Theoretical determination of stress-strain curve of two-dimensional amorphous solids of dispersed frictional grains with finite shear strain

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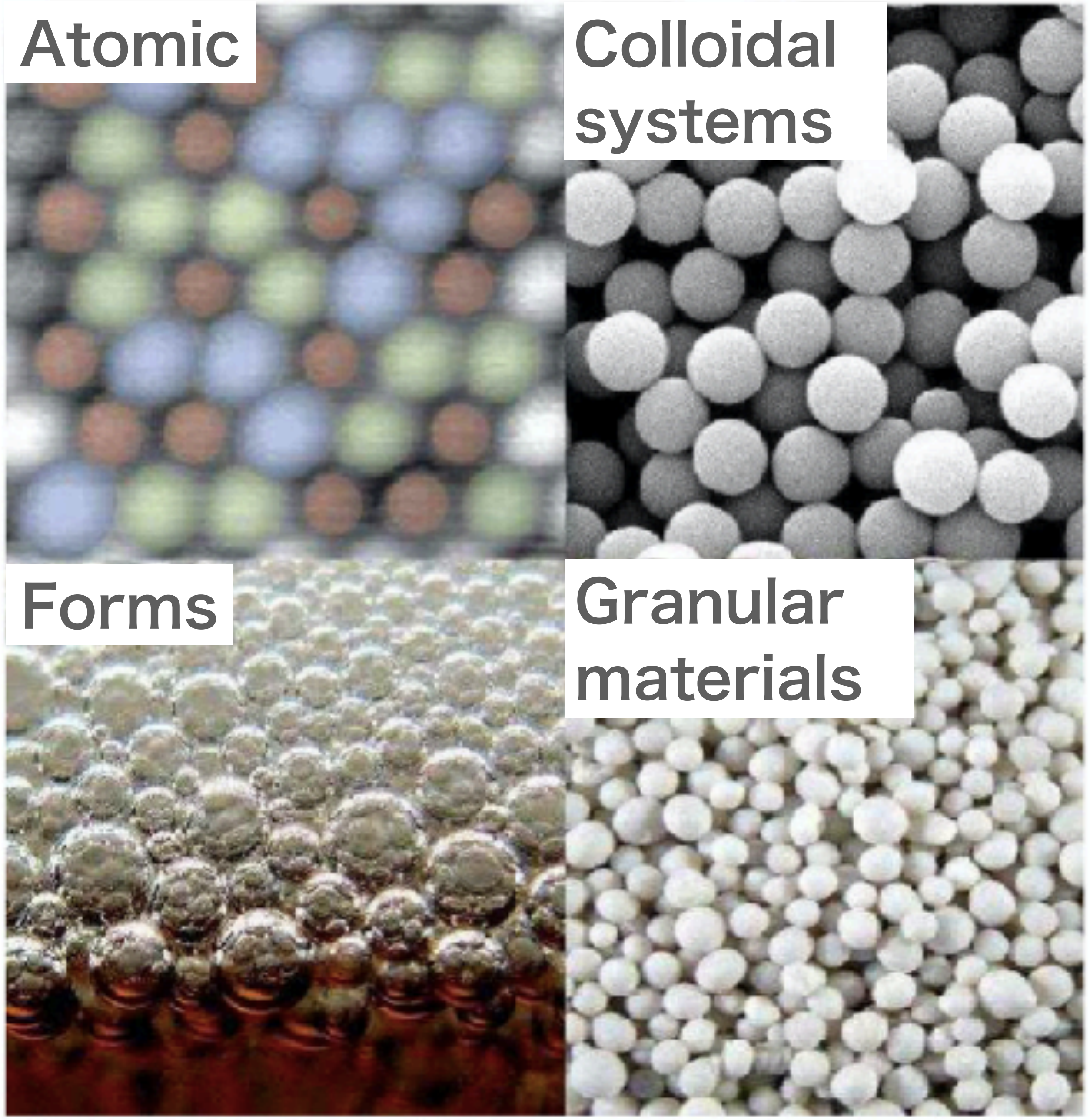
Introduction

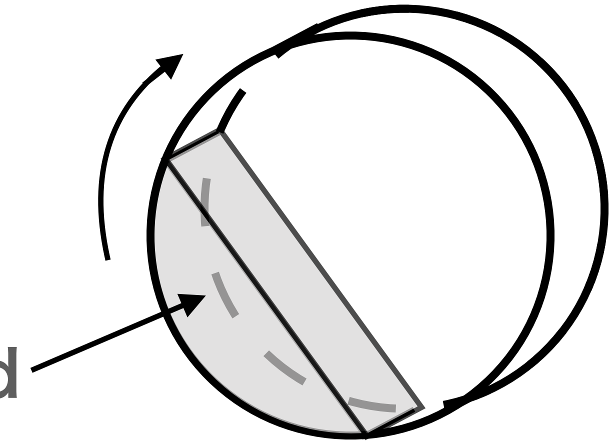
Examples of amorphous materials



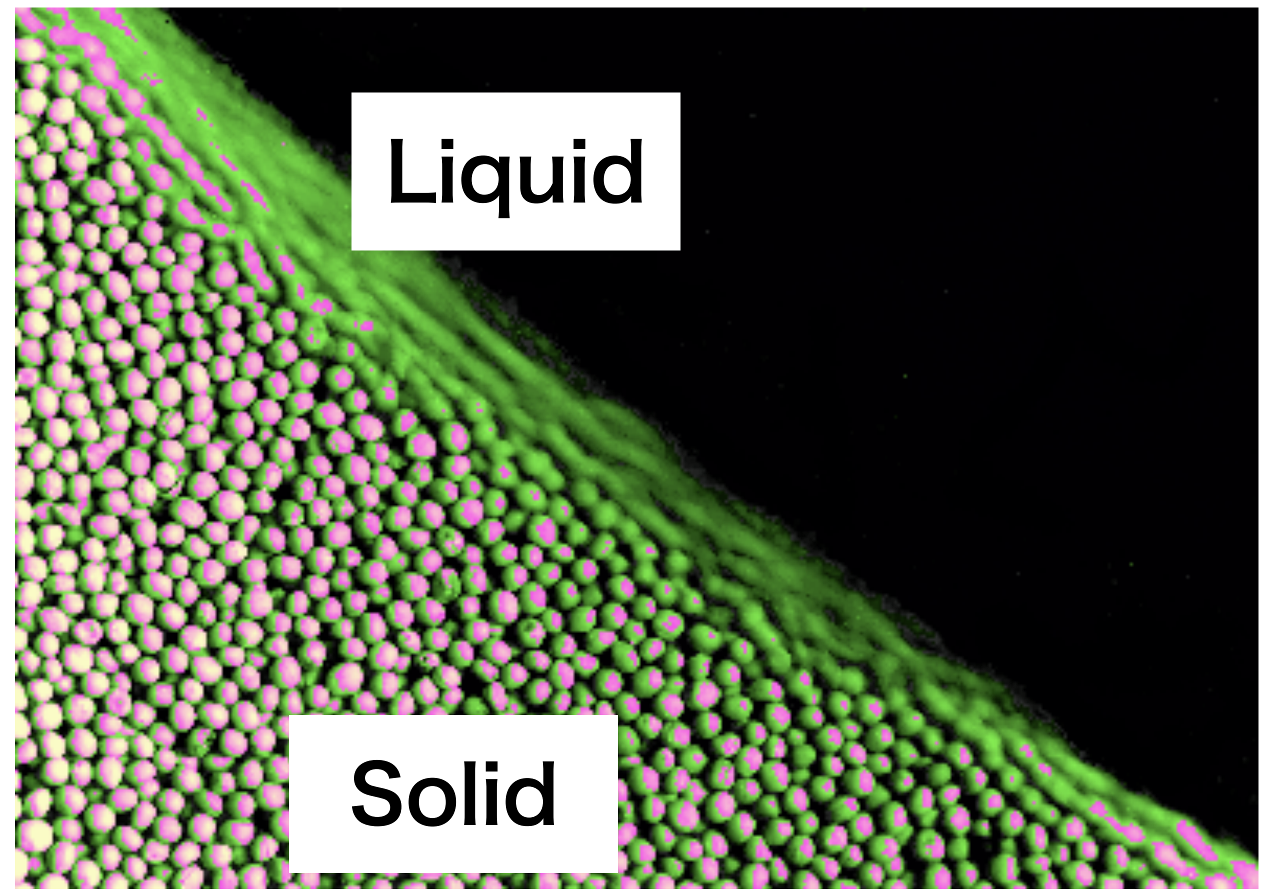
L. Berthier and G. Biroli, Rev. Mod. Phys., ***83***, *587 (2011).*

Introduction

Behavior of an amorphous materials



"*https://www.youtube.com/watch?v=SIkRUv39SoI*"

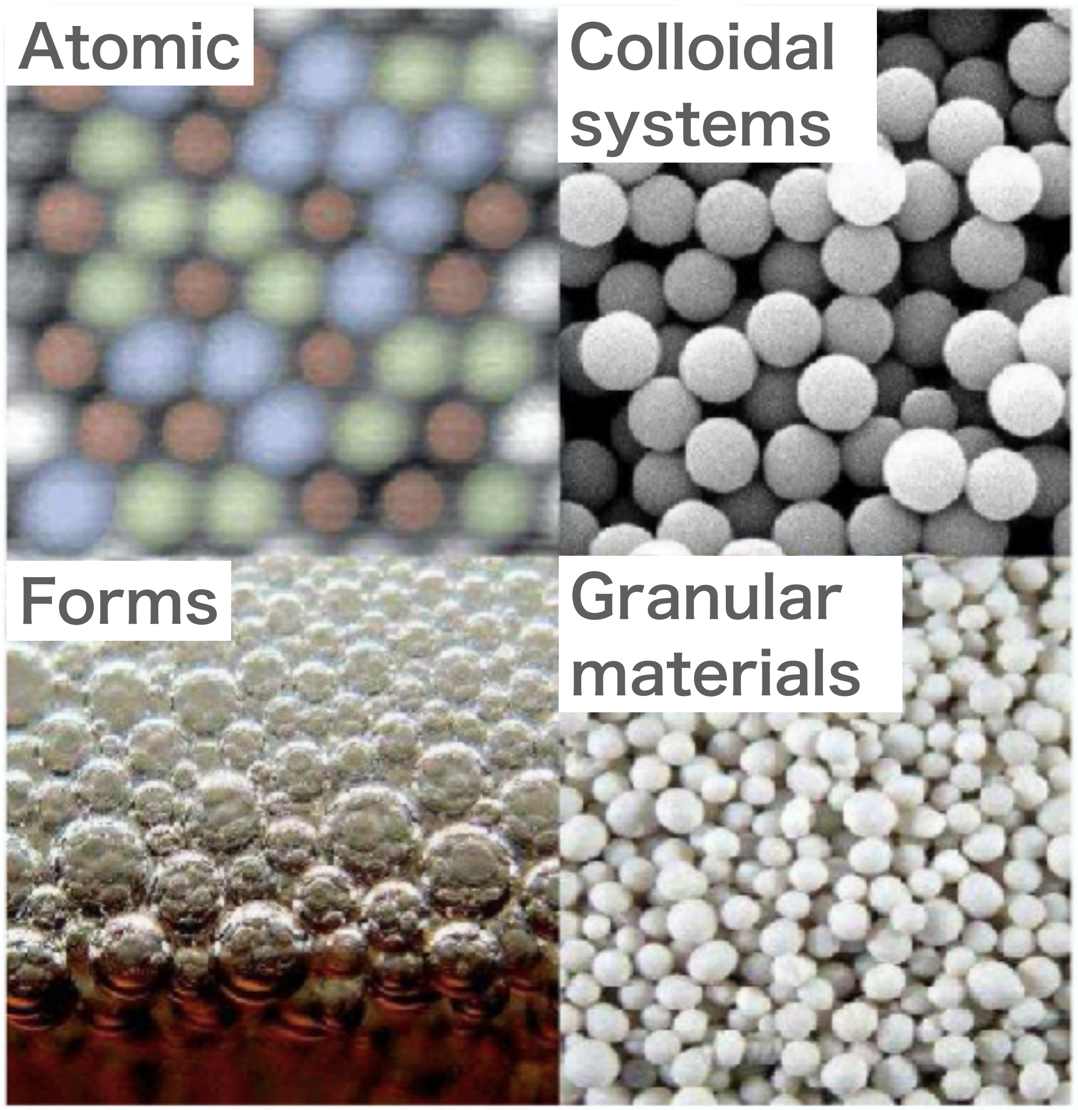


H. M. Jaeger, and S. R. Nagel, Rev. Mod. Phys. ***68****, 4 (1996).*

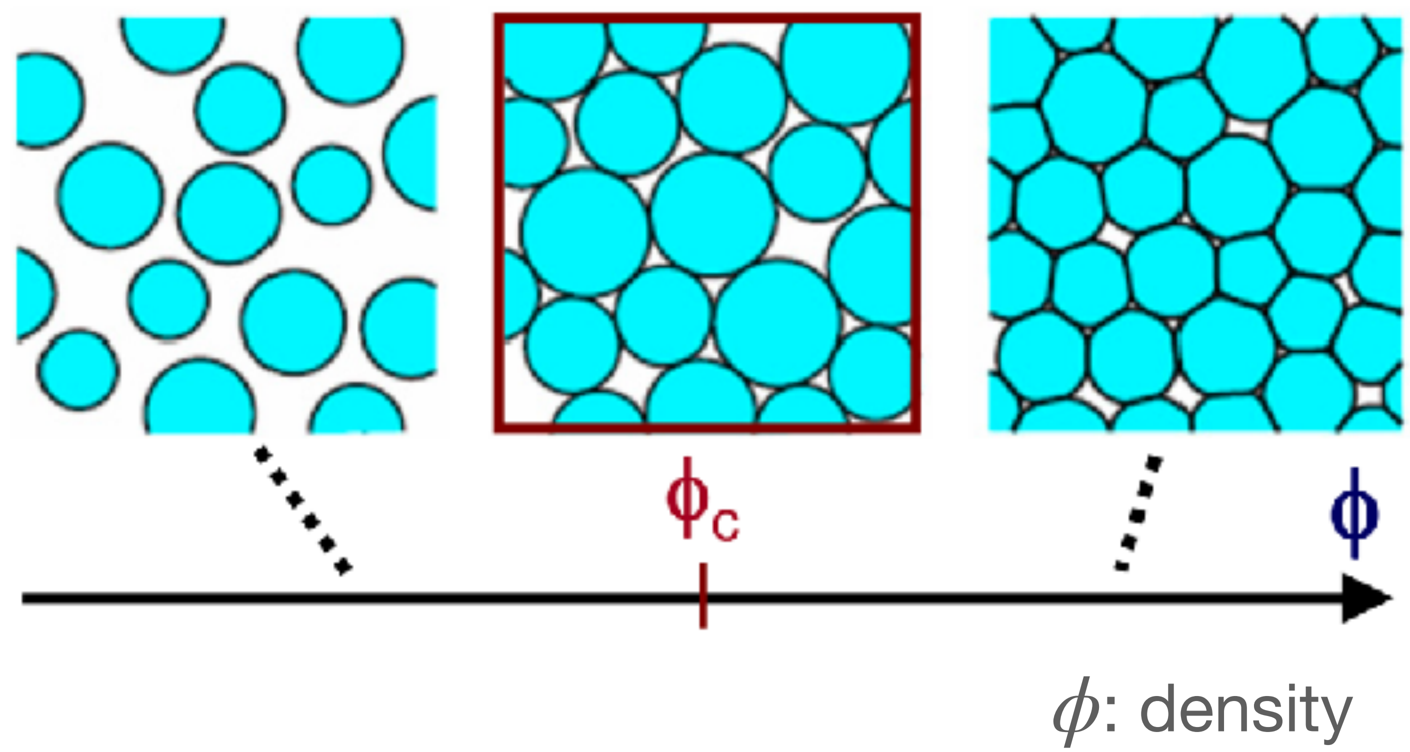
The system behave as solid or liquid

Introduction: Amorphous solids

Amorphous materials



L. Berthier and G. Biroli, Rev. Mod. Phys., ***83****, 587 (2011).*



M. Van Hecke, J. Phys. Cond. Matt., ***22****, 033101 (2010).*

They have rigidity above critical density ϕ_c

Previous research

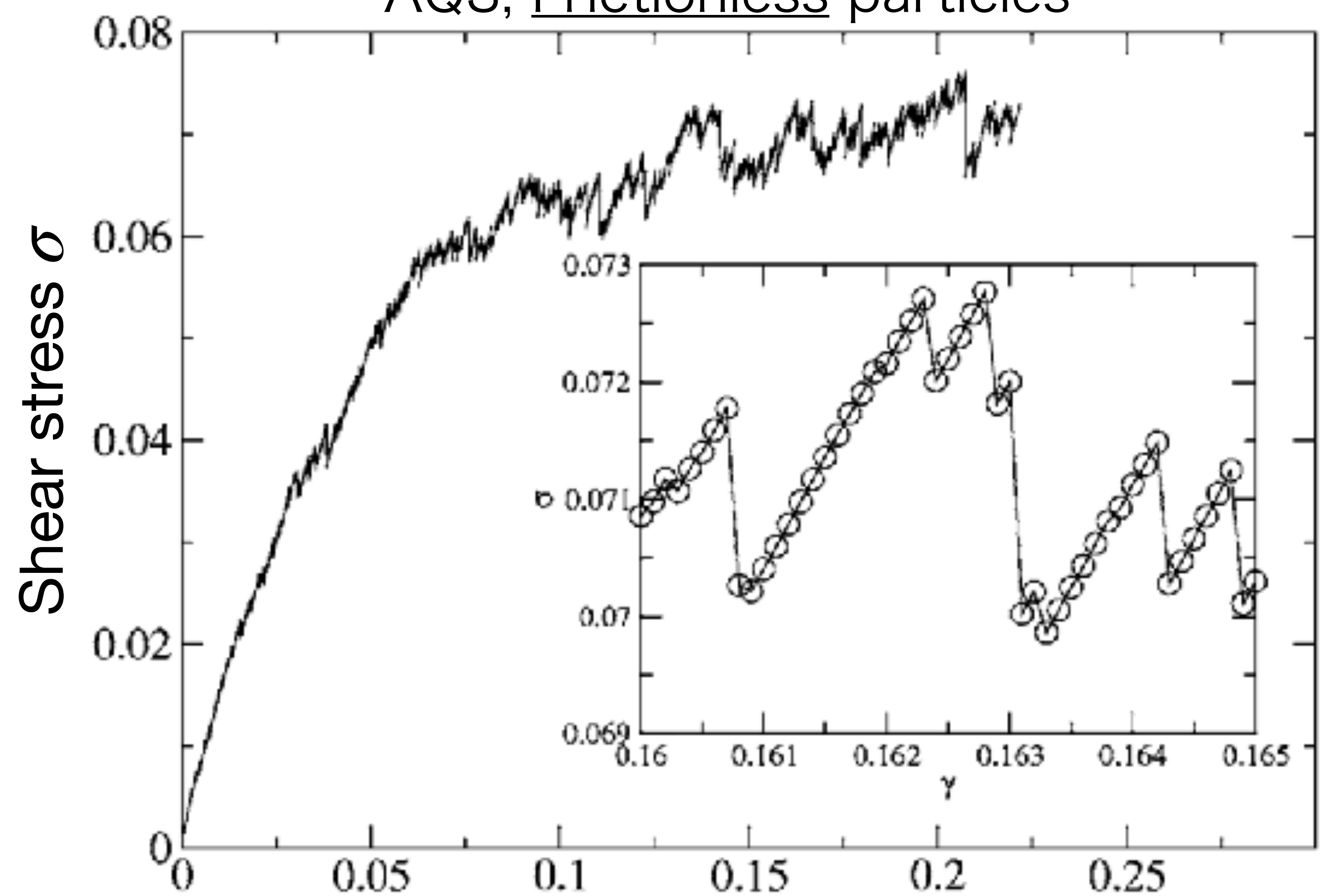
Definition of Hessian $H_{ij}^{\alpha\beta}$

$$H_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial r_i^\alpha \partial r_j^\beta}$$

U : Potential energy,

r_i^α : α coordinate of i-th particle.

AQS, Frictionless particles

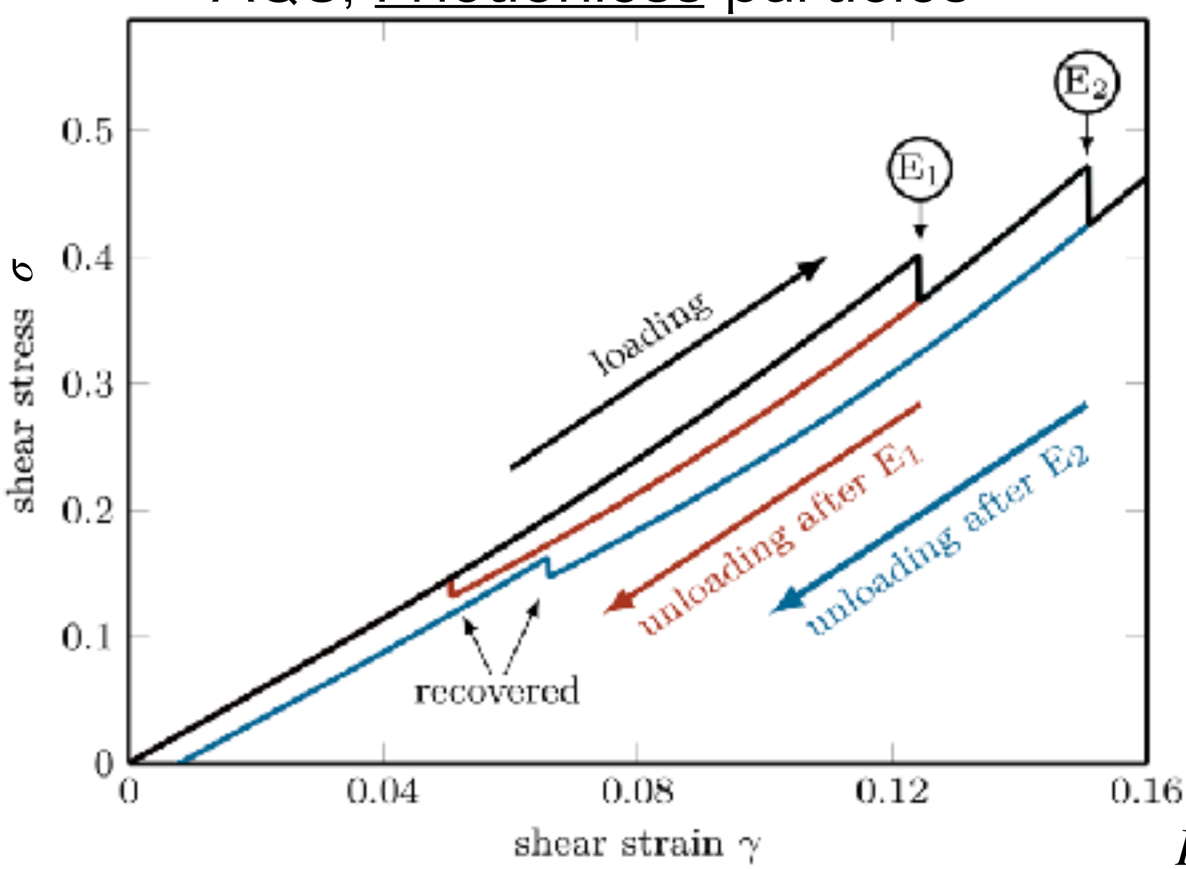


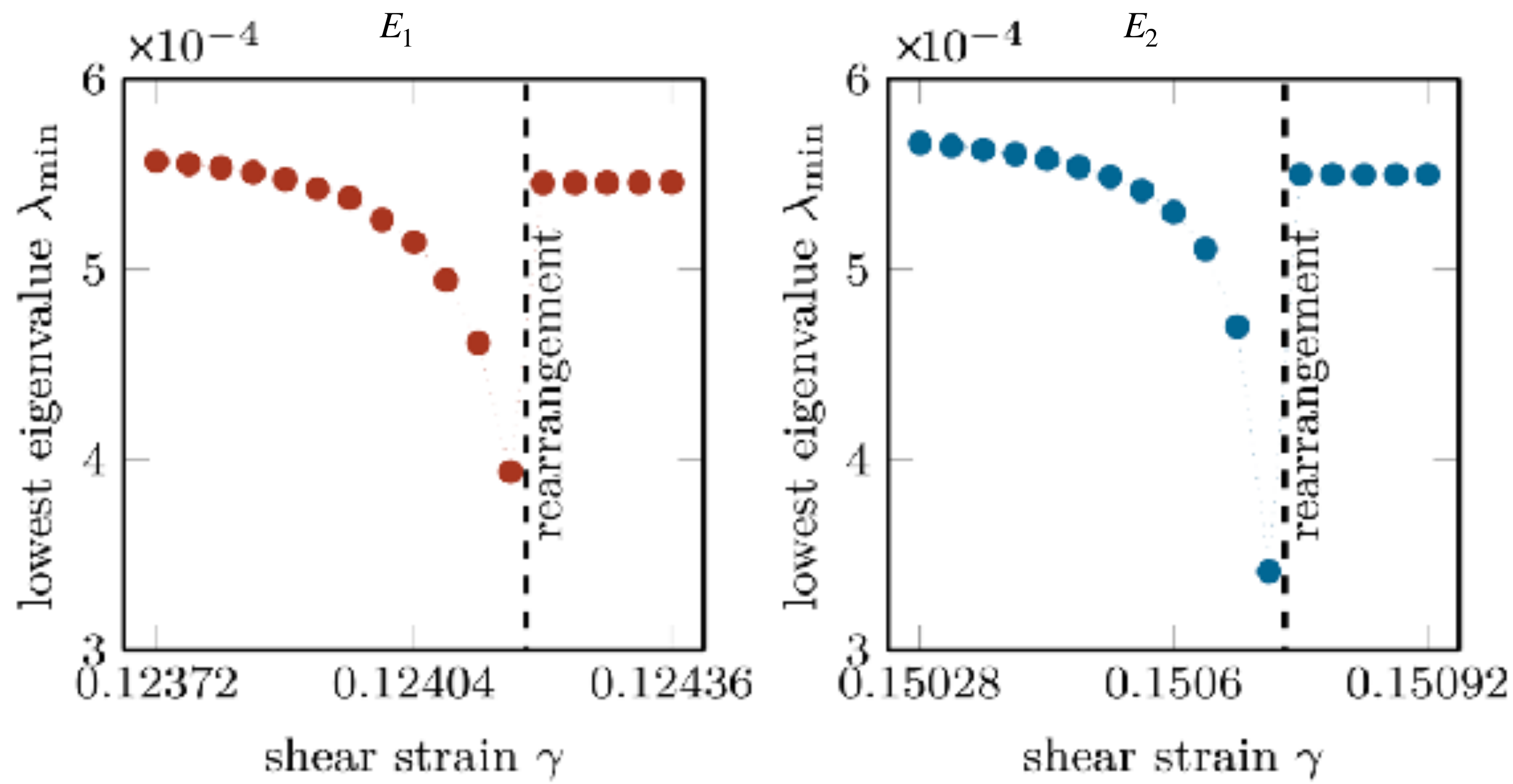
C. C. Maloney & A. Lemaître, Phys. Rev. E ***74****, 016118 (2006).*

They proposed that the eigenvalue analysis of H can predict the rigidity

Previous research

AQS, Frictionless particles



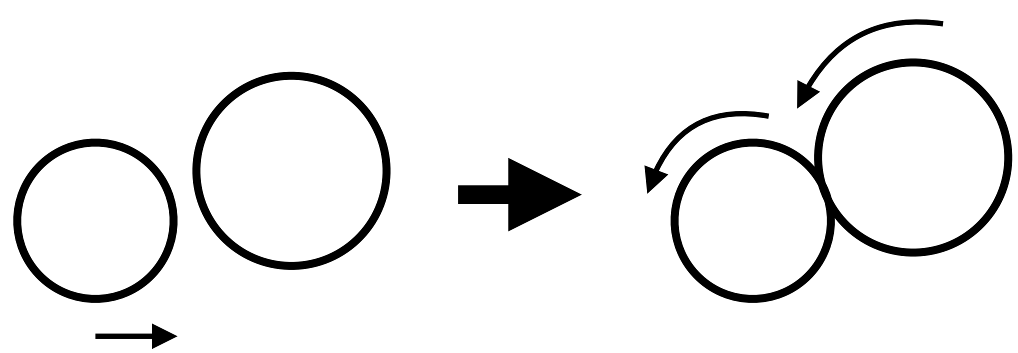


*F. Ebrahem, F. Bamer, & B. Markert, Phys. Rev. E **102**, 033006 (2020).*

They suggest minimum eigenvalue of H
is precursor for stress drop

Purpose

	Frictionless grains	Frictional grains
Prediction of G by eigenvalue analysis	✔	?
Precursor for stress drop	✔	



Problem

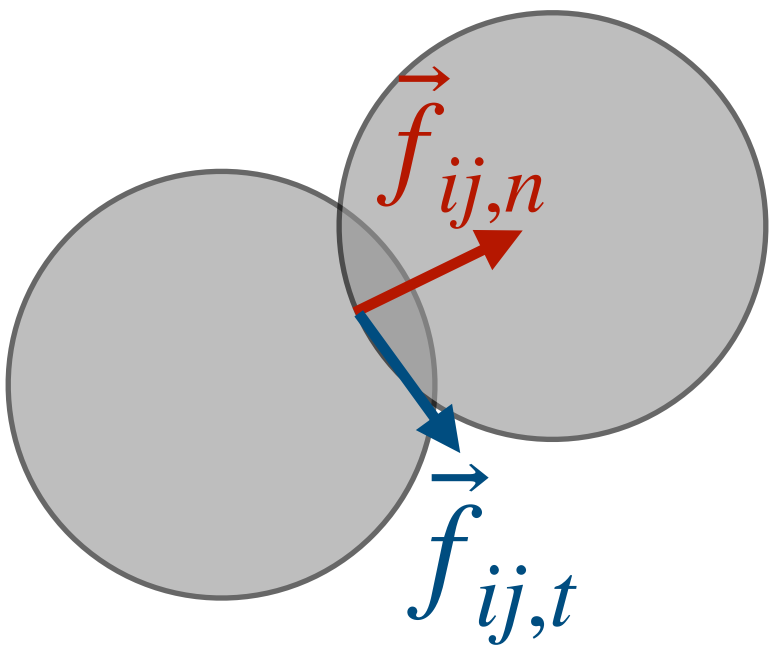
We cannot ignore the mutual friction between grains

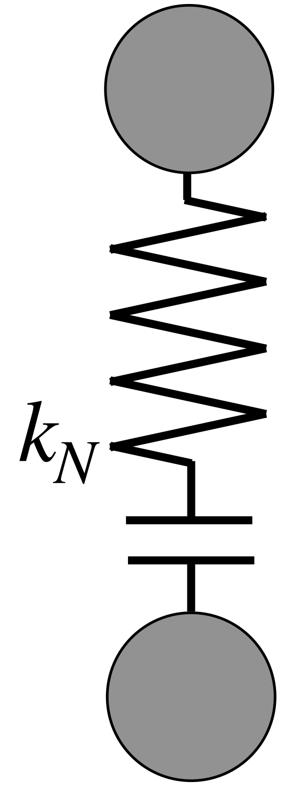
Purpose

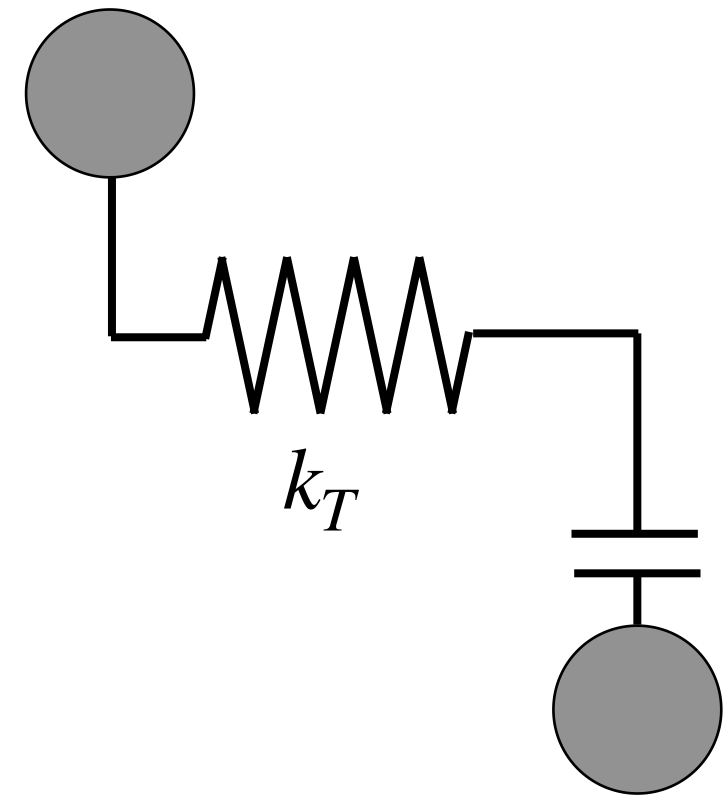
We conduct the eigenvalue analysis for <u>frictional grains</u>

Numerical methods

Contact force: linear spring







Normal force $\vec{f}_{ij,n}$

Tangential force $\vec{f}_{ij,t}$

*nonslip model

S. Luding, Granular Matter ***10****, 235 (2008).*

Our simulated system

2 dimensional frictional binary disks ($N = 128$),

Density: $\phi = 0.90$,

Tangential spring constant $k_T = k_N$.

Our protocol

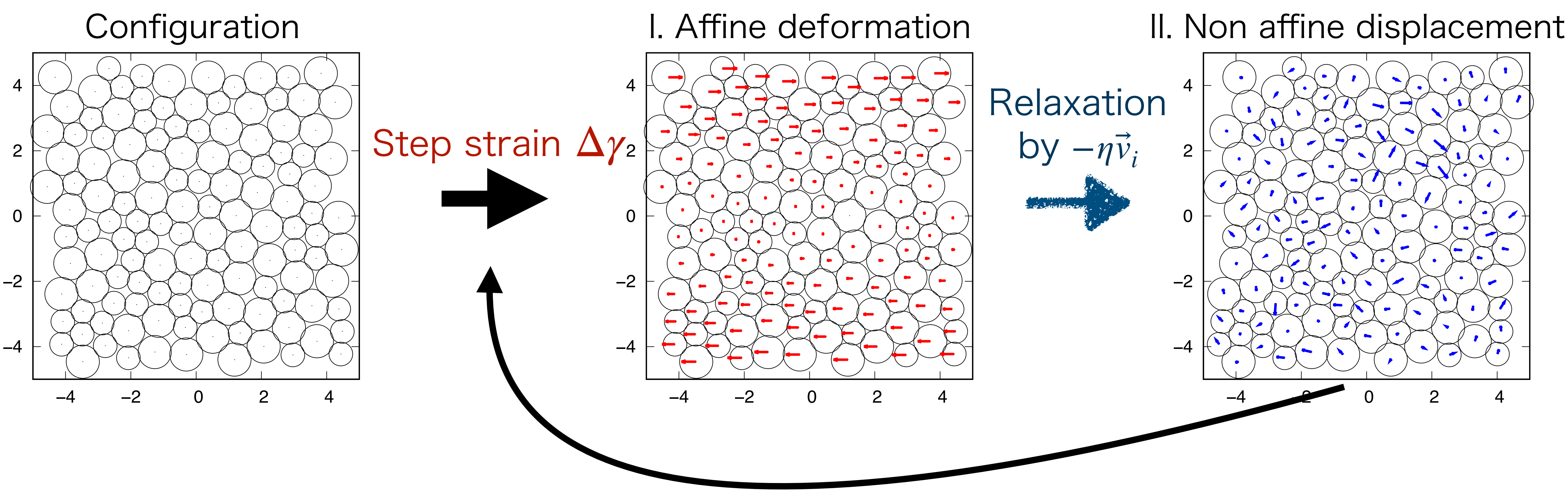
Athermal quasistatic shear (AQS) protocol

I. Applying affine shear deformation $\Delta\gamma^*$ to the system with Lees-Edwards boundary condition

*Range of $\Delta\gamma$: $1.0 \times 10^{-8} \leq \Delta\gamma \leq 1.0 \times 10^{-4}$

II. Relaxation by dissipation $-\eta\vec{v}_i$ until $|F_i^\alpha| < F_{\mathrm{Th}}{}^*$

*Threshold value of mechanical equilibrium condition: $F_{\mathrm{Th}}/(k_N d_0) = 10^{-14}$



Repeating AQS protocol we apply finite shear strain γ to the system

Protocol to change $\Delta\gamma$

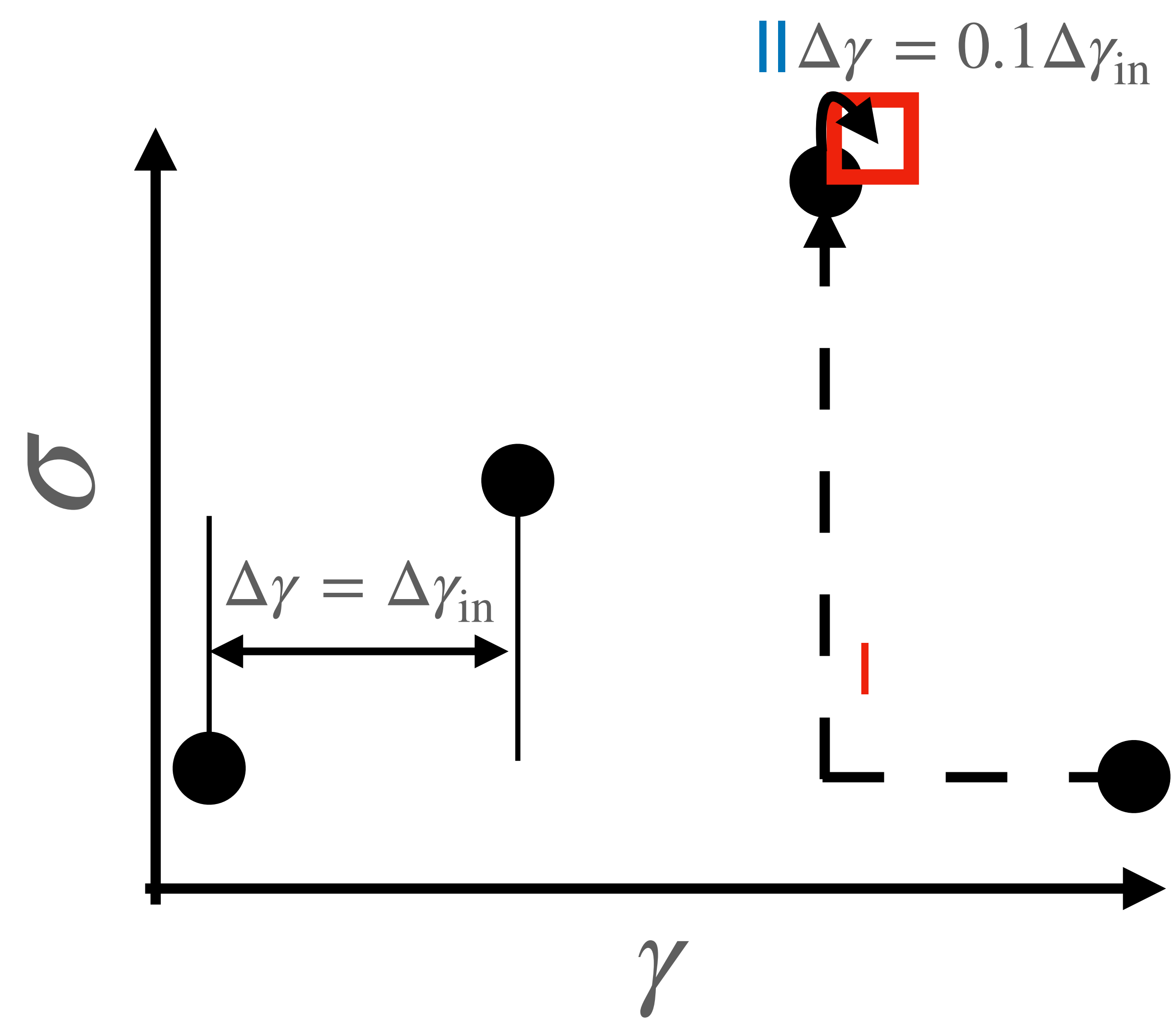
When the stress drop occurs, we have changed $\Delta\gamma$ until $\Delta\gamma < \Delta\gamma_{\mathrm{Th}}$ repeating following protocol:

I. The system comes back to the state before stress drop.

II. We change $\Delta\gamma$ to $0.1\Delta\gamma$.

We have used

$\Delta\gamma_{\mathrm{Th}} = 1.0 \times 10^{-8}$, $\Delta\gamma_{\mathrm{in}} = 1.0 \times 10^{-4}$.



Eigenvalue analysis

Definition of Hessian $H_{ij}^{\alpha\beta}$ for our system

$$H_{ij}^{\alpha\beta} := \frac{\partial \delta e_{ij}}{\partial q_i^{\alpha} \partial q_j^{\beta}},$$

δe_{ij} : Effective potential between frictional i & j grains $\delta e_{ij} := \frac{k_N}{2}\delta r_{N,ij}^2 + \frac{k_T}{2}\delta r_{T,ij}^2$
with normal displacement $\delta r_{N,ij}$ and tangential displacement $\delta r_{T,ij}$

q_i^{α} : α component of generalized i particle coordinate $q_i := (r_i^x, r_i^y, \theta_i)$,

θ_i : Rotational degree of i particle.

Eigenvalue equation:

$$H|\Phi_n\rangle = \lambda_n|\Phi_n\rangle$$

We obtain eigenvalue λ_n and $|\Phi_n\rangle$ from Hessian H.

Results: Stress-strain curve

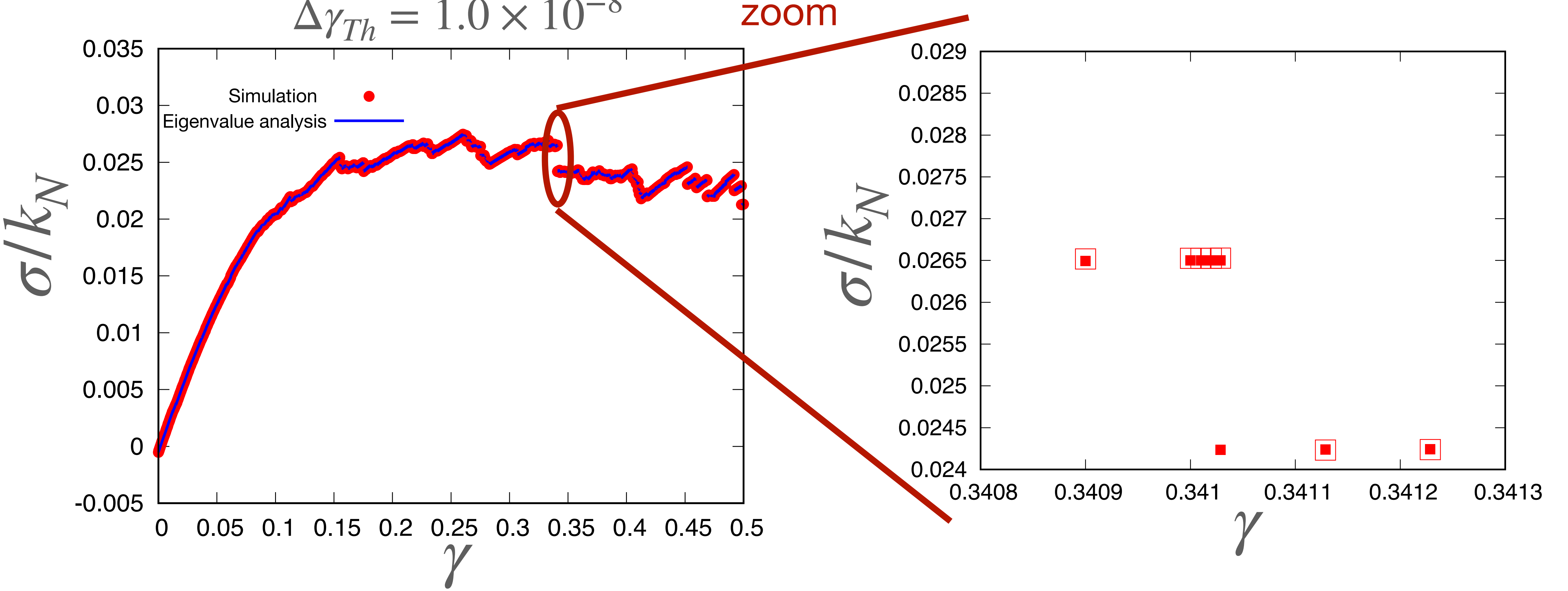
To obtain rigidity G

Simulated $G(\gamma)$ uses the information about γ and $\gamma + \Delta\gamma$ $\left(\because G(\gamma) := \frac{\sigma(\gamma + \Delta\gamma) - \sigma(\gamma)}{\Delta\gamma} \right)$.

$G(\gamma)$ obtained by eigenvalue analysis uses the eigenvalue & eigenfunction for Hessian with stable configuration at γ.

$$\sigma(\gamma + \Delta\gamma) = \sigma(\gamma) + G(\gamma)\Delta\gamma$$

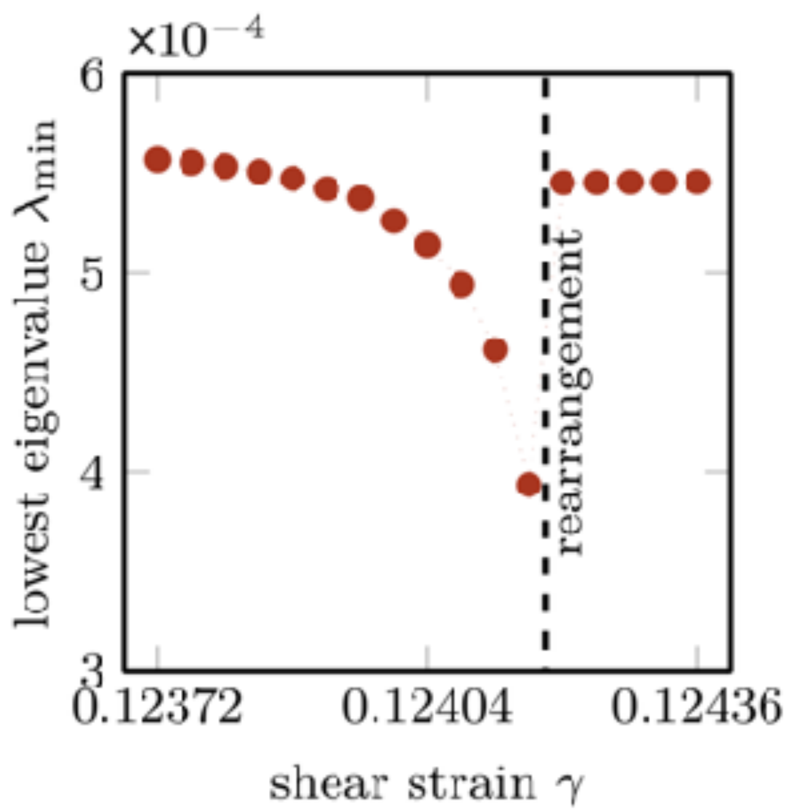
$$\Delta\gamma_{Th} = 1.0 \times 10^{-8}$$



Eigenvalue analysis agrees with simulated G except for stress drop strain

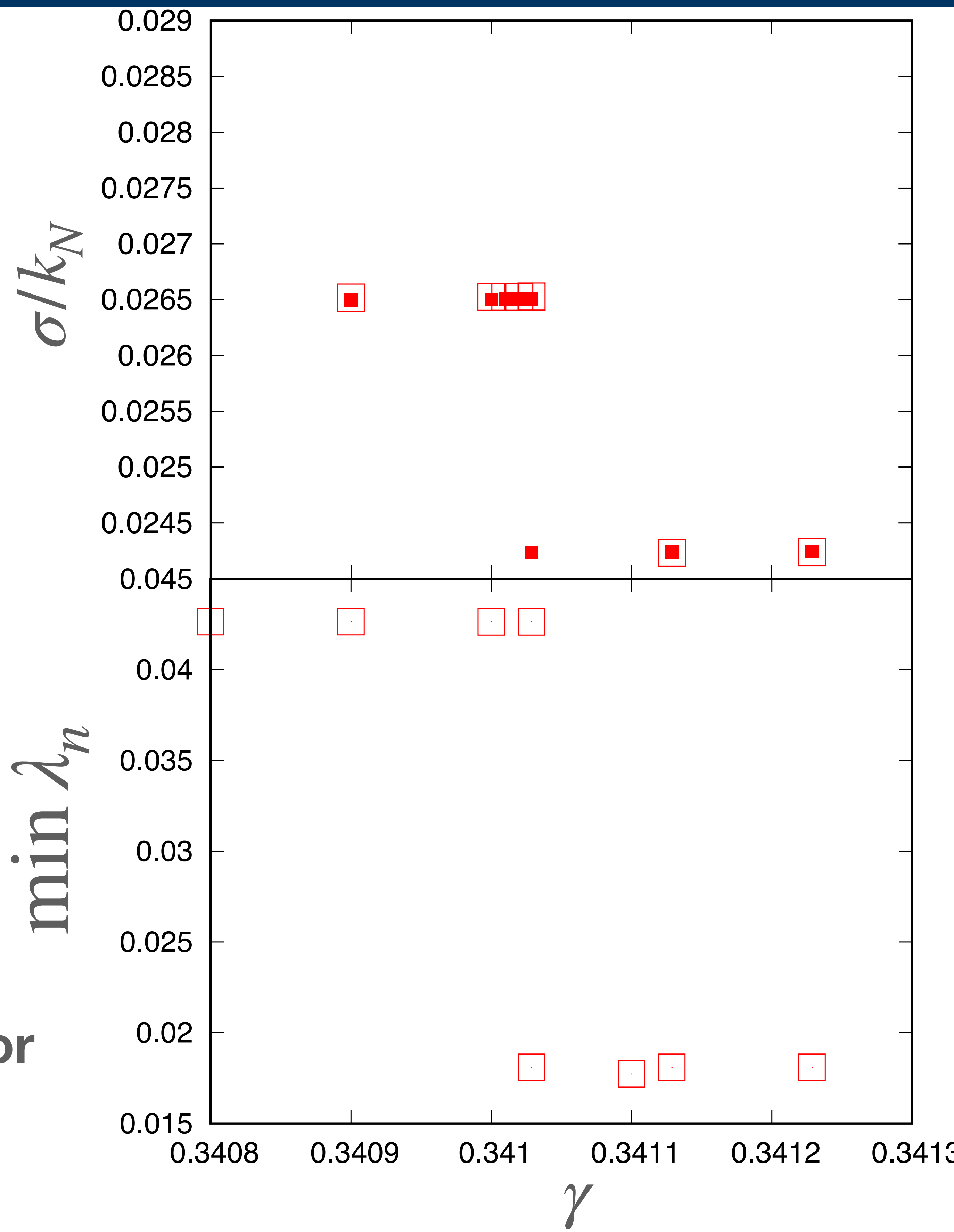
Stress drop event

Previous study suggests precursor for stress drop



F. Ebrahem et al., PRE ***102****, 033006 (2020).*

We cannot observe the precursor for stress drop, at least, for frictional linear spring system.



Discussion: NO Precursor for stress drop

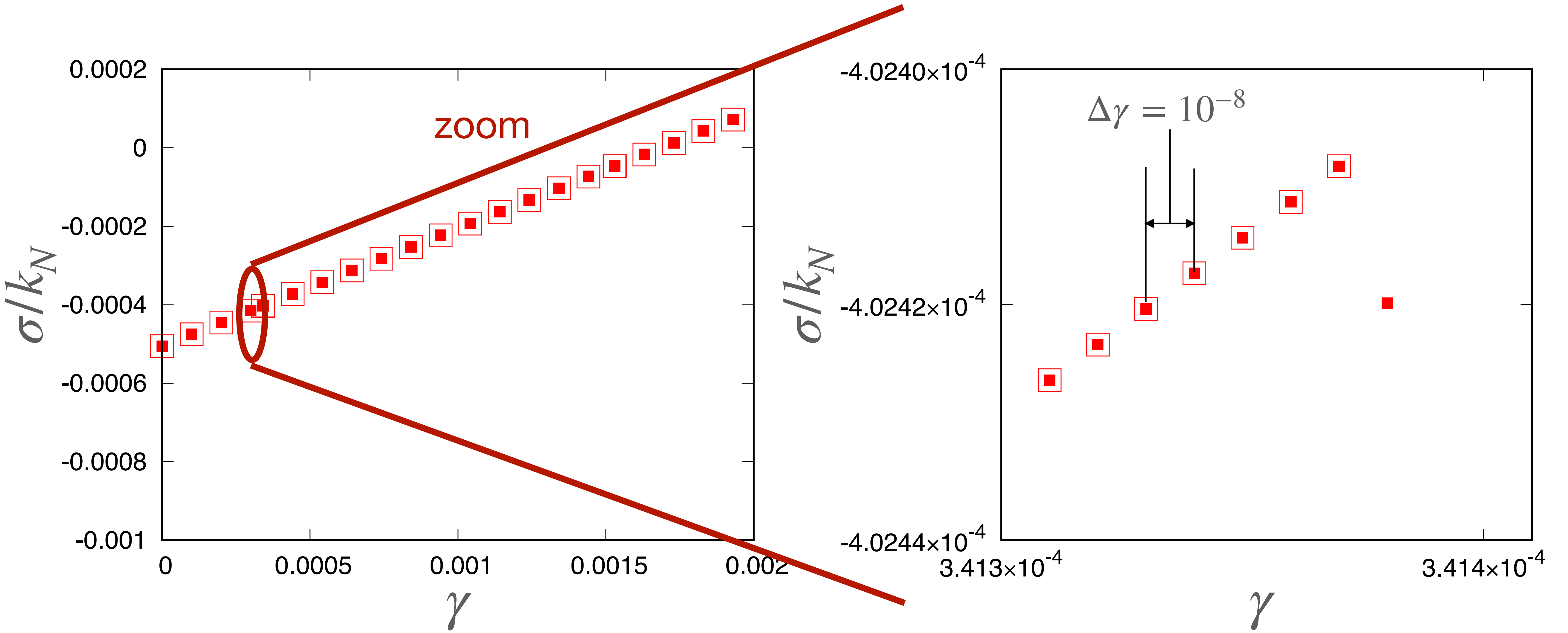
	Previous research	Our research
Precursor	○	✖
Friction between grains	✖	○
Nonlinearity of potential	○	✖

Nonlinearity of potential is important for the precursor

Because Hessian for linear potential does not have the information about displacements between particle:

$$H := \frac{\partial^2 \delta e_{ij}}{\partial q_i^\alpha \partial q_j^\beta} \quad \text{with} \quad \delta \mathrm{e}_{\mathrm{ij}} := \frac{\mathrm{k_N}}{2}\delta \mathrm{r}_{\mathrm{N,ij}}^2 + \frac{\mathrm{k_T}}{2}\delta \mathrm{r}_{\mathrm{T,ij}}^2$$

Another event: contact change

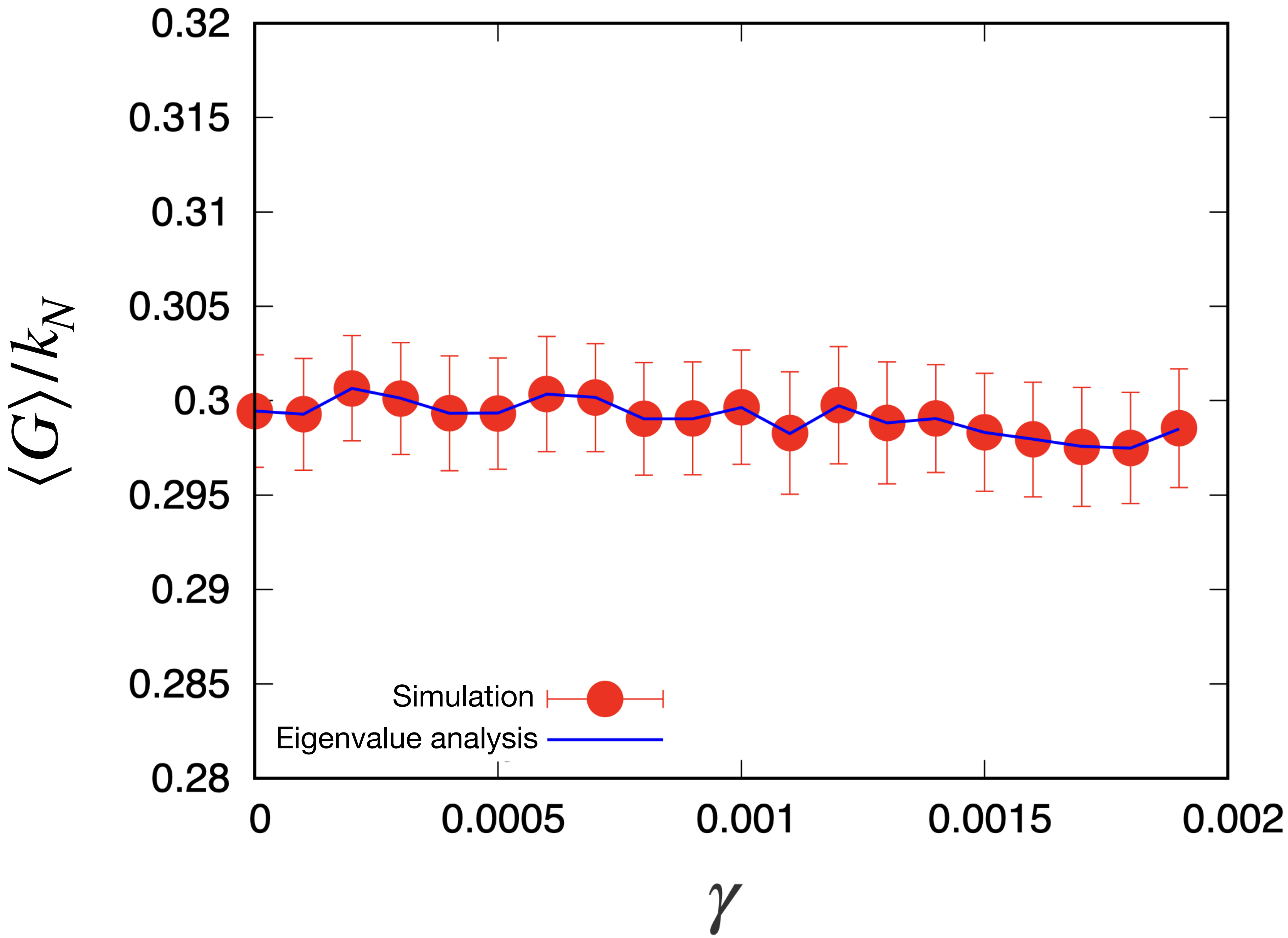


We have found a tiny stress drop by the contact changes

Another event: contact change

$\langle G \rangle$: ensemble averaged G*

*we eliminate G at γ if stress drops



We confirmed that the eigenvalue analysis can predict $\langle G \rangle$ correctly

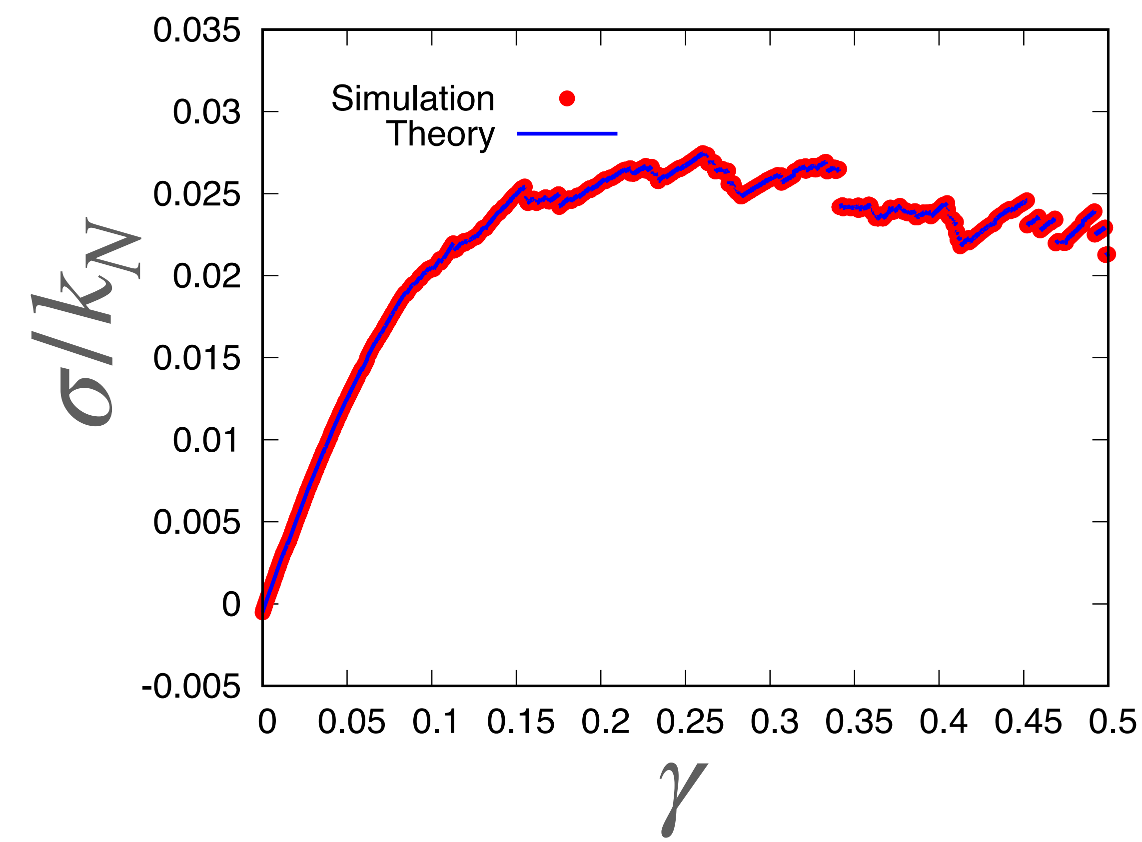
Summary

We have conducted the eigenvalue analysis of amorphous solid consisting of frictional grains under quasi-static shear.

❖ **Rigidity of amorphous solids consisting of frictional grains is determined by Hessian*.**

*Once the stable configuration is given, theory can predict the rigidity except for stress drop point.

- There is no precursor for stress drop, at least, for frictional linear spring system.



Future work

- We will update our theory for slipping contact cases.
- We will investigate system size effects.