXiv:2209.08861, 2022
Glass

Snapshots have no feature

Low $T$ liquid

High $T$ liquid

$T_g$

Temperature $T$
Dynamical heterogeneity

Snapshot
Low $T$ liquid

Dynamics
Red: Mobile
Blue: Immobile

The mechanism of dynamical heterogeneity is unclear
Many theories and scenarios

- Thermodynamic scenarios
  Adam and Gibbs, JCP 1965
  Kirkpatrick, Thirumalai, and Wolyness, PRA 1989
  Bouchaud and Biroli, JCP 2004

- Dynamic facilitation
  Chandler and Garrahan, Annu. Rev. Phys. Chem. 2010
  Hedges, Jack, Garrahan, and Chandler, Science 2009

- Elasticity scenarios
  Dyre, RMP 2006
  Lemaitre, PRL 2014

- Geometrical considerations
  Tarjus, Kivelson, Nussinov, and Viot, J. Phys. Condens. Matter 2005
  Tanaka, Kawasaki, Shintani, and Watanabe, Nat. Mater 2010

- Etc..
Different approaches

Solid that flows
Dyre, RMP 2006
Lemaitre, PRL 2014

Viscous fluid

Majority of theories

Glass $T_g$

Liquid

Temperature $T$
Thermodynamic scenario

Relaxation time

\[ \tau_\alpha \sim e^{\frac{\xi \psi}{T}} \]

Adam and Gibbs, JCP 1965
Kirkpatrick, Thirumalai, and Wolyness, PRA 1989
Bouchaud and Biroli, JCP 2004

Cooperative rearranging region
Cooperative rearranging region is too small compared with dynamical heterogeneity
Plastic events induced by
- Thermal fluctuation
- Elastic interaction

Chacko, Landes, Biroli, Dauchot, Liu, and Reichman PRL 2021

Lerbinger, Barbot, Vandembroucq, and Patinet, PRL 2022

Cascade of events: Facilitation

Chandler and Garrahan, Annu. Rev. Phys. Chem. 2010
Molecular simulation

Elastoplastic model

Many variations

Nicolas, Ferrero, Martens, and Barrat, RMP 2018
Bulatov and Argon, Mod. Sim. 1994
Baret, Vandembroucq, and Roux, PRL 2002
Onuki, PRE 2003
Jagla, PRE 2007
Lin, Lerner, Rosso, and Wyart PNAS 2014
1) Local dynamics condition for local stress $\sigma_i$

i) $\sigma_i \leq \sigma_{i}^{th}$: Elastic (immobile)

ii) $\sigma_i > \sigma_{i}^{th}$: Plastic (mobile) with a stress drop $\sigma_i \rightarrow \sigma_i - \delta \sigma_i$

iii) Thermal fluctuation: Elastic $\rightarrow$ Plastic with probability $e^{-E(\sigma_i)/T}$

$E(\sigma_i) = (\sigma_{i}^{th} - \sigma_i)^{3/2}$

Ferrero, Martens, and Barrat, PRL 2014
Popovic, de Geus, Ji, and Wyart, PRE 2021
Lerbinger, Barbot, Vandembroucq, and Patinet, PRL 2022

2) Elastic interaction

$\sigma_j \rightarrow \sigma_j + g(r_{ij})\delta \sigma_i$

$g(r_{ij}) = \frac{\cos(4\theta)}{r_{ij}^2}$

Picard, Ajdari, Lequeux, and Bocquet, EPJE 2004

3) Repeat 1) - 2)
Movie

Mobile

Immobile
$N_{\text{corr}}$ : Size of dynamically correlated region

**Experiments**

Dalle-Ferrier, Thibierege, Alba-Simionesco, Berthier, Biroli, Bouchaud, Ladieu, L’Hote, and Tarjus, PRE 2007

Dauchot, Ladieu, and Royall, arXiv 2022
Mean-field theory

\[
\frac{\partial P(\sigma, t)}{\partial t} = \alpha \Gamma(t) \frac{\partial^2 P(\sigma, t)}{\partial \sigma^2} - \nu(\sigma, \sigma_c) P(\sigma, t) + \Gamma(t) y(\sigma)
\]

Magnitude of elastic interaction

\[
\alpha = \frac{1}{2} \sum_{j \neq i} \left( g(r_{ij}) \delta \sigma_j \right)^2
\]

\[
\tau_\alpha \approx \Gamma^{-1} \approx \tau_0 e^{\frac{E}{T}}
\]

Elasticity-induced facilitation