Softening and loop trajectories of jammed grains under oscillatory shear

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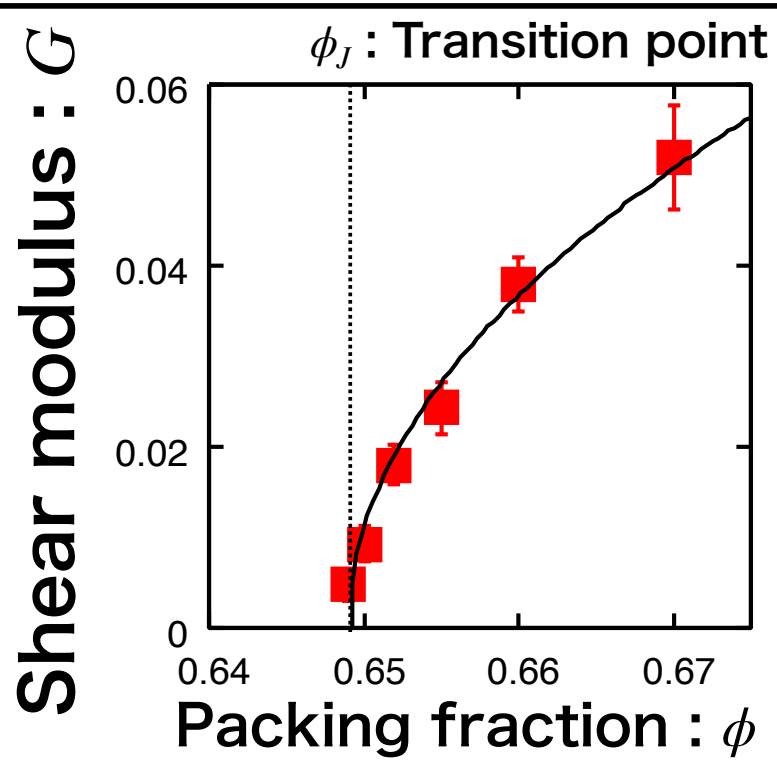
Hisao Hayakawa（Kyoto Univ.)

arXiv:2101.07473
arXiv:2103.14457 (to be published in EPJE)

Rheology of jammed materials

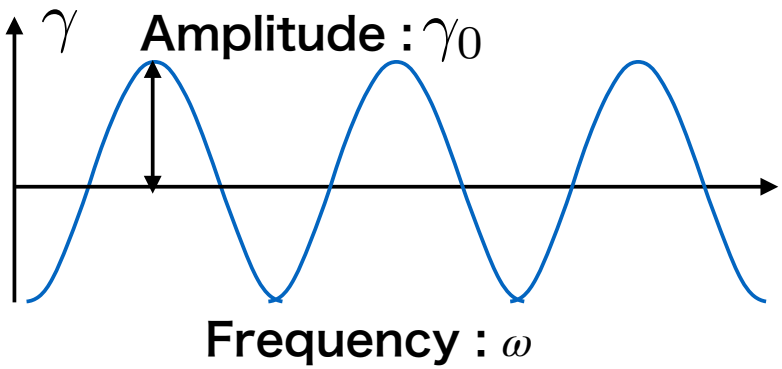
Jammed materials : collections of grains (sand, emulsion)



Dense jammed materials exhibit elasticity.

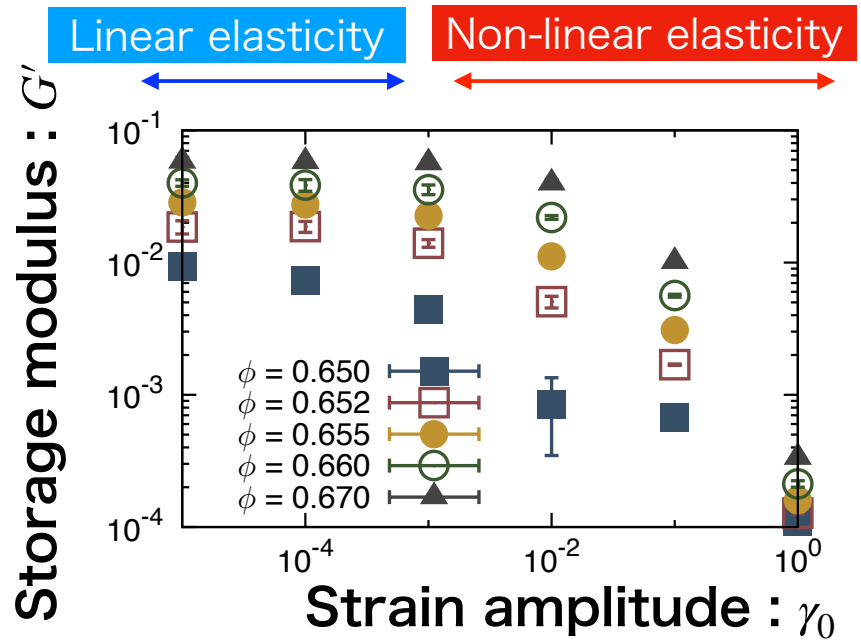
Elasticity of jammed materials under oscillatory shear

Shear strain : $\gamma(t) = \gamma_0 \sin(\omega t)$



MO and H. Hayakawa, 90, 042202 (2014)

Amplitude dependence of G'



Natural conjecture

Origin of non-linear elasticity : Irreversible plastic deformation?

Recent studies suggest

J. Boschan, et. al.,(2016), S. Dagois-Bohy, et. al., (2017), T. Kawasaki and K. Miyazaki, (2020)

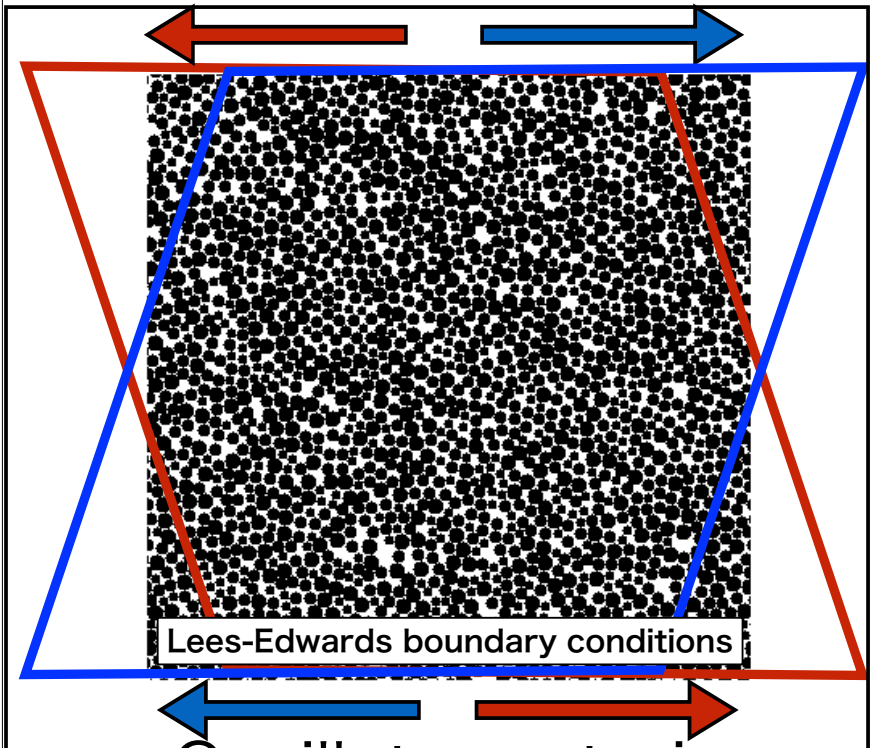
Nonlinear elasticity appears without plastic deformation.

Origin of nonlinear elasticity ?

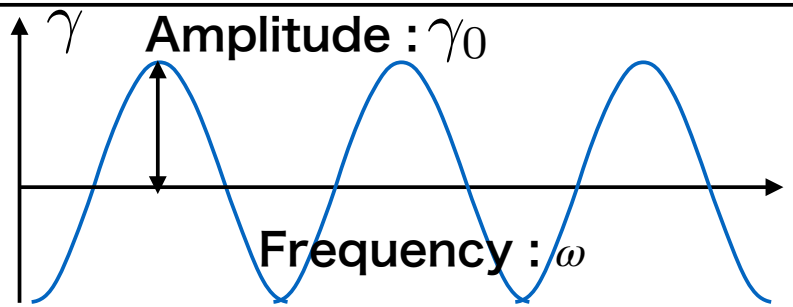
Outline

1. Introduction : Elasticity of jammed grains
2. **Frictionless grains** arXiv:2101.07473
3. Frictional grains arXiv:2103.14457 (to be published in EPJE)
4. Summary

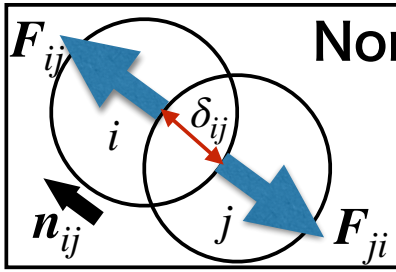
Model : 2D frictionless grains



Oscillatory strain



Strain : $\gamma(t) = \gamma_0 \sin(\omega t)$



Normal repulsive force :

$$\boldsymbol{F}_{ij} = \left(k\delta_{ij} + \eta\dot{\delta}_{ij}\right)\boldsymbol{n}_{ij}$$

Contact length : δ_{ij}

Position : $\boldsymbol{r}_i$

Over-damped eq. :

$$\frac{d}{dt}r_i = \dot{\gamma}(t)y_i\boldsymbol{e}_x + \sum_{j\neq i}\boldsymbol{F}_{ij}/\eta$$

c.f. The same results for under-damped systems

Shear stress : $\sigma(t)$

Storage modulus : elasticity

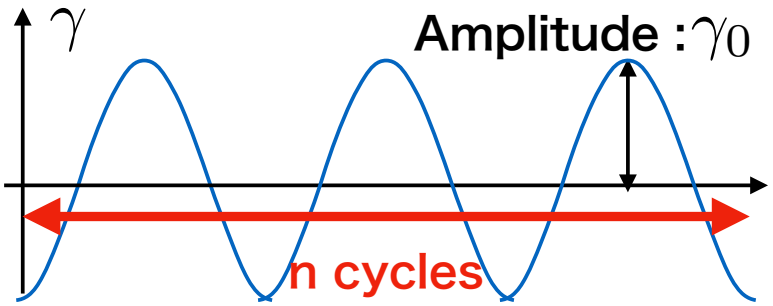
$$G' = \frac{\omega}{\pi}\int_0^{2\pi/\omega} d\theta\, \frac{\sigma(t)\sin(\omega t)}{\gamma_0}$$

Loss modulus : dissipation

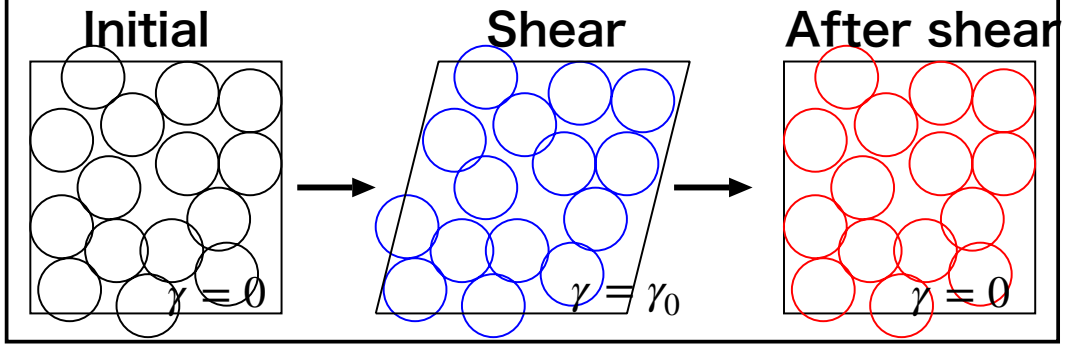
$$G'' = \frac{\omega}{\pi}\int_0^{2\pi/\omega} d\theta\, \frac{\sigma(t)\cos(\omega t)}{\gamma_0}$$

Detecting plastic deformation

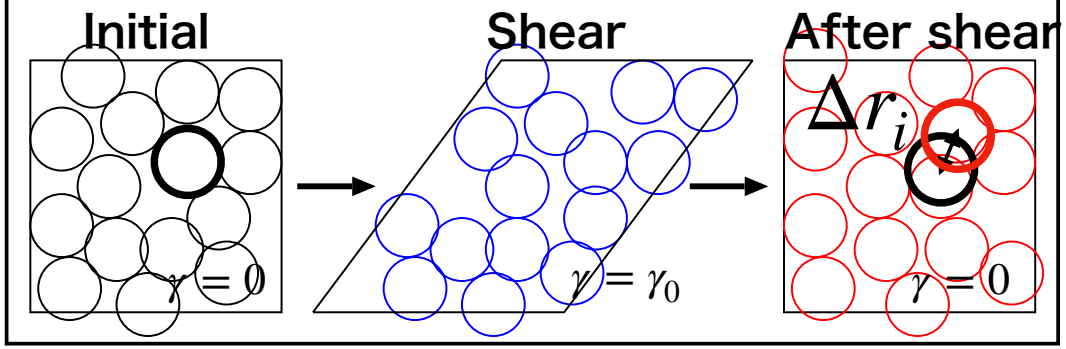
c.f. T. Kawasaki and L. Breathier, Phys. Rev. E 94, 022615 (2016)



Small strain amplitude : no displacement

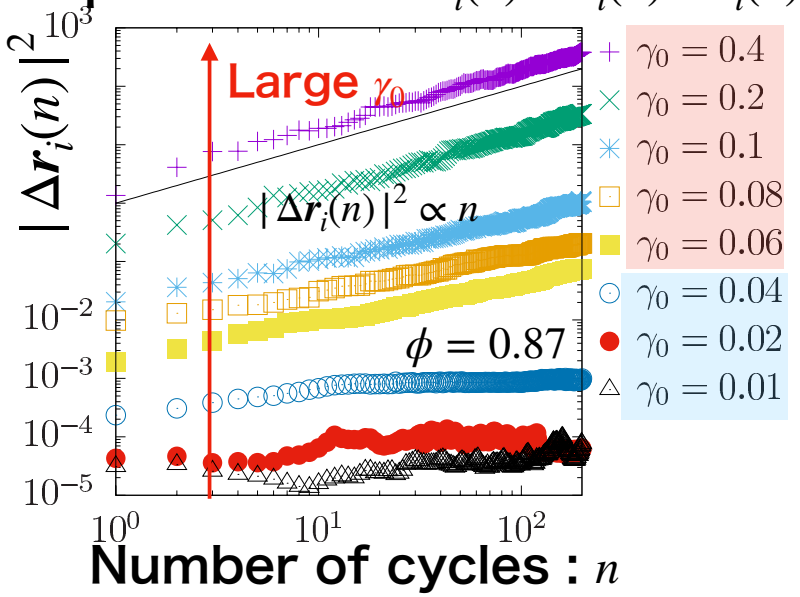


Large strain amplitude : finite displacement

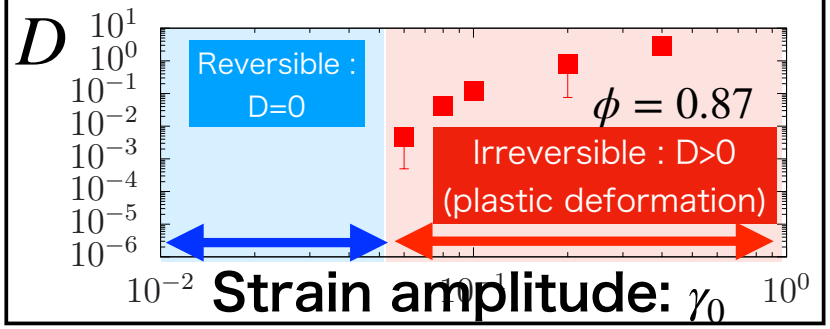


Position after n cycle : $\boldsymbol{r}_i(n)$

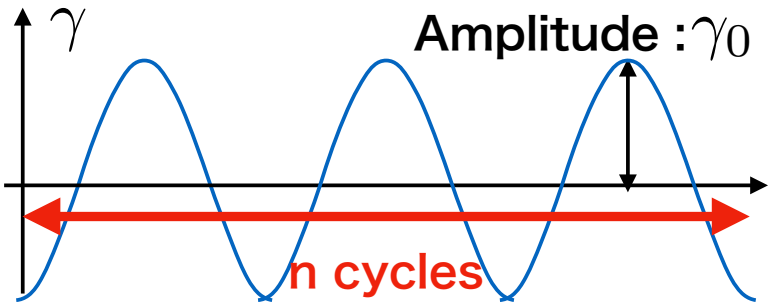
Displacement : $\Delta \boldsymbol{r}_i(n) = \boldsymbol{r}_i(n) - \boldsymbol{r}_i(0)$



Diffusion coefficient : $D = \lim_{n \to \infty} \Delta \boldsymbol{r}_i / n$



Loop trajectory in reversible phase



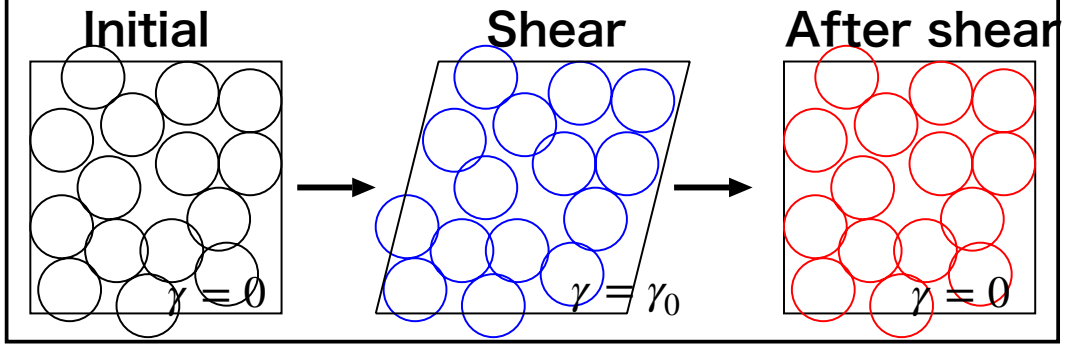
Position : $\boldsymbol{r}_i(t) = \boldsymbol{R}_i + \gamma(t) Y_i \boldsymbol{e}_x + \tilde{\boldsymbol{r}}_i(t)$

Initial position : $\boldsymbol{R}_i = (X_i, Y_i)$ (Macroscopic shear)

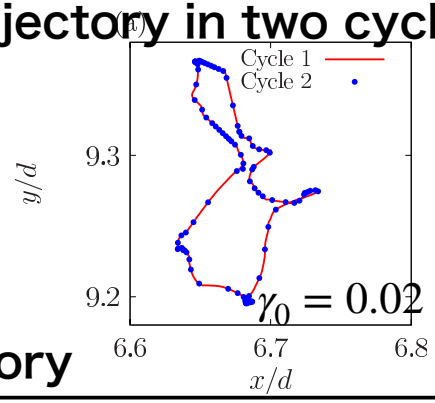
Affine motion : $\gamma(t) Y_i \boldsymbol{e}_x$

Non-affine motion : $\tilde{\boldsymbol{r}}_i(t)$

Small strain amplitude : no displacement

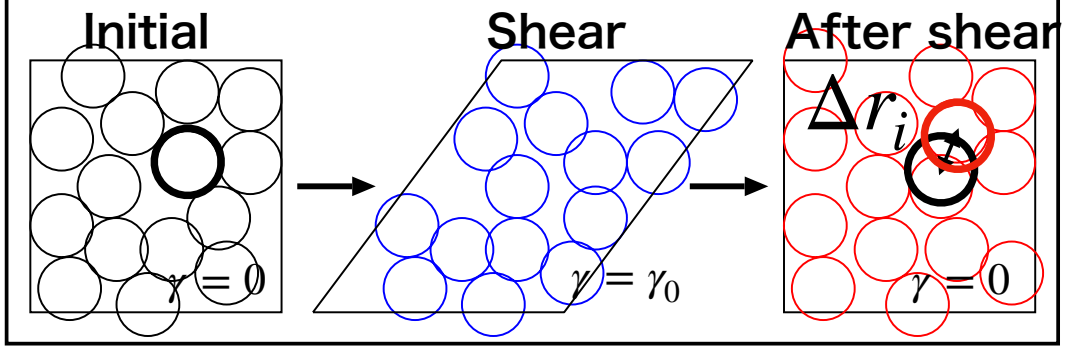


Reversible Trajectory in two cycle

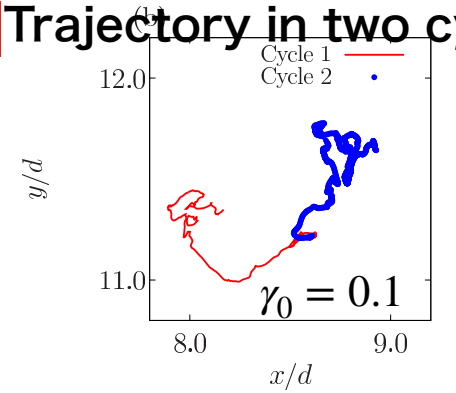


Loop trajectory

Large strain amplitude : finite displacement

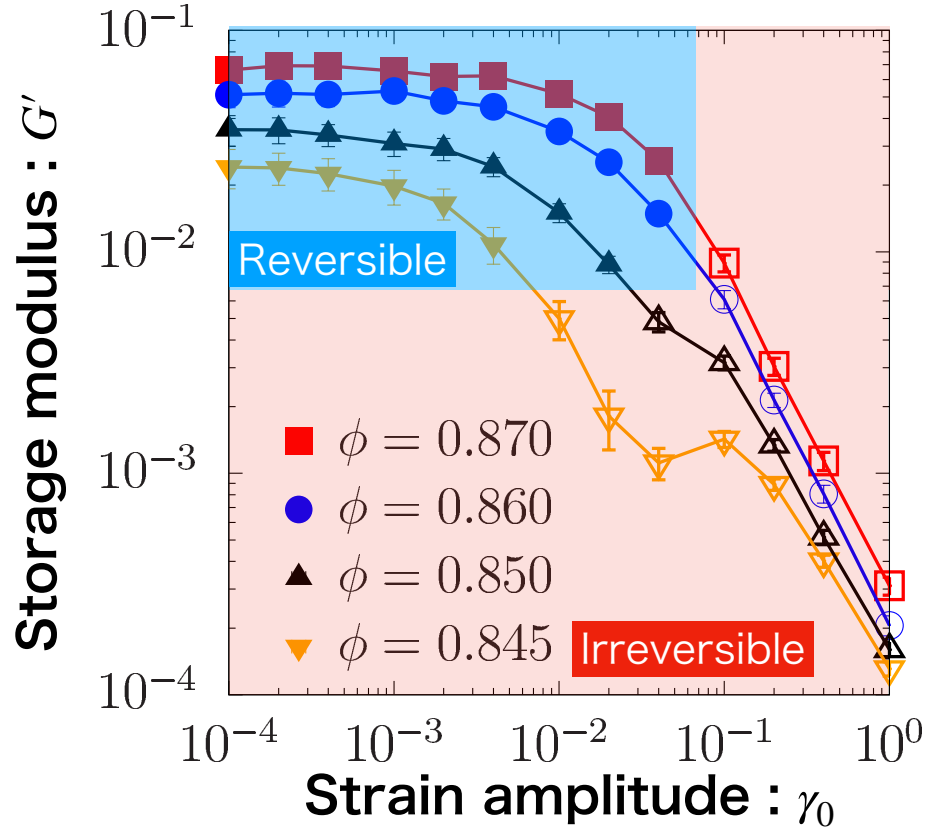


Irreversible Trajectory in two cycle

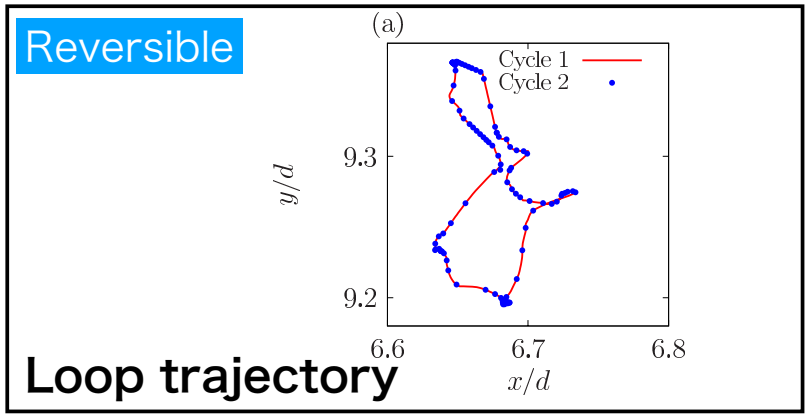


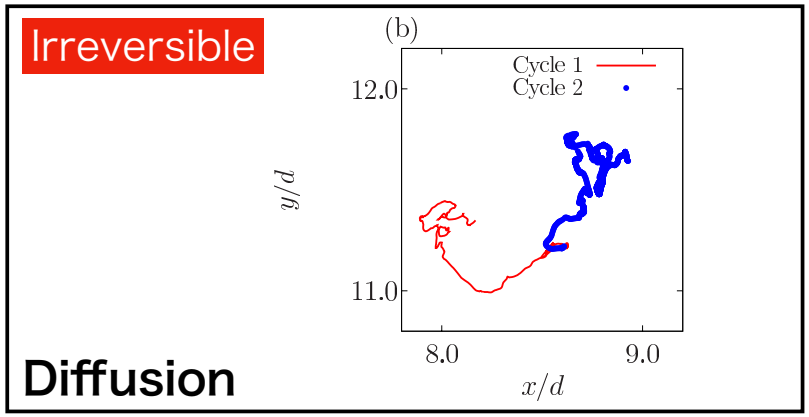
Diffusion

Storage modulus



G' decreases even in the reversible phase.

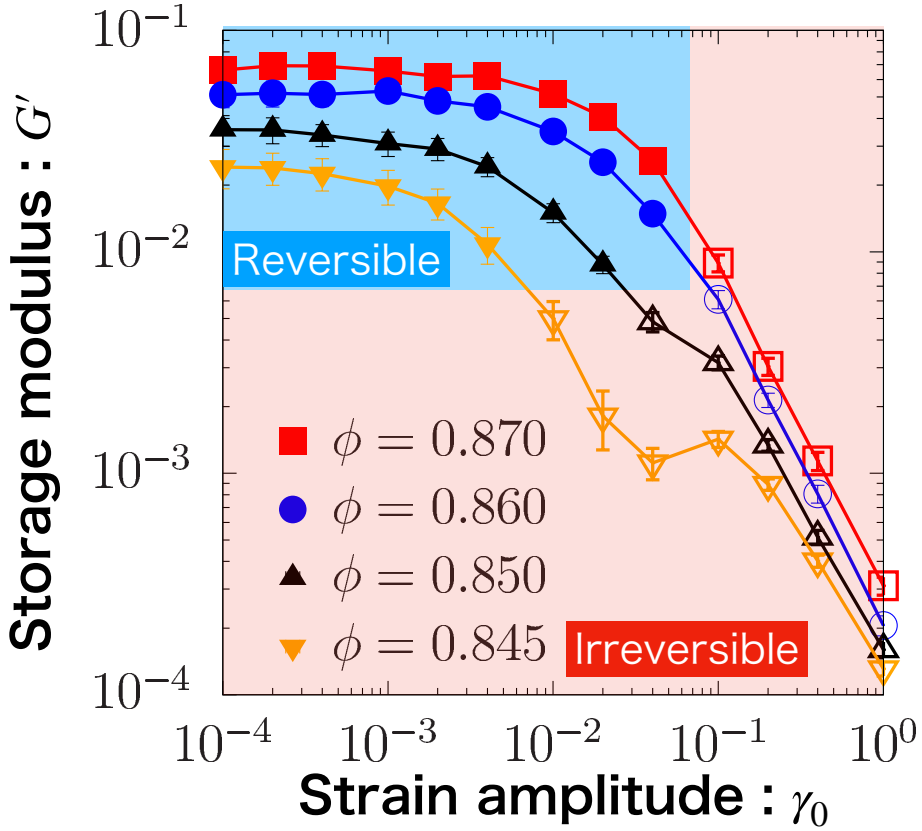


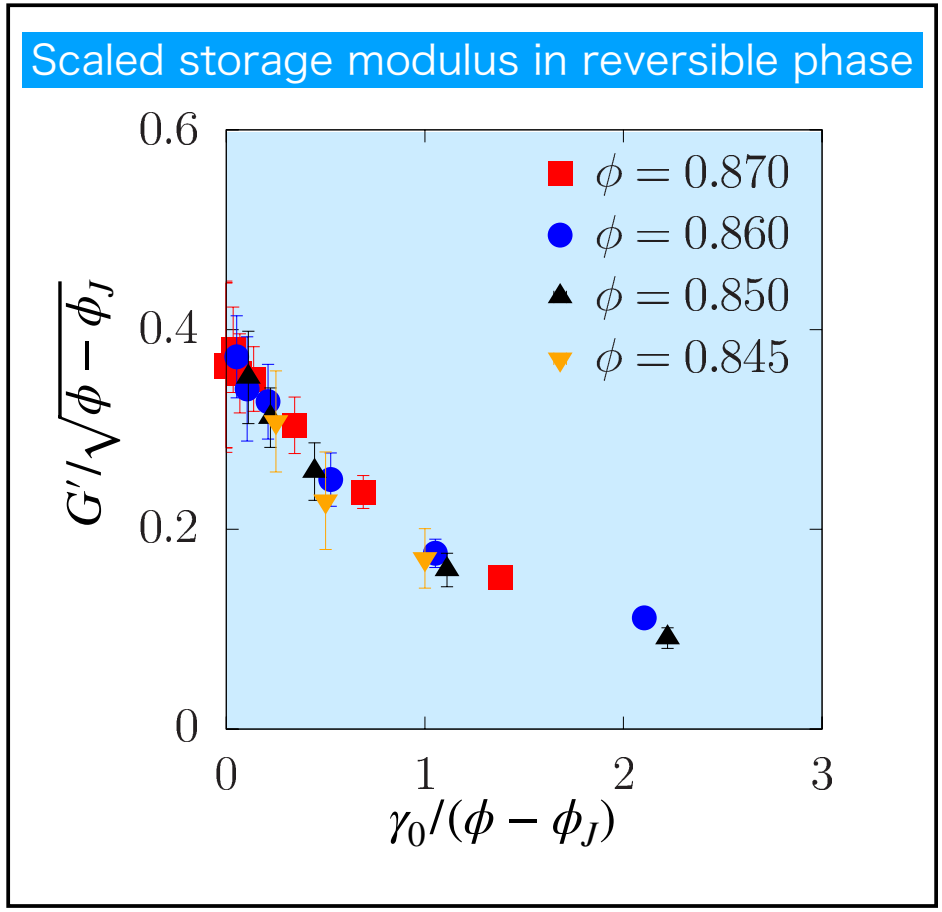


Irreversible yielding : Decrease of G' in the irreversible phase.

Reversible softening : Decrease of G' in the reversible phase.

Reversible softening



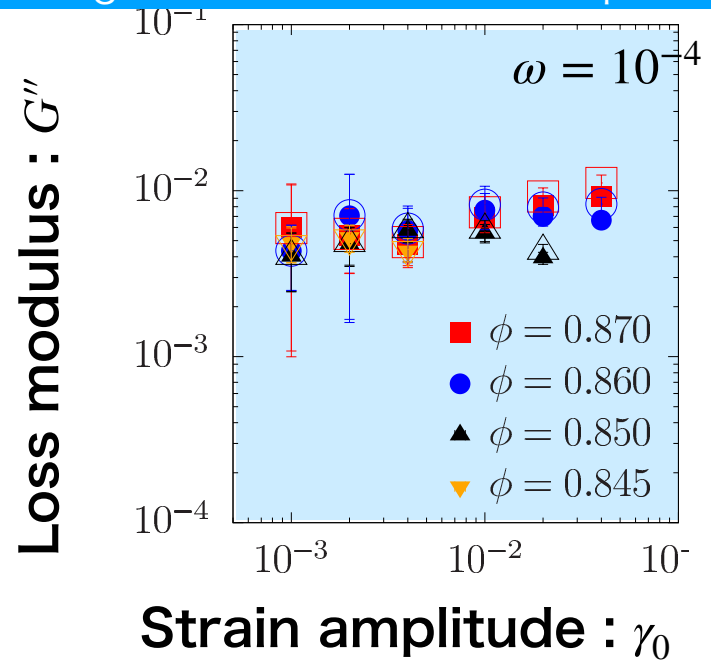


Reversible softening : Decrease of G' in the reversible phase.

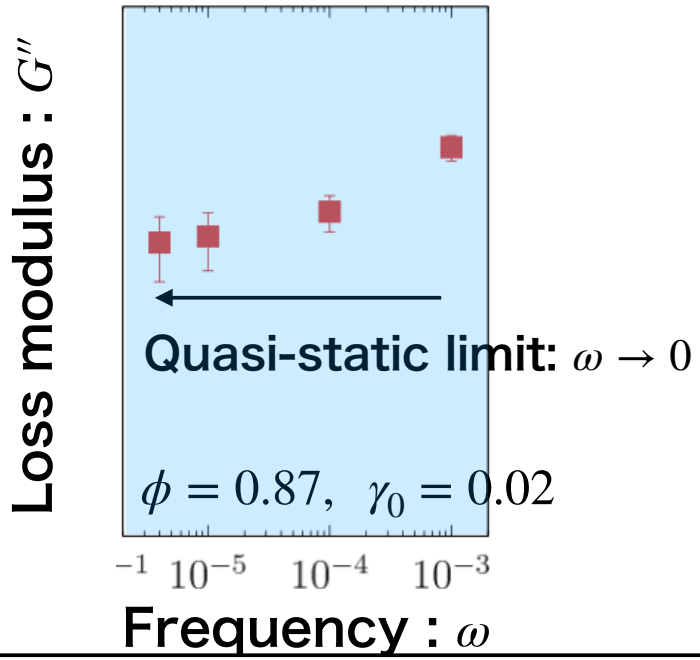
G' decreases to less than half.

Residual loss modulus

Storage modulus in reversible phase



Loss modulus for different ω



G" is almost independent of ϕ and γ_0.
Residual loss modulus : G" remains for $\omega \to 0$ without plastic deformation.

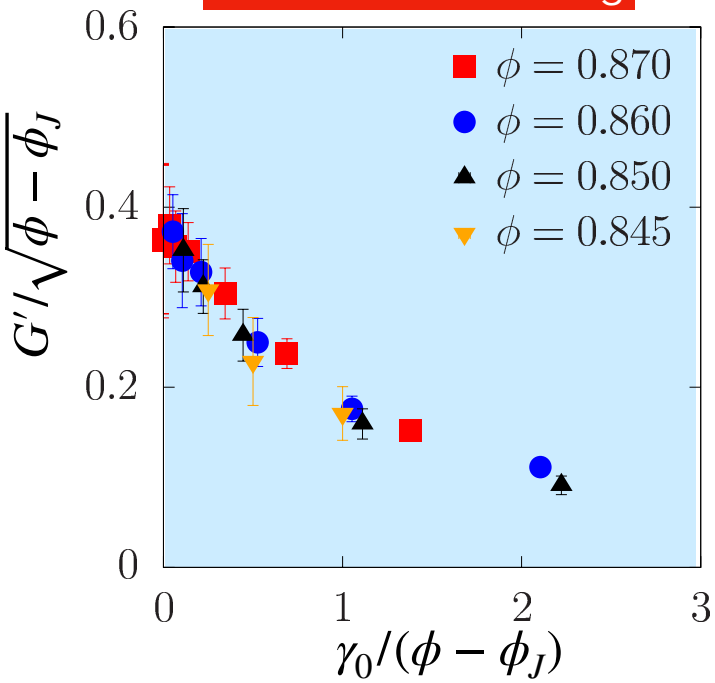
cf. Linear visco elasticity : $\sigma = G\gamma + \eta\dot{\gamma}$

(Kelvin-Voigt model) $G' = G, \ G'' = \eta\omega$

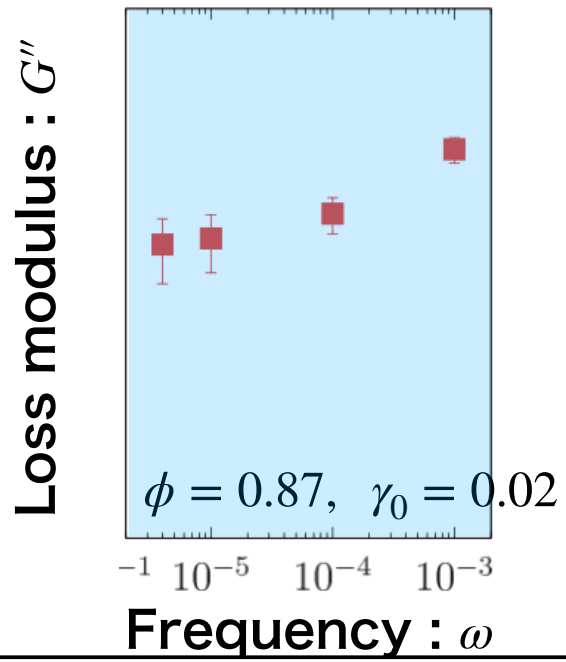
Dissipation (G") disappears for $\omega \to 0$.

Origin of anomalous response?

Reversible softening



Residual loss modulus

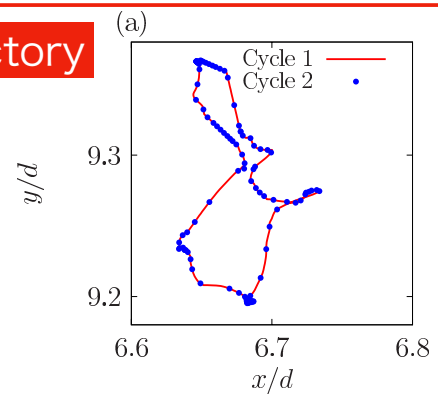


Origin of anomalous response:
Loop trajectory ?

↓

We analytically check this conjecture.

Loop trajectory



Fourier analysis of loop trajectories

Phase : $\theta = \omega t$ **(quasi-static limit)**

Shear strain : $\gamma(\theta) = \gamma_0 \sin\theta$

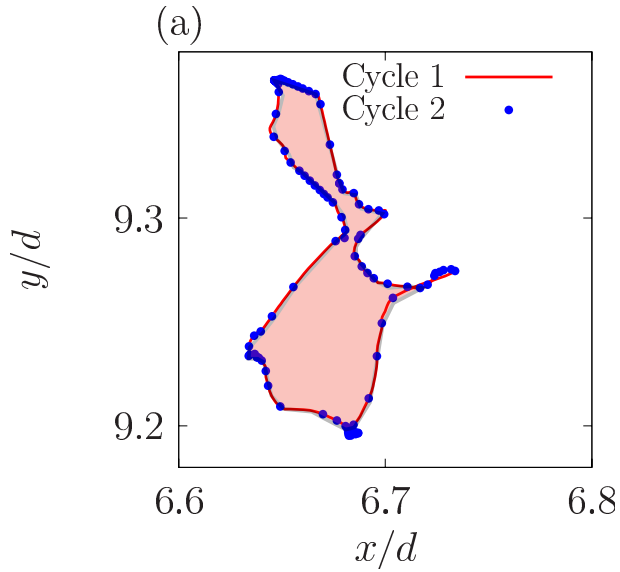
Reversible phase **(periodic function)**

Position : $\boldsymbol{r}_i(\theta) = \boldsymbol{r}_i(\theta + 2\pi)$

Non-affine motion :

$$\tilde{\boldsymbol{r}}_i(\theta) = \tilde{\boldsymbol{r}}_i(\theta + 2\pi)$$

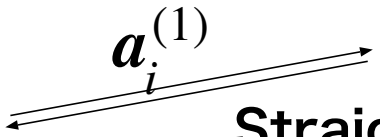
Non-affine trajectory : $\boldsymbol{r}_i(t) - \gamma(t) Y_i \boldsymbol{e}_x$



Fourier series of non-affine motion

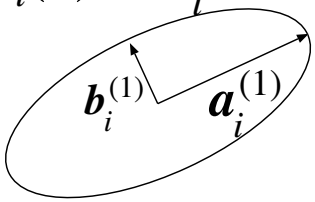
$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

Examples 1: $\tilde{\boldsymbol{r}}_i(\theta) = \boldsymbol{a}_i^{(1)} \sin\theta$



Straight line

Examples 2: $\tilde{\boldsymbol{r}}_i(\theta) = \boldsymbol{a}_i^{(1)} \sin\theta + \boldsymbol{b}_i^{(1)} \cos\theta$



Ellipse

Area of loop

$$A_i = \oint \tilde{x}_i(\theta) d\tilde{y}_i(\theta) = \pi \sum_n n \{ \boldsymbol{b}_i^{(n)} \times \boldsymbol{a}_i^{(n)} \}_z$$

Fourier coefficients characterizes the area.

Fourier coefficients

Fourier series of non-affine motion

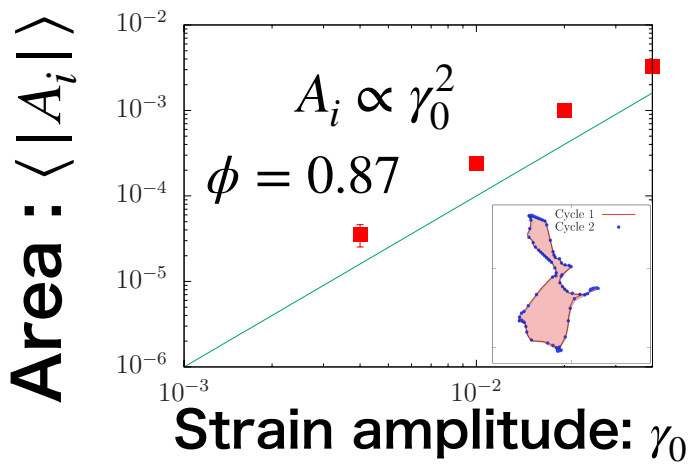
$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

Shear strain : $\gamma(\theta) = \gamma_0 \sin\theta$

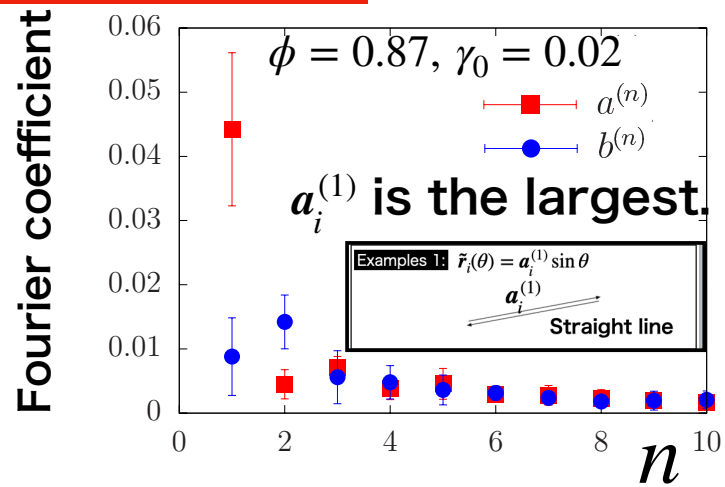
Area of loop

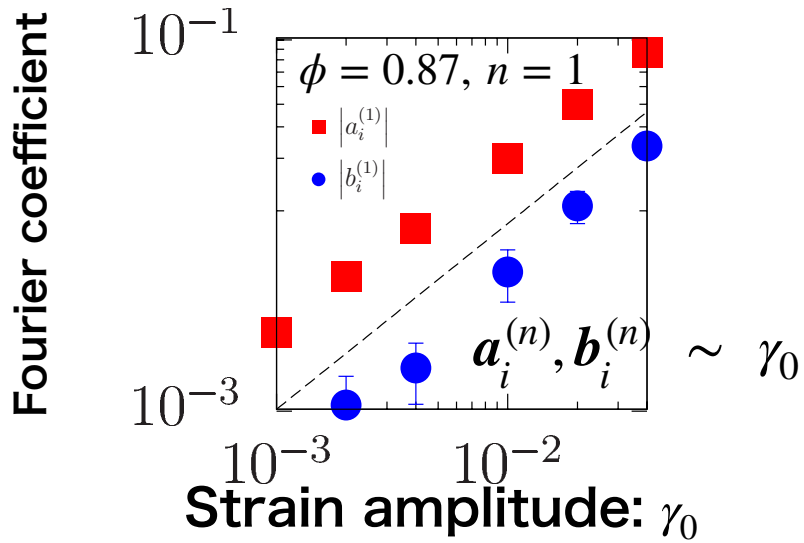
$$A_i = \oint \tilde{x}_i(\theta) d\tilde{y}_i(\theta) = \pi \sum_n n \{ \boldsymbol{b}_i^{(n)} \times \boldsymbol{a}_i^{(n)} \}_z$$

Fourier coefficients characterizes the area.



Fourier coefficient





c.f. $\boldsymbol{a}_i, \boldsymbol{b}_i \sim (\gamma_0 d)$, $A \sim (\gamma_0 d)^2$ **indicate the trajectory is scaled by** $\gamma_0 d$. d **: diameter of grain**

Analysis : Reversible softening

Shear strain : $\gamma(\theta) = \gamma_0 \sin\theta$
(quasi-static limit)

Storage modulus :

$$G' = \frac{1}{\pi}\int_0^{2\pi} d\theta \, \frac{\sigma(t)\sin\theta}{\gamma_0}$$

Stress : $\sigma(\theta) = -\sum_{i,j} \frac{x_{ij}(\theta)y_{ij}(\theta)}{L^2 r_{ij}(\theta)} F(r_{ij}(\theta))$

Normal repulsive force : $F(r)$

Position : $\boldsymbol{r}_i(\theta) = \boldsymbol{R}_i + \gamma(\theta) Y_i \boldsymbol{e}_x + \tilde{\boldsymbol{r}}_i(\theta)$

Initial position : $\boldsymbol{R}_i = (X_i, Y_i)$

Non-affine motion : Loop

$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

First order approximation of γ_0, $\boldsymbol{a}_i^{(n)}$, and $\boldsymbol{b}_i^{(n)}$

Only modes with $n = 1$ $(\sin\theta)$ remain in the integral of θ.

$$G' \simeq G'_1 = \langle A' \rangle - \sum_i \left\langle \boldsymbol{B}'_i \cdot \frac{\boldsymbol{a}_i^{(1)}}{\gamma_0} \right\rangle$$

$A', \boldsymbol{B}'_i$: functions of $\boldsymbol{R}_i$

G' depends only on $\boldsymbol{a}_i^{(1)}$.

Detail :

$$\begin{aligned} G'_1 = & -\left\langle \frac{1}{L^2}\sum_{i,j}\left\{ \frac{X_{ij}^2 Y_{ij}^2}{R_{ij}}\Psi'(R_{ij}) + Y_{ij}^2 \Psi(R_{ij}) \right\} \right\rangle \\ & -\left\langle \frac{1}{L^2}\sum_{i,j}\left(\frac{a_{ij,x}^{(1)}}{\gamma_0} Y_{ij} + X_{ij}\frac{a_{ij,y}^{(1)}}{\gamma_0} \right)\Psi(R_{ij}) \right\rangle \\ & -\left\langle \frac{1}{L^2}\sum_{i,j} X_{ij}Y_{ij}\Psi'(R_{ij}) \frac{\boldsymbol{R}_{ij}\cdot \boldsymbol{a}_{ij}^{(1)}}{\gamma_0 R_{ij}} \right\rangle, \end{aligned}$$

Fourier coefficient (n=1) for loop trajectories → Reversible Softening

Analysis : Residual loss modulus

Shear strain : $\gamma(\theta) = \gamma_0 \sin\theta$

(quasi-static limit)

Loss modulus :

$$G'' = \frac{1}{\pi}\left\langle \int_0^{2\pi} d\theta \, \frac{\sigma(t)\cos\theta}{\gamma_0} \right\rangle$$

Stress : $\sigma(\theta) = -\sum_{i,j} \frac{x_{ij}(\theta) y_{ij}(\theta)}{L^2 r_{ij}(\theta)} F(r_{ij}(\theta))$

Normal repulsive force : $F(r)$

Position : $\boldsymbol{r}_i(\theta) = \boldsymbol{R}_i + \gamma(\theta) Y_i \boldsymbol{e}_x + \tilde{\boldsymbol{r}}_i(\theta)$

Initial position : $\boldsymbol{R}_i = (X_i, Y_i)$

Non-affine motion : Loop

$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

First order approximation of γ_0, $\boldsymbol{a}_i^{(n)}$, and $\boldsymbol{b}_i^{(n)}$

Only modes with $n = 1$ $(\cos\theta)$ remain in the integral of θ.

$$G'' \simeq G''_1 = \sum_i \left\langle \boldsymbol{B}''_i \cdot \frac{\boldsymbol{b}_i^{(1)}}{\gamma_0} \right\rangle$$

B''_i : function of $\boldsymbol{R}_i$

G'' depends only on $\boldsymbol{b}_i^{(1)}$.

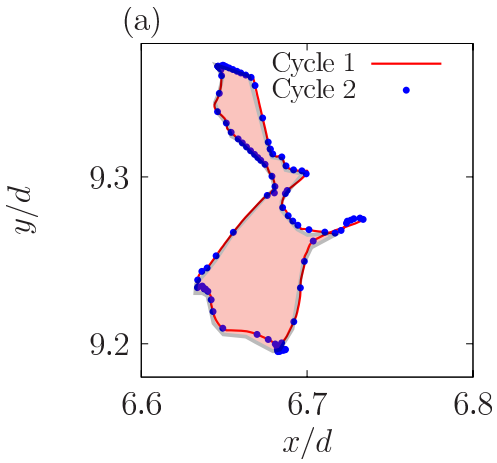
Detail :

$$G''_1 = -\left\langle \frac{1}{L^2} \sum_{i,j} \left(\frac{b_{ij,x}^{(1)}}{\gamma_0} Y_{ij} + X_{ij} \frac{b_{ij,y}^{(1)}}{\gamma_0} \right) F(R_{ij}) \right\rangle - \left\langle \frac{1}{L^2} \sum_{i,j} X_{ij} Y_{ij} F'(R_{ij}) R_{ij} \frac{\boldsymbol{R}_{ij} \cdot \boldsymbol{b}_{ij}^{(1)}}{\gamma_0 R_{ij}^2} \right\rangle$$

Fourier coefficient (n=1) for loop trajectories → Residual loss modulus

Validity of theoretical prediction

Fourier analysis of loop trajectory



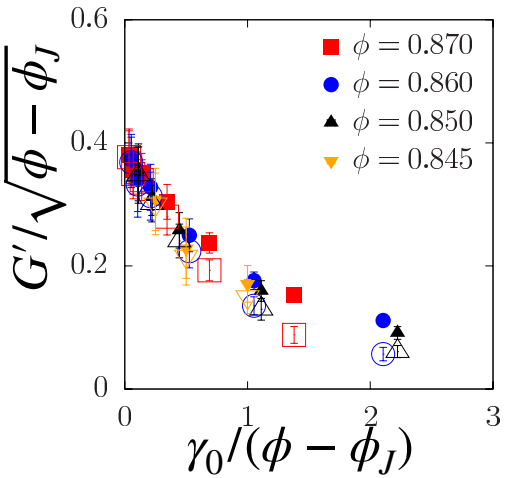
$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

Theoretical prediction

$$G' \simeq G'_1 = \langle A' \rangle - \sum_i \left\langle \boldsymbol{B}'_i \cdot \frac{\boldsymbol{a}_i^{(1)}}{\gamma_0} \right\rangle$$

$$G'' \simeq G''_1 = \sum_i \left\langle \boldsymbol{B}''_i \cdot \frac{\boldsymbol{b}_i^{(1)}}{\gamma_0} \right\rangle$$

Reversible softening

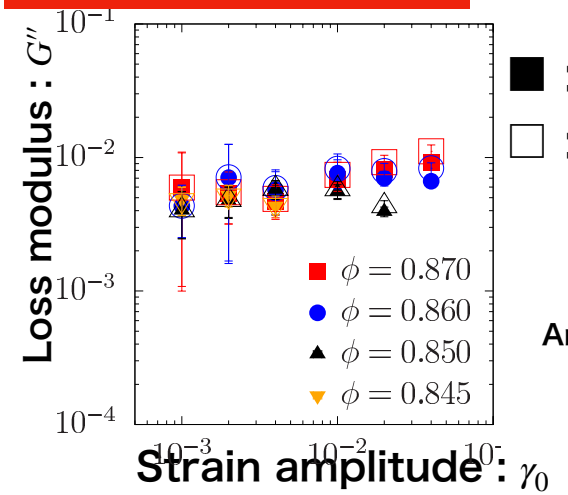


■ : **Original** (closed symbol)

□ : **Analytical** (open symbol)

Analytical results are consistent with the numerical data.

Residual loss modulus



■ : **Original** (closed symbol)

□ : **Analytical** (open symbol)

Analytical results are consistent with the numerical data.

The anomalous response is connected with the loop trajectory in frictionless system.

Outline

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2. Frictionless grains arXiv:2101.07473
3. **Frictional grains** arXiv:2103.14457 (to be published in EPJE)
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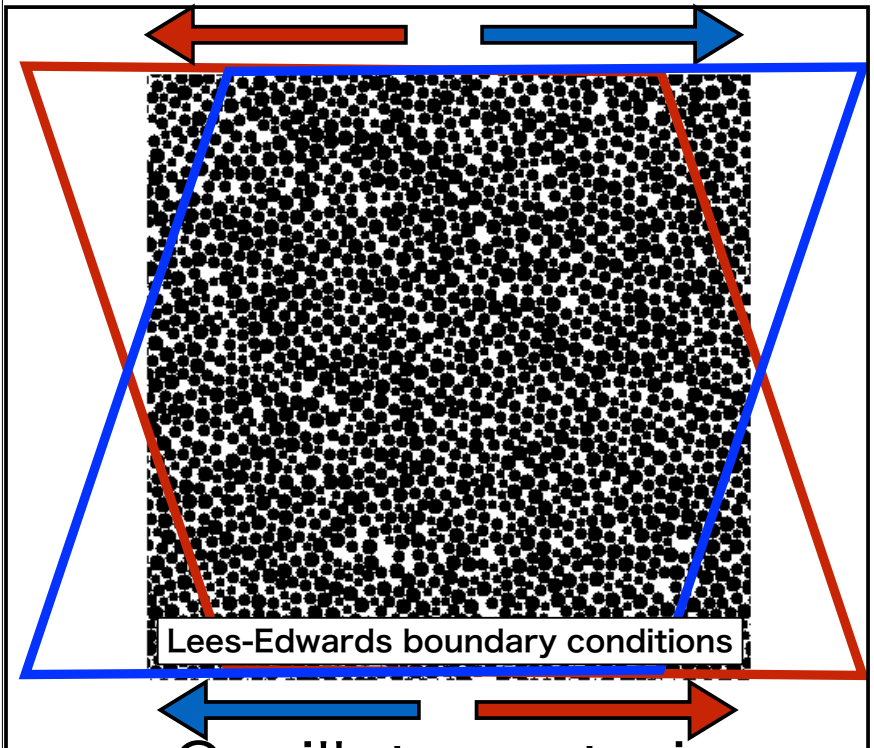
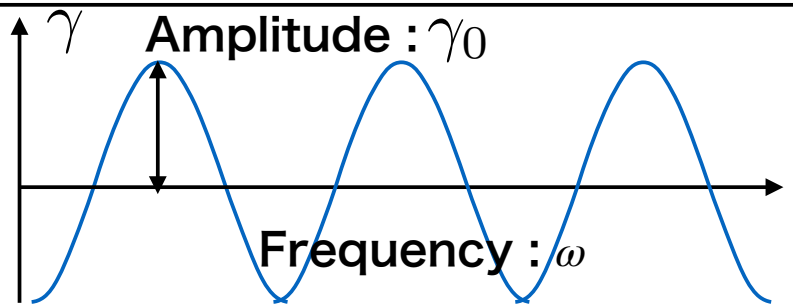
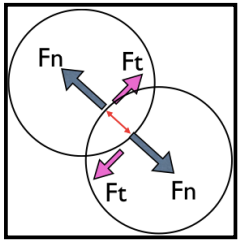
Model : 2D frictional grains



Oscillatory strain



Strain : $\gamma(t) = \gamma_0 \sin(\omega t)$



F_n : Normal force

F_t : Tangential friction

Coulomb law : $F_t \leq \mu F_n$

μ : Friction coefficient

SLLOD eq. :

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m_i} + \dot{\gamma}(t) r_{i,y} \hat{\boldsymbol{x}},$$

$$\frac{d\boldsymbol{p}_i}{dt} = \sum_{j \neq i} \boldsymbol{F}_{ij} - \dot{\gamma}(t) p_{i,y} \hat{\boldsymbol{x}},$$

Shear stress : $\sigma(t)$

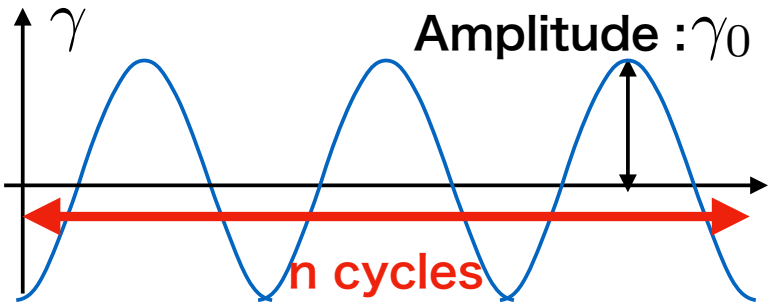
Storage modulus : elasticity

$$G' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\sin(\omega t)}{\gamma_0}$$

Loss modulus : dissipation

$$G'' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\cos(\omega t)}{\gamma_0}$$

Trajectory in reversible phase

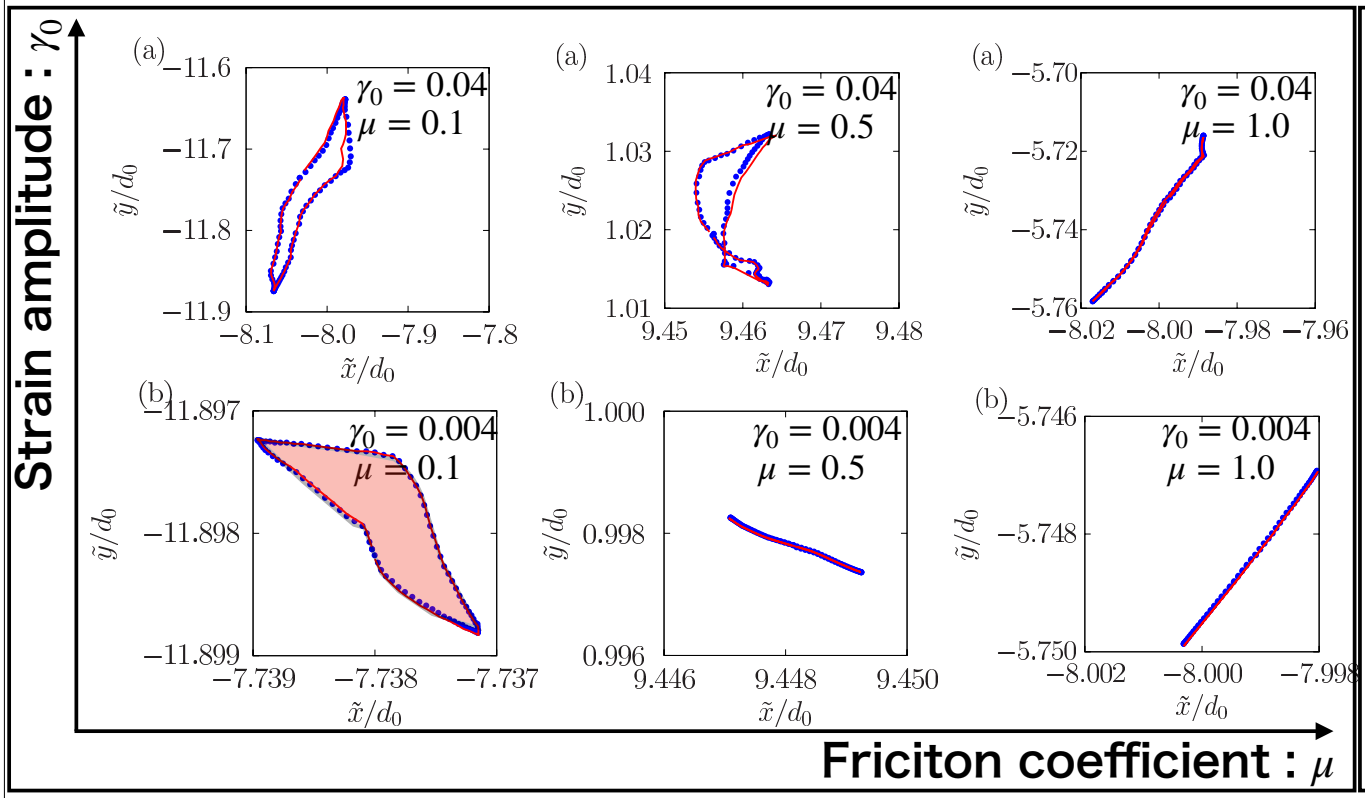


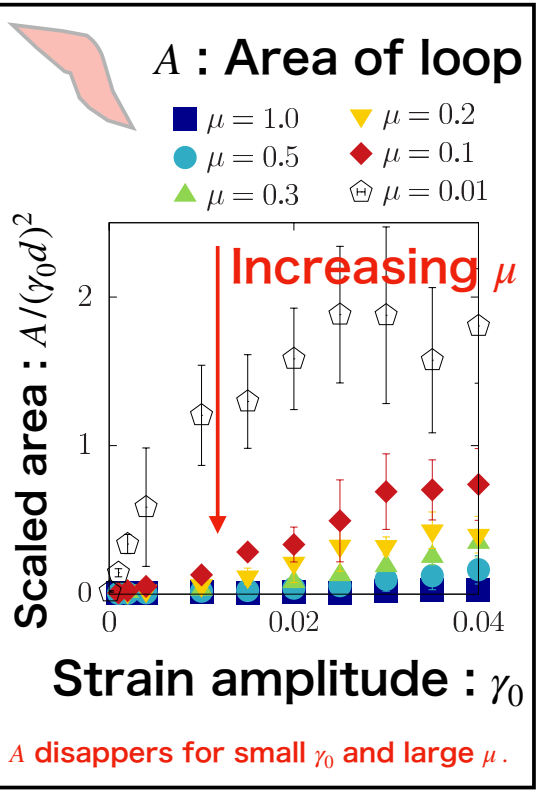
Position : $\boldsymbol{r}_i(t) = \boldsymbol{R}_i + \gamma(t) Y_i \boldsymbol{e}_x + \tilde{\boldsymbol{r}}_i(t)$

Initial position : $\boldsymbol{R}_i = (X_i, Y_i)$ (Macroscopic shear)

Affine motion : $\gamma(t) Y_i \boldsymbol{e}_x$

Non-affine motion : $\tilde{\boldsymbol{r}}_i(t)$



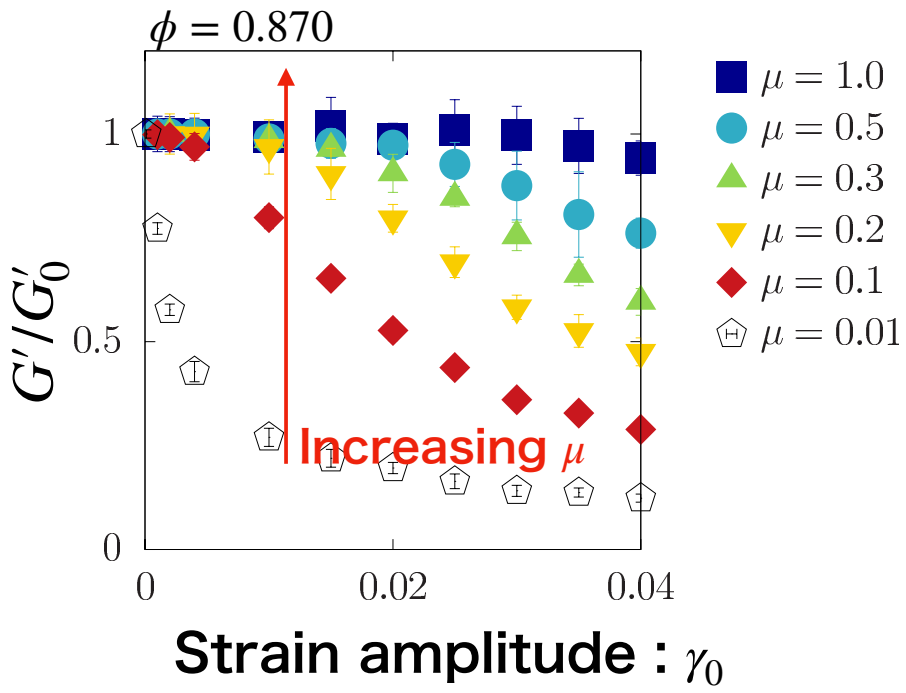


A disappers for small γ_0 and large μ.

c.f. $A \sim (\gamma_0 d)^2$ if the trajectory is scaled by $\gamma_0 d$ with the diameter of grain d.

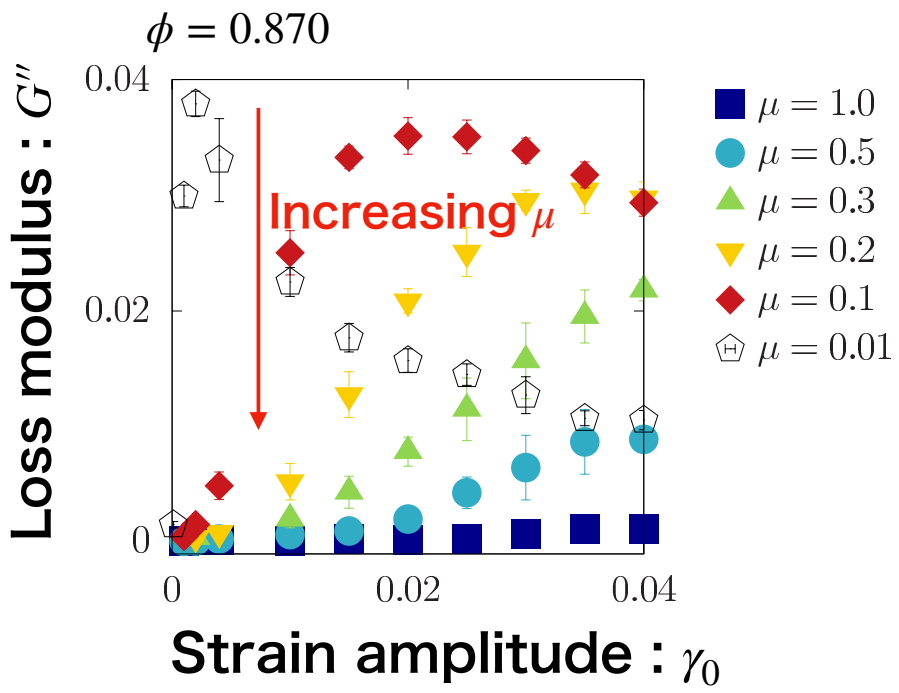
Rheological properties in reversible phase

Storage modulus in reversible phase



G'_0 : Storage modulus in the limit of $\gamma_0 \to 0$.

Loss modulus in reversible phase



Reversible softening : G' decreases in the reversible phase.

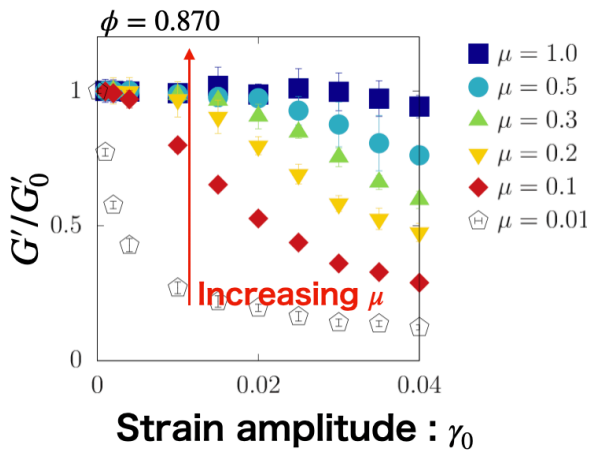
The softening disappears for small γ_0 and large μ.

Residual loss modulus : G'' remains in the reversible phase.

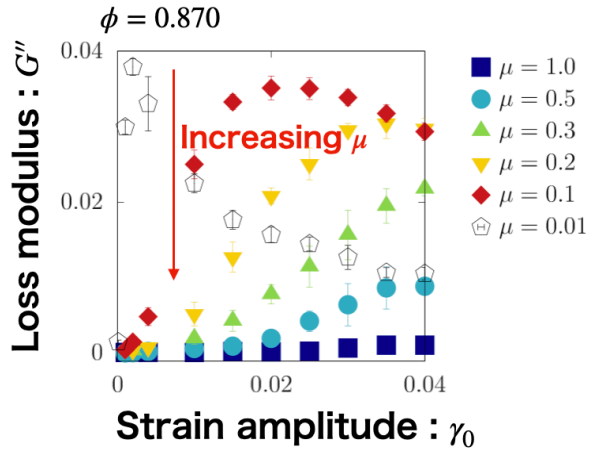
The loss modulus disappears for small γ_0 and large μ.

Rheological properties and loop

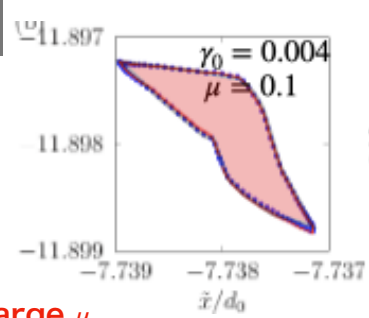
Reversible softening

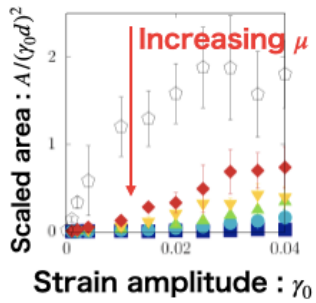


Residual loss modulus



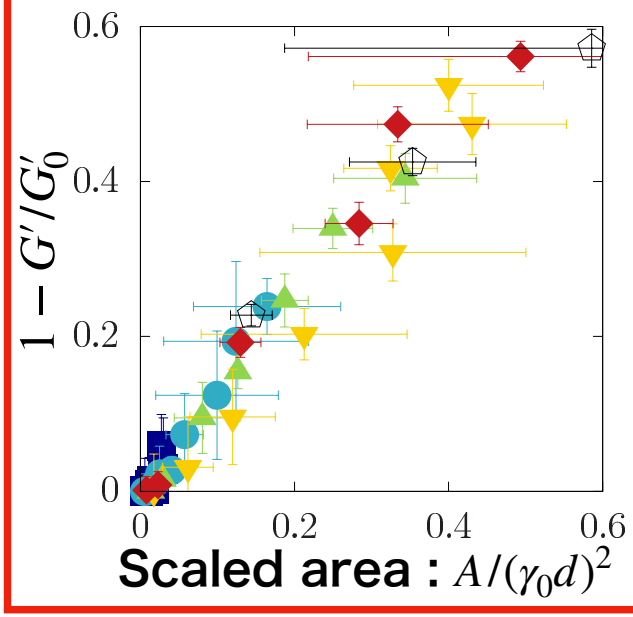
Area of loop trajectory

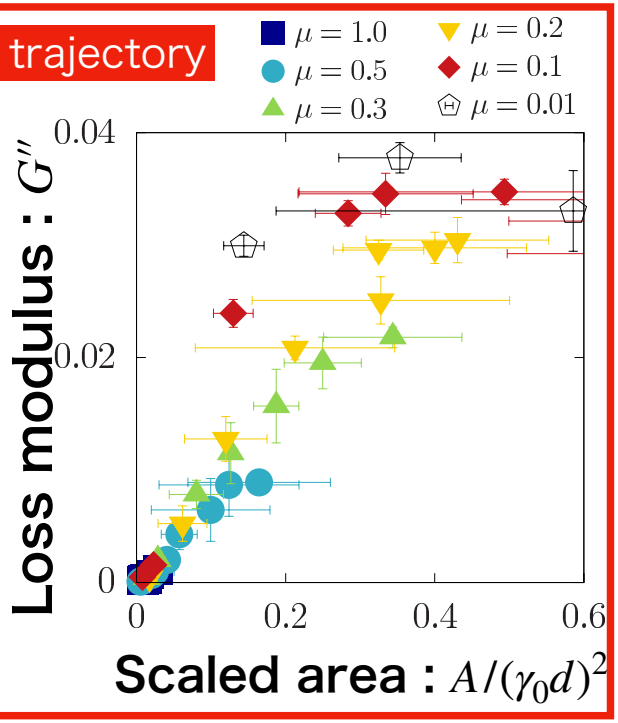




A disappers for small γ_0 and large μ.

Anomalous response and loop trajectory





Anomalous response is scaled by the area of loops.

Outline

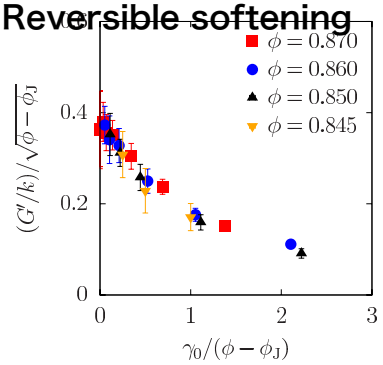
1. Introduction : Elasticity of jammed grains
2. Frictionless grains arXiv:2101.07473
3. Frictional grains arXiv:2103.14457 (to be published in EPJE)
4. **Summary**

Summary

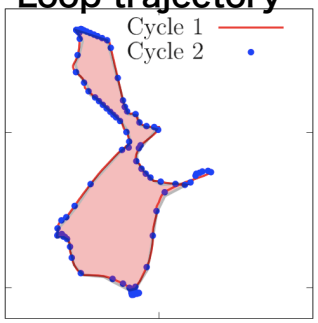
arXiv:2101.07473
arXiv:2103.14457

- Topic : Non-linear elasticity of jammed grains.
- Result 1 : Non-linear elasticity (reversible softening and residual loss modulus) .
- Result 2 : Loop trajectories in the reversible phase.
- Result 3 : The non-linear elasticity is analytically related to the Fourier coefficients of loop trajectories for frictionless grains.
- Result 4 : We numerically connect the non-linear elasticity with the area of loop trajectories in frictional systems.
- Future work : Analysis for frictional grains.

Reversible softening



Loop trajectory



Analysis (frictionless) :

$$\tilde{\boldsymbol{r}}_i(\theta) = \sum_n \left\{ \boldsymbol{a}_i^{(n)} \sin n\theta + \boldsymbol{b}_i^{(n)} \cos n\theta \right\}$$

$$G_1' = \langle A' \rangle - \sum_i \left\langle \boldsymbol{B}_i' \cdot \frac{\boldsymbol{a}_i^{(1)}}{\gamma_0} \right\rangle$$

$$G_1'' = \sum_i \left\langle \boldsymbol{B}_i'' \cdot \frac{\boldsymbol{b}_i^{(1)}}{\gamma_0} \right\rangle$$

Frictional grains :