Cavitation instabilities in amorphous solids

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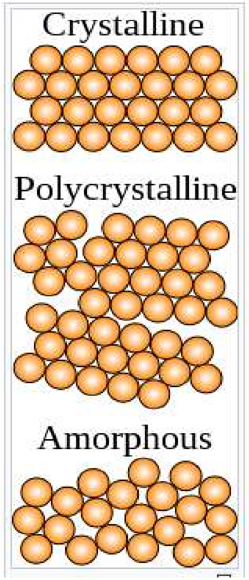
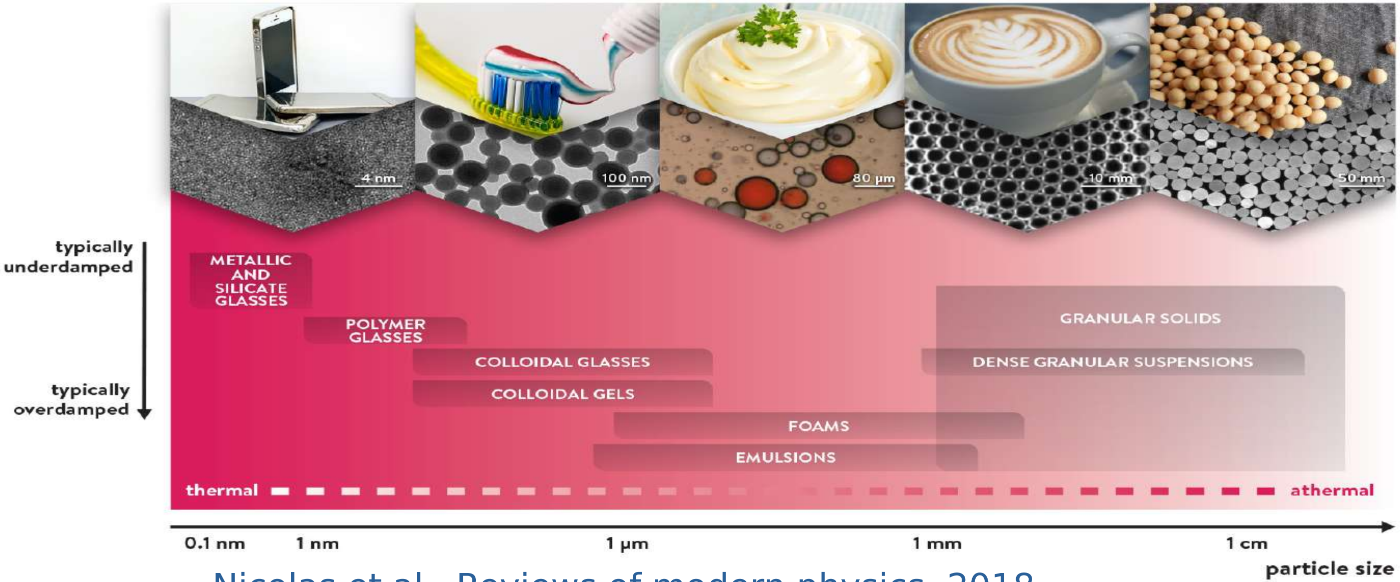
Introduction: amorphous solids

- **Amorphous solids lack long-range order**
- **They exist in diverse forms**



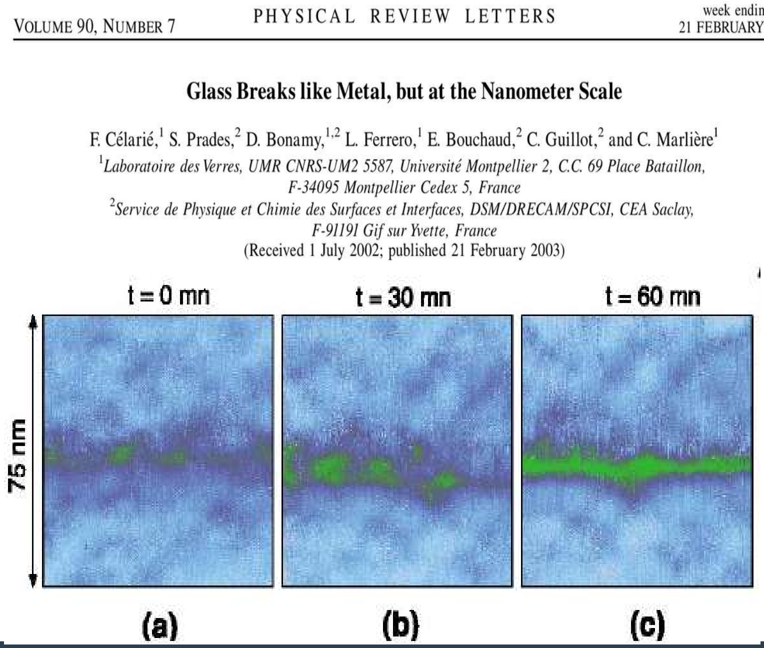
wikipedia



Nicolas et al., Reviews of modern physics, 2018

Introduction

- **Amorphous solids known to fracture via coalescence of small-cavities/voids**


VOLUME 90, NUMBER 7 PHYSICAL REVIEW LETTERS week ending 21 FEBRUARY 2003

Glass Breaks like Metal, but at the Nanometer Scale

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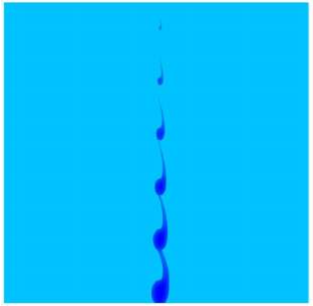
March, 2021




SCIENCE ADVANCES | RESEARCH ARTICLE

CONDENSED MATTER PHYSICS

Observation of cavitation governing fracture in glasses

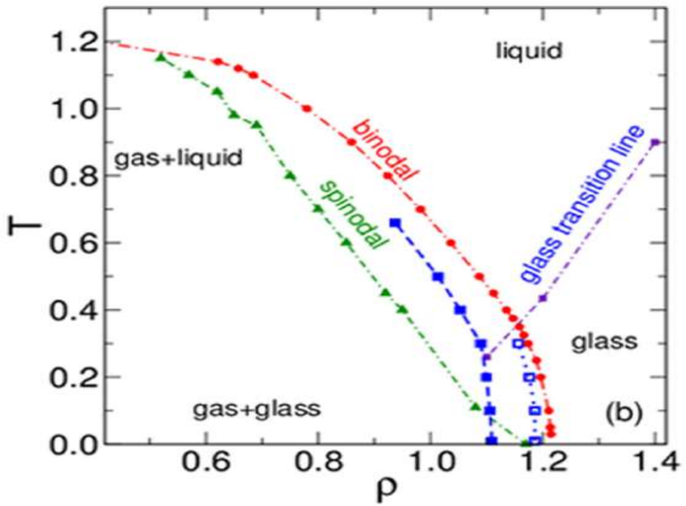
Lai-Quan Shen[1,2,3], Ji-Hao Yu[1,3], Xiao-Chang Tang[1,3], Bao-An Sun[1,2]*, Yan-Hui Liu[1,2,3], Hai-Yang Bai[1,2,3]*, Wei-Hua Wang[1,2,3]

Background: Numerical simulations

- **Intersection of glass-transition line with spinodal at finite temperature(Sastry, PRL, 1999)in the $T - \rho$ plane**

- **Mechanical instability below glass-transition temperatures due to gas-glass coexistence**

Phase diagram of attractive glass-forming system



Testard, Berthier & Kob, PRL, 2011

Outline

- **Cavitation instabilities in amorphous solids under uniform expansion**

  Umang A. Dattani, Smarajit Karmakar & Pinaki Chaudhuri. Phys. Rev. E 106, 055004, 2022.

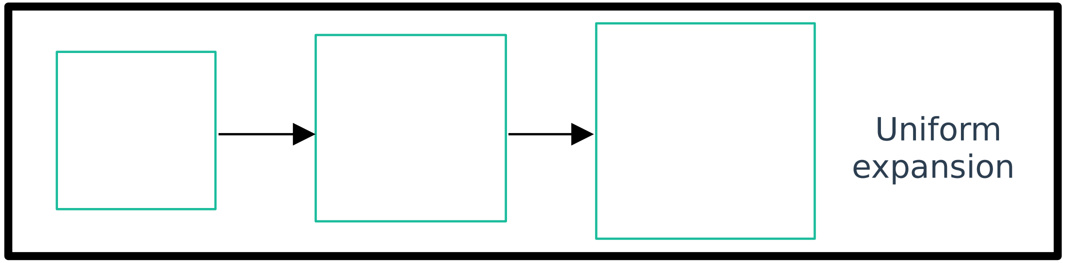
- **Cavitation instabilities in amorphous solids via secondary mechanical perturbations**

  Umang Dattani, Rishabh Sharma, Smarajit Karmakar & Pinaki Chaudhuri. arXiv: 2303.04529, March, 2023

Protocol: athermal quasistatic expansion

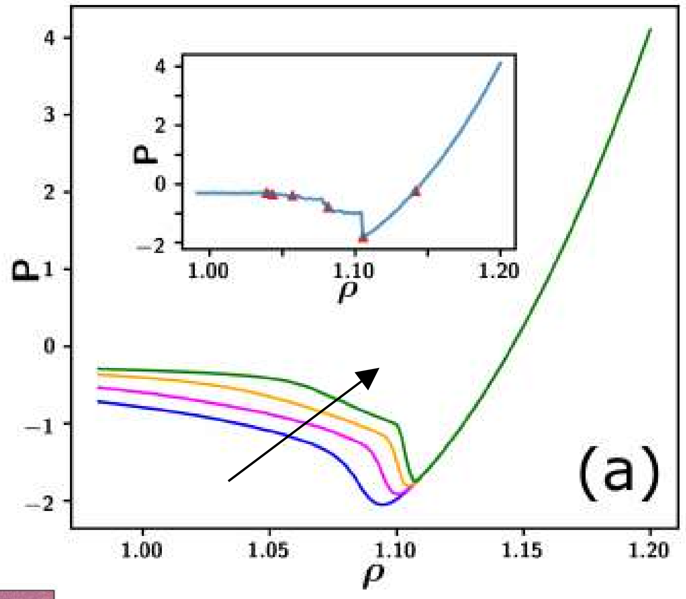
- **Initial states prepared by cooling a high temperature liquid (MD, 2D Lennard-Jones system)**

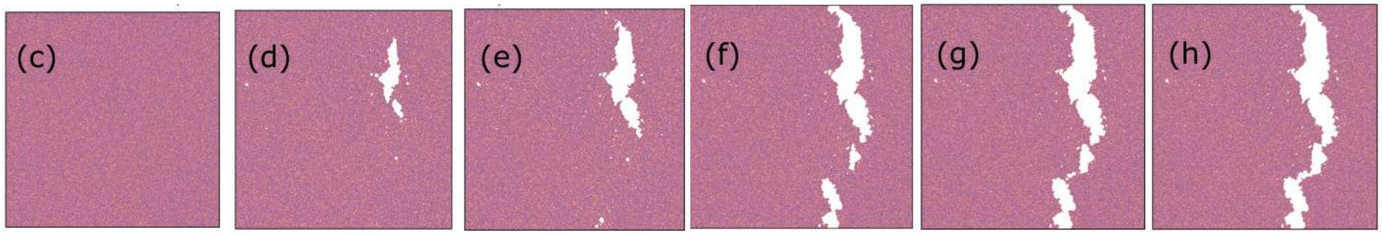
- **Protocol: apply a constant volume strain in each step of the simulation followed by energy minimization(conjugate gradient)**



Stress-strain curves

- On expansion pressure decreases, even goes negative
- A large pressure jump beyond a certain density
- Pressure jumps correspond to cavitation
- Cavities eventually merge and lead to complete fracture [(c)-(h)]



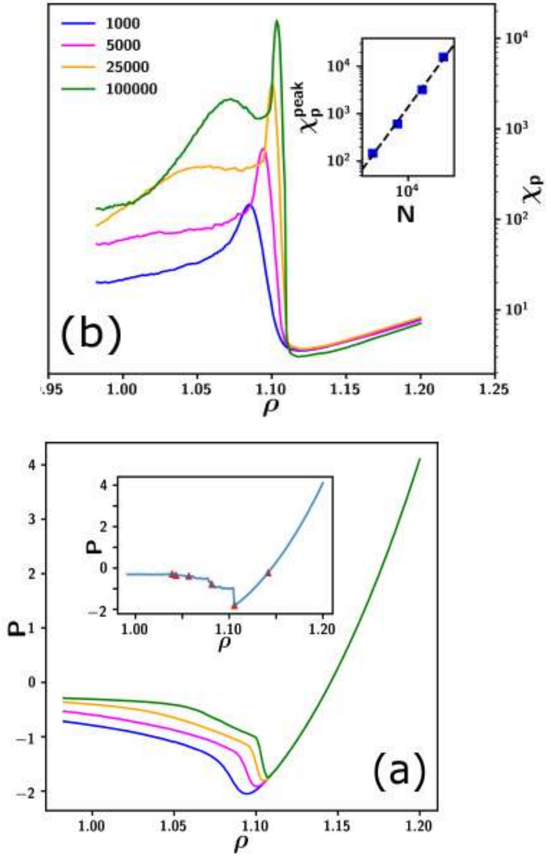


Pressure fluctuations

- **Ensemble fluctuations in pressure as function of density define a susceptibility** $\chi_p(\rho) = N\left(\langle P^2(\rho)\rangle - \langle P(\rho)\rangle^2\right)$

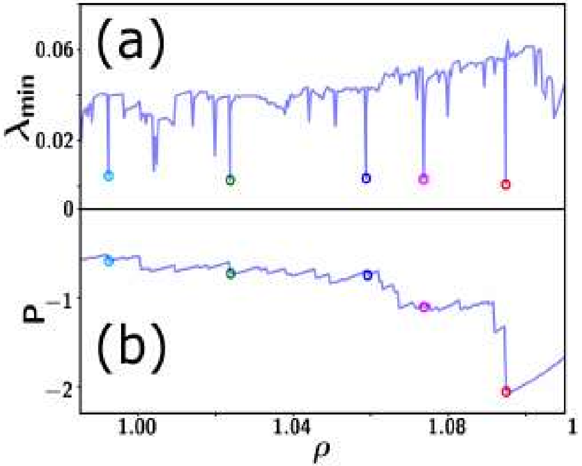
- **Sharp peak with increasing system sizes implies a yielding like transition**

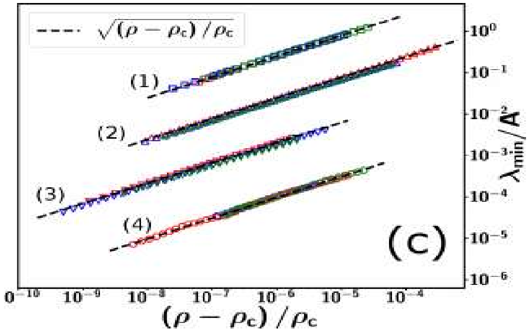
- **The peak height goes as** $\chi_p^{peak} \sim N$**; brittle-like yielding with a macroscopic pressure drop** (Ozawa et al, PNAS 2018)



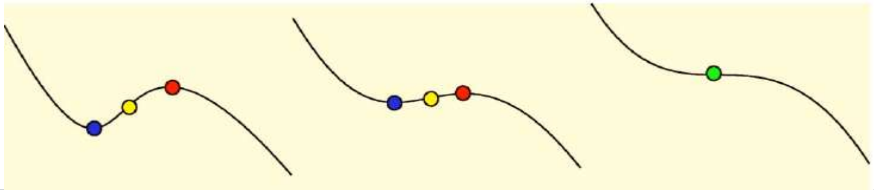
Pressure jumps and plastic events

- Pressure jumps correspond to irreversible plastic events
- We diagonalize the hessian of potential energy to probe the stability near a plastic drop $\mathrm{H}_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial x_i^\alpha \partial x_j^\beta}$
- Near each plastic jump, the lowest non-zero eigenvalue of the hessian goes to zero as a power law: $\lambda_{min} \sim \sqrt{(\rho - \rho_c)/\rho_c}$
- Saddle-node bifurcation on the potential energy landscape; seen under shear too





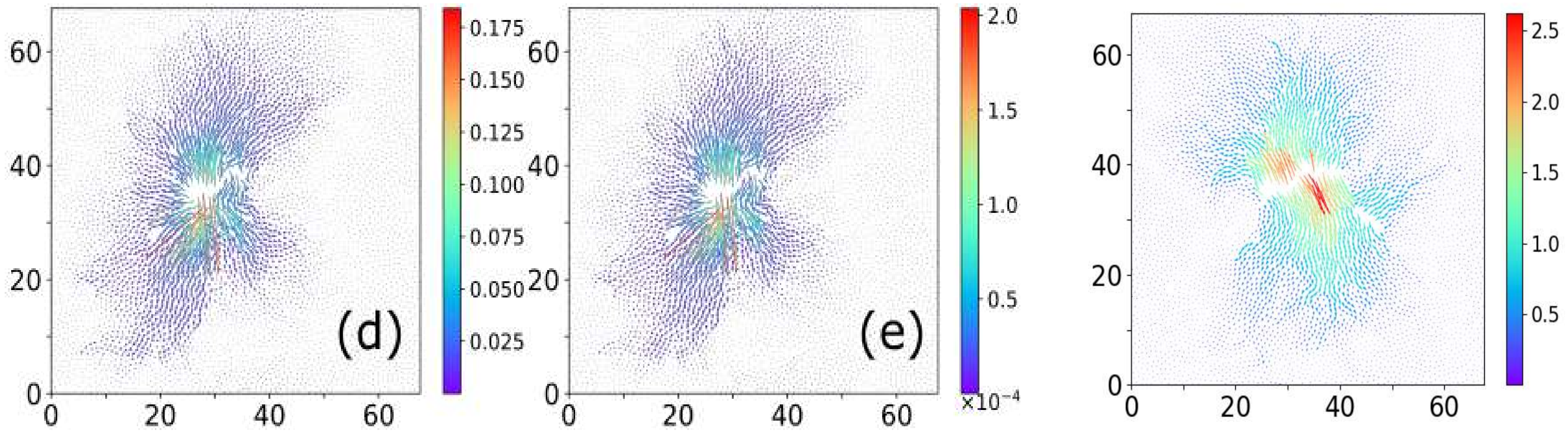
(Maloney & Lemaitre, PRE 2005)



eigenmodes & displacement fields

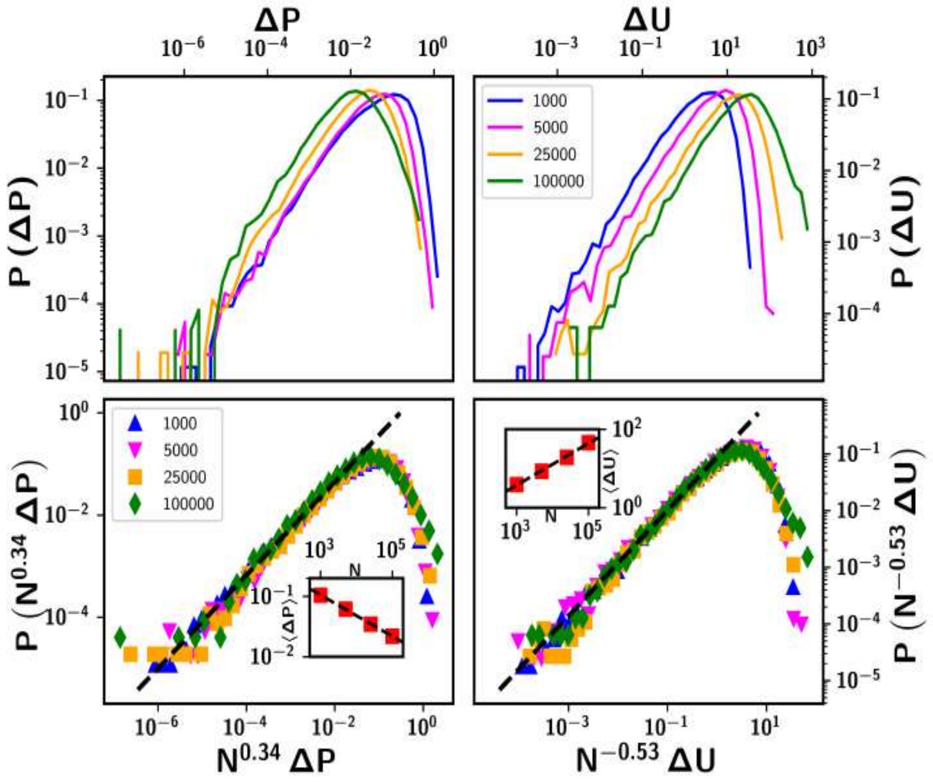
- **On approach to a plastic jump, the eigenmode of λ_{min} predicts the displacement field**
- **Across the plastic jump, the displacement field has a smaller overlap with the eigenmode; cascade/avalanche nature of cavitation**

$\hat{e} \cdot \hat{d} = 0.99$ $\hat{e} \cdot \hat{d} = 0.57$



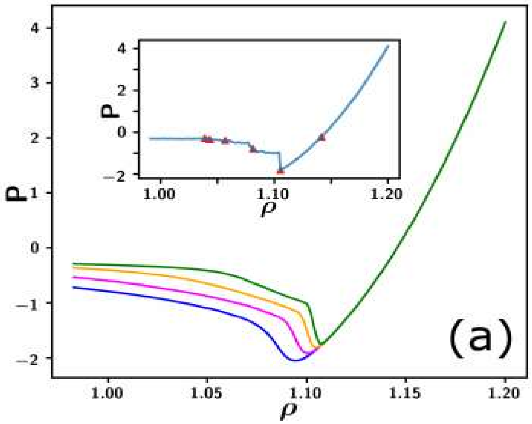
Statistics of avalanches: post-yield

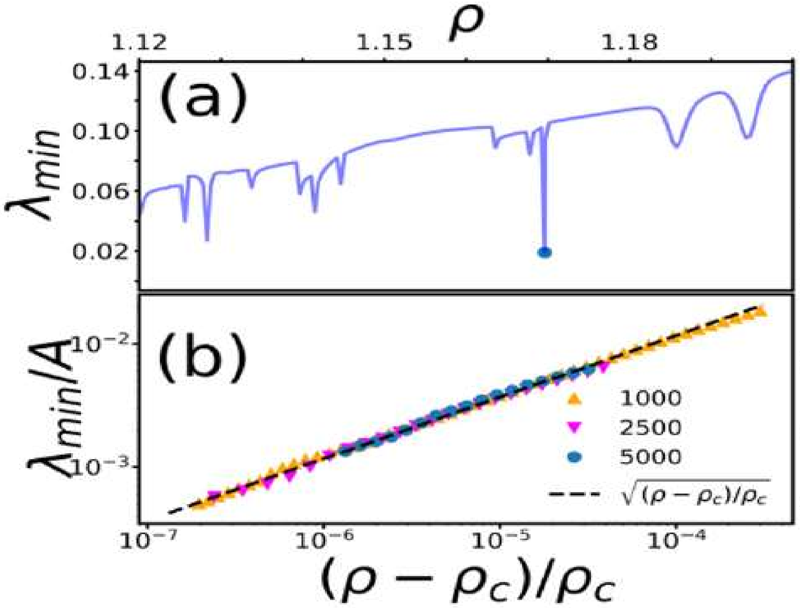
- **Absence of a post-yield steady state**
- **Distributions of size of pressure jumps and energy drops collapse on scaling N by exponents -0.34 and 0.53**
- **The mean sizes of pressure jumps and energy drops too scale with same exponents**

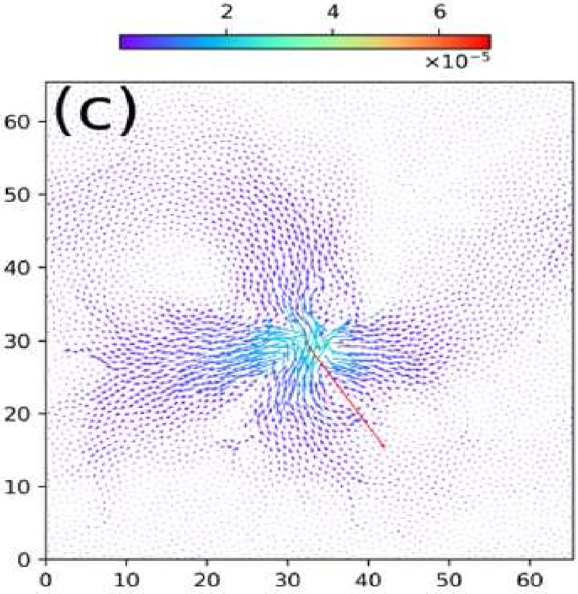


Pre-yield plastic events

- λ_{min} goes to zero multiple times even before cavities start to form
- These plastic events have a quadruopolar shape just like the events seen under shear







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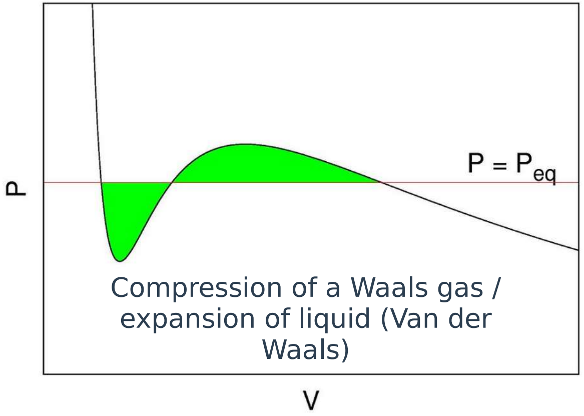
Motivation

- **Negative pressure states in liquids are metastable(maxwell's construction), but our the liquid is below the glass-transition temperature?**



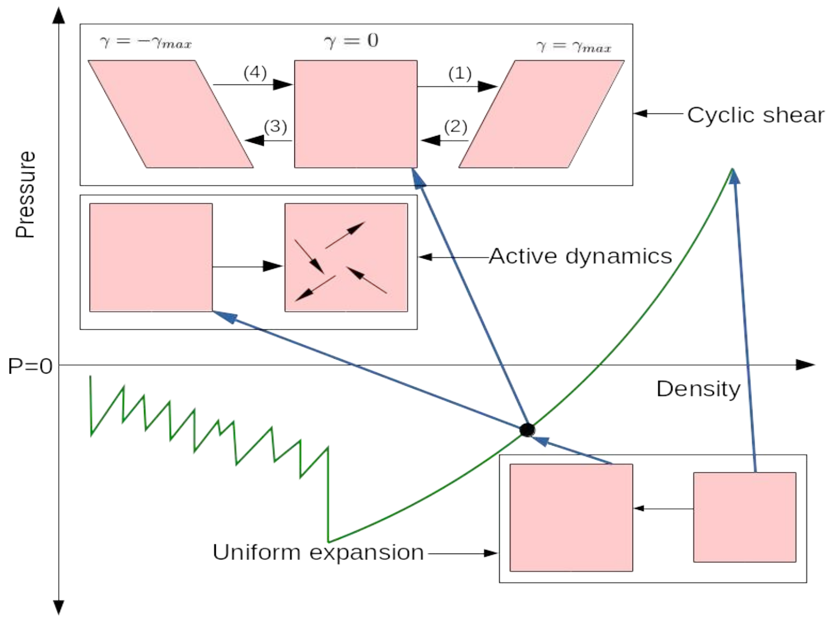
Compression of a Waals gas / expansion of liquid (Van der Waals)

- **In real-life scenarios, the modes of deformation are always a combination of volume strains and shear strains, how to account for this?**

Part II: Secondary defomation of the expanded solid

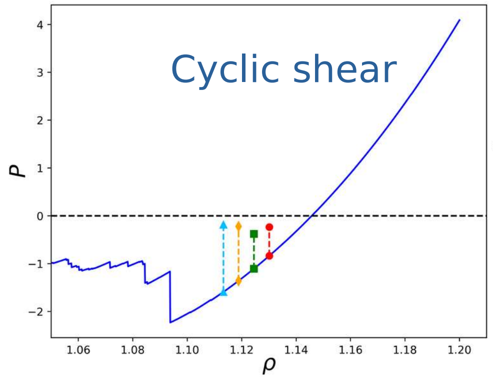
- **Uniform expansion states subject to cyclic shear(T=0) and local random deformation via activity(T=0.01)**

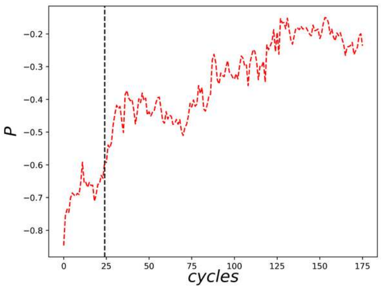
- **Control parameters:**
  - Amplitude of cyclic shear: γ_{max}
  - Magnitude of active force: f_0

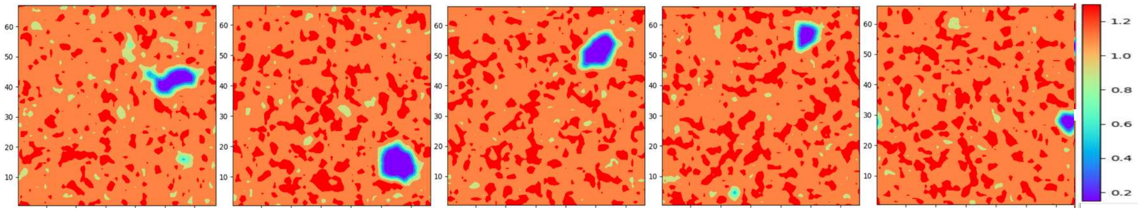


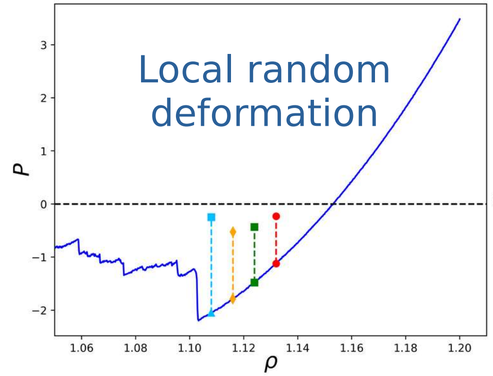
Results: high density cavitation

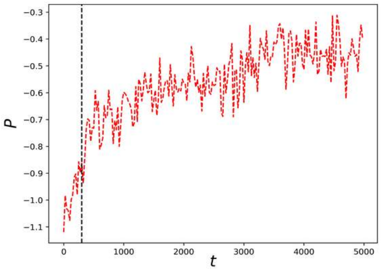
Cavitation at higher densities for both secondary deformations

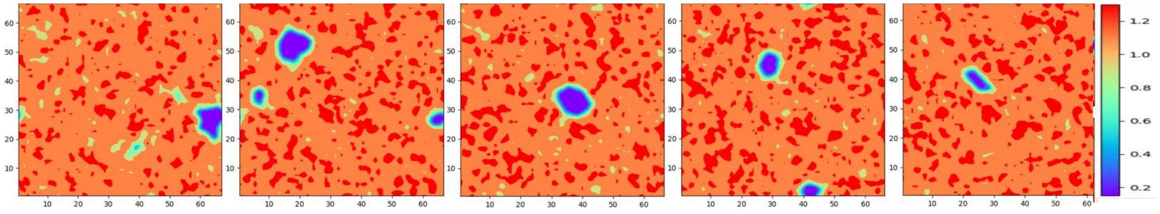






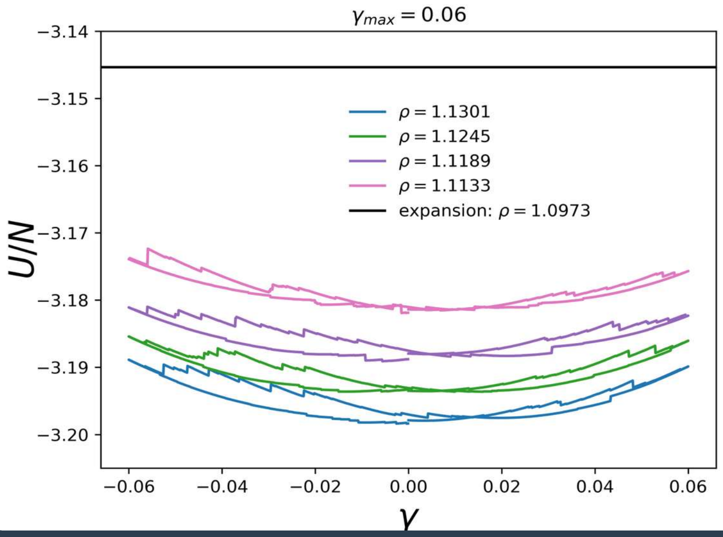


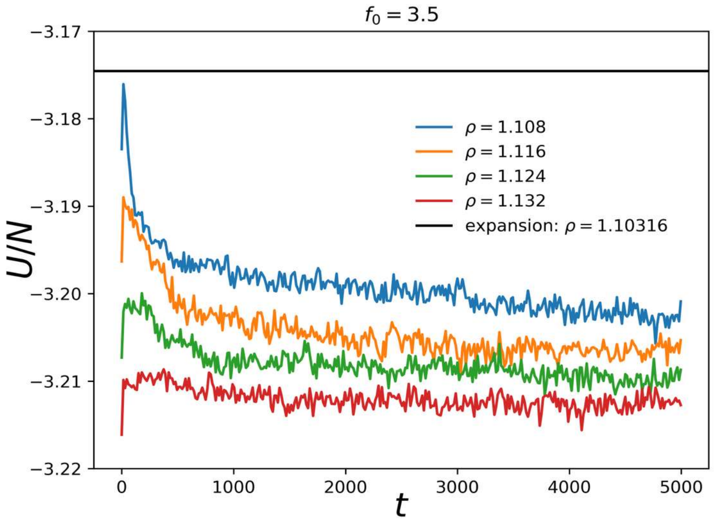




Energy barriers

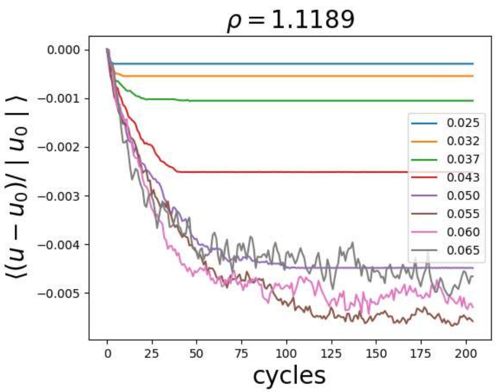
- **Lower energy barriers/thresholds to cavitation under secondary deformations**
- **Shear deformation and local random deformation couple better to cavitation instabilities than expansion**

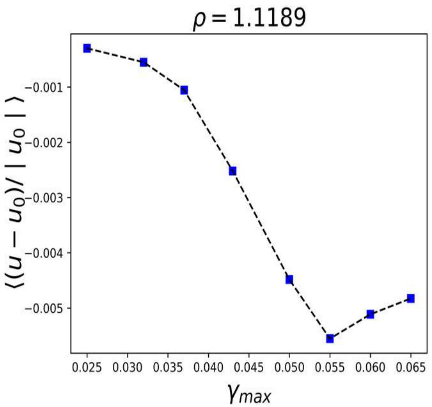


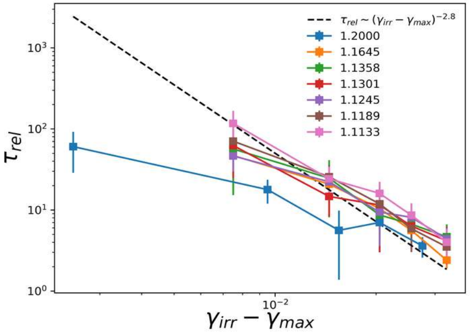


Yielding under cyclic shear

- **Stroboscopic energy relaxation shows yielding under cyclic shear**
- **No limit cycles above yielding**
- **Cusp in average steady-plateau energy (Bhowmik, Foffi & Sastry, PNAS, 2021)**
- **Divergence of timescales to reach limit cycles with an exponent -2.8**

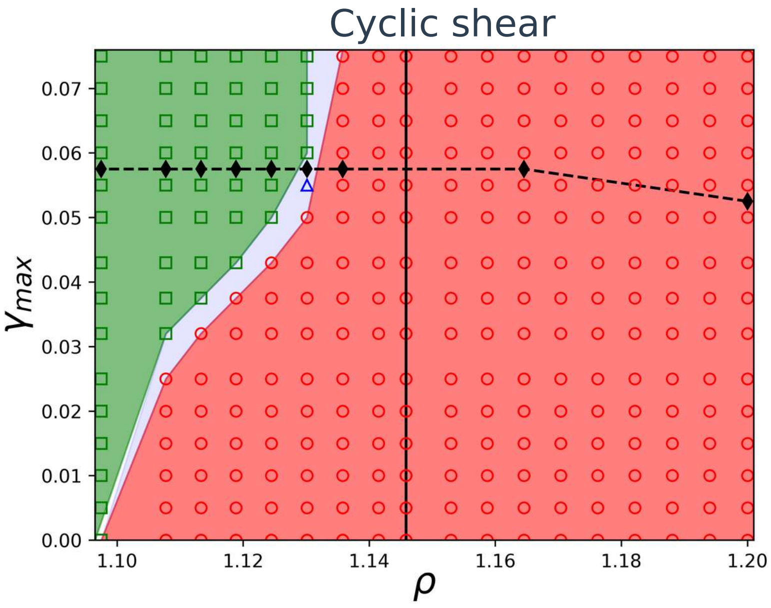


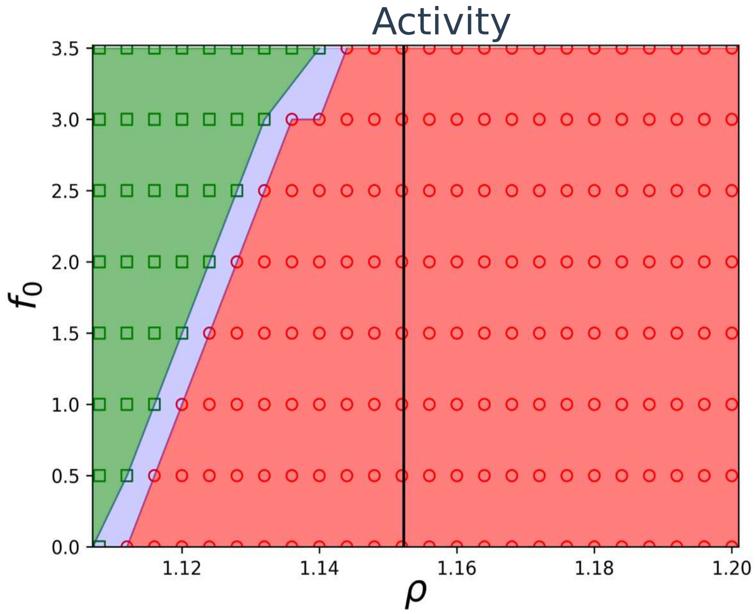




Dependence on control parameters

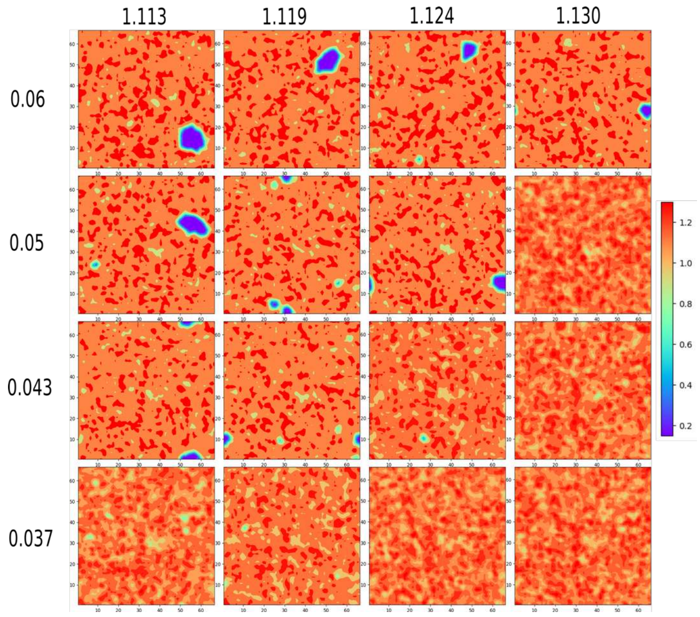
- **Cavitation region marked in two-parameter phase diagrams**
- **Cavitation occurs both, below and above, yield / fluidisation thresholds**



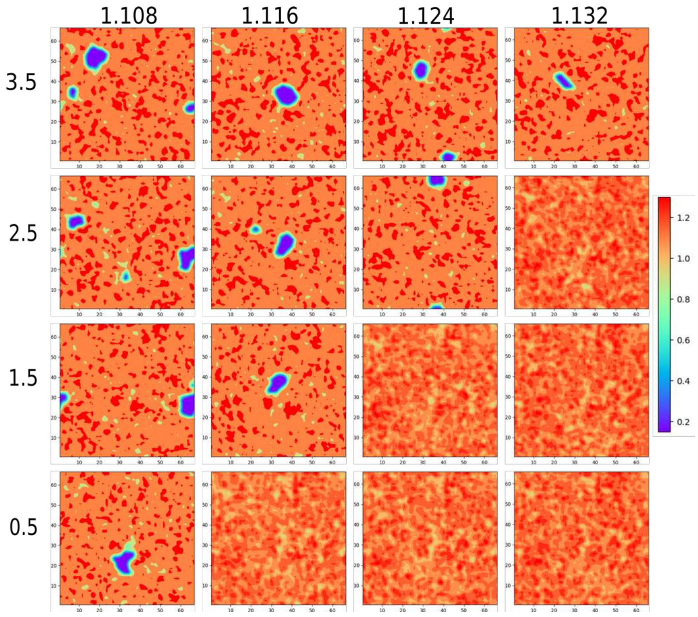


Soft spots

- **For a same expansion trajectory the soft spots for different phase parameters are different – abundance of soft cavitation modes**



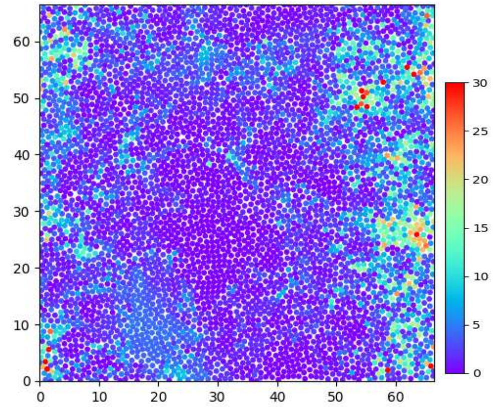
Cyclic shear



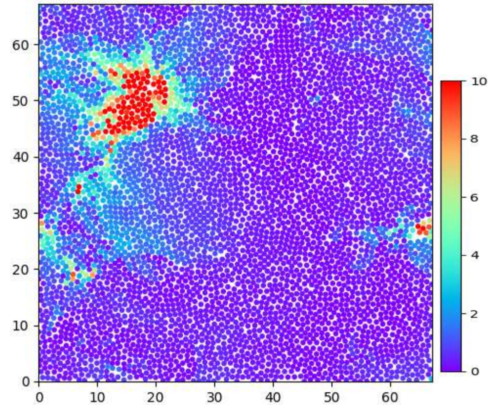
Activity

Spatial maps of plasticity: squared displacements

- **Cyclic shear: system spanning avalanche-like structures at high values of γ_{max}**
- **Local random deformation: spatially localised bursts of plasticity**
- **Both local and system-spanning pathways lead to cavitation under secondary deformations**



Cyclic shear



Activity

Summary

- **Under expansion, the amorphous solids cavitate via a yielding-like transition**
- **The cavities grow with expansion resulting in a system-spanning crack**
- **Plastic pressure jumps correspond to saddle-node bifurcations on the PEL**
- **Early onset of cavitation for both secondary deformations, cyclic shear & local random deformation**
- **Lower energy barriers to cavitation under cyclic shear & local random deformation than expansion**

Thank you!