イオン渋滞学
科研費・学術変革(A)

創発的研究支援事業
Fusion Oriented REsearch for disruptive Science and Technology

MOONSHOT
RESEARCH & DEVELOPMENT PROGRAM

ML PhYs
Foundation of "Machine Learning Physics"

Unified understanding of nonlinear rheology near jamming

Nagoya University

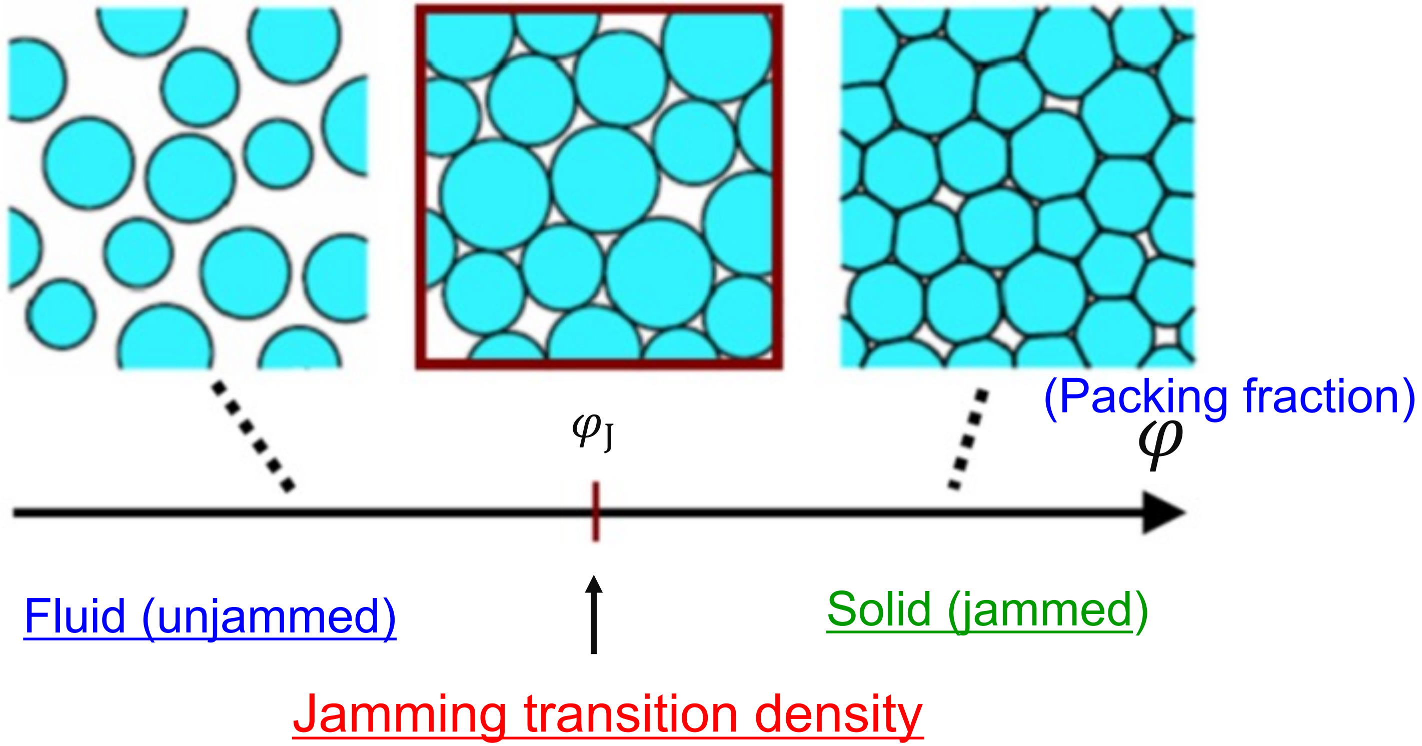
Takeshi Kawasaki

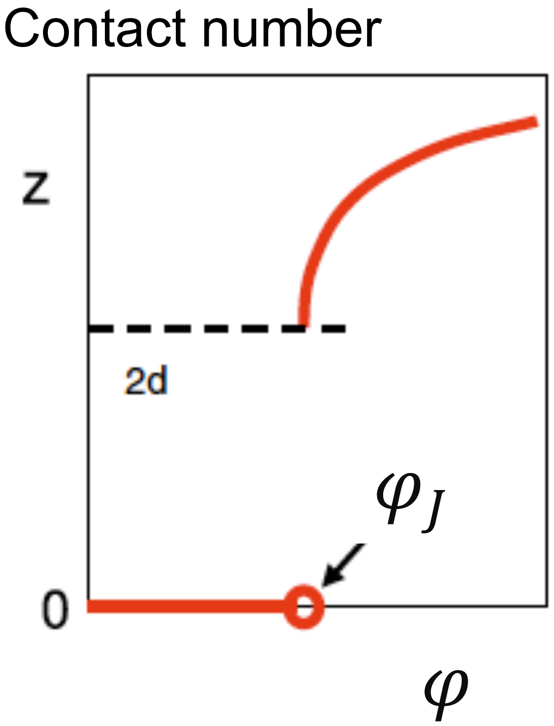
Collaboration with Kunimasa Miyazaki (Nagoya Univ.)

Ref: T. Kawasaki and K. Miyazaki, Phys. Rev. Lett. **132**, 268201 (2024)

Intro: Jamming transition

- Increasing the density of "athermal" particles:
  - ➡ Fluid – solid state transition: jamming transition





- In the vicinity of the jamming transition point $(\varphi = \varphi_J)$, mechanical property and mechanical response of the system are critical and nonlinear.

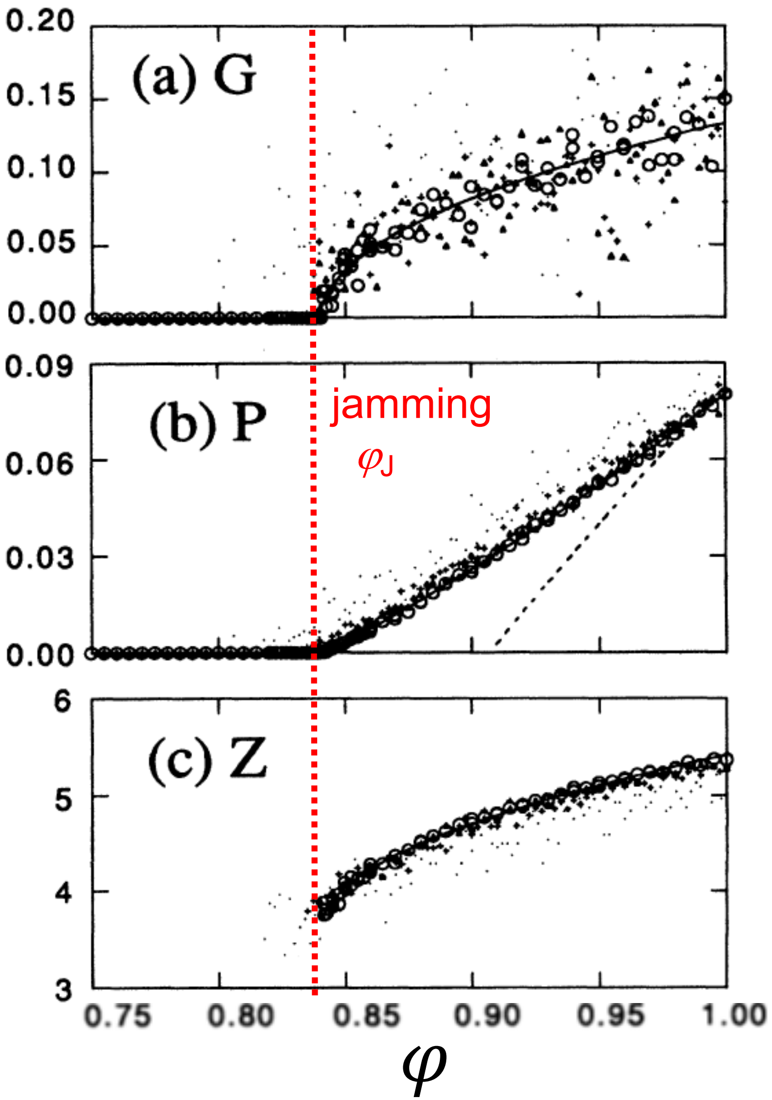
M. van Hecke, J. Phys.: Condens. Matter **22**, 033101 (2010).

Intro: Critical behaviors near jamming

(a) Shear modulus

(b) Pressure

(c) Contact number



D. J. Durian, Phys. Rev. Lett. **75**, 4780 (1995)

$$G \sim (\varphi - \varphi_J)^{\alpha - \frac{3}{2}}$$

$$P \sim (\varphi - \varphi_J)^{\alpha - 1}$$

α: Hyper-elasticity exponent of the inter-particle potential

$$\Delta Z = Z - 2d \sim (\varphi - \varphi_J)^{\frac{1}{2}}$$

ΔZ: Number of excess contact points

M. Wyart et al., Phys. Rev. E 72, 051306 (2005)

Intro: Typical interaction potential of jammed systems

■ Inter-particle potential (contact force potential)

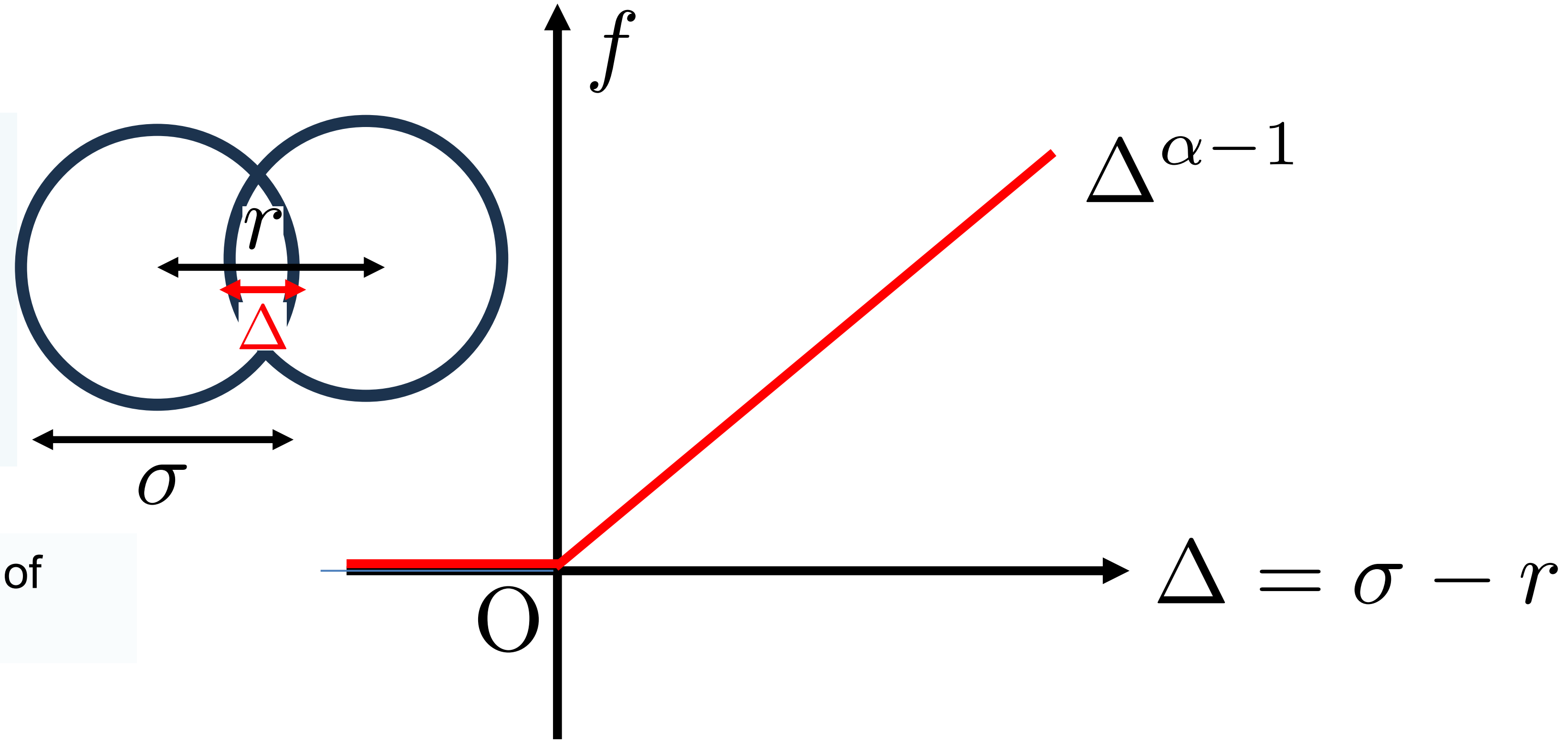
$$U = \sum_{i<j} \epsilon \left(\frac{\sigma_{ij} - r_{ij}}{\sigma_{ij}} \right)^{\alpha} = \sum_{i<j} k \, \Delta_{ij}^{\alpha}$$

$\sigma_{ij} = (\sigma_i + \sigma_j)/2$
Δ_{ij}: overlap length
r_{ij} : interparticle distance

■ Supported by Hertzian contact theory

$\alpha = \frac{5}{2}$ (3d)

$\alpha = 2$ (2d)



L.D.Landau and E.M.Lifshitz: Theory of Elasticity (1959)

Intro: Criticality of mechanical properties

■ Minute changes in packing fraction from φ_J :

$$\varphi \quad \to \varphi_\mathrm{J} + \delta\varphi$$
$$\sigma_i \quad \to \sigma_{\mathrm{J}i} + \delta\sigma_i$$

φ: packing fraction of particles

σ_i: diameter of particle *i*

$$\varphi = \varphi_\mathrm{J} + \delta\varphi = \frac{\pi}{6V}\sum_i\left(\sigma_{\mathrm{J}i} + \delta\sigma_i\right)^3 \sim \frac{\pi}{6V}\sum_i \sigma_{\mathrm{J}i}^3\left(1 + \frac{3\delta\sigma_i}{\sigma_{\mathrm{J}i}}\right)$$

$\delta\varphi \propto \delta\sigma \propto \Delta$ (interparticle overlap length)

■ Criticality of mechanical properties

$$U \sim Nz\Delta^{\alpha} \propto \delta\varphi^{\alpha} \quad (\delta\varphi = \varphi - \varphi_J)$$
$$P \sim U' \sim Nz\Delta^{\alpha-1} \propto \delta\varphi^{\alpha-1}$$
$$B \sim U'' \sim Nz\Delta^{\alpha-2} \propto \delta\varphi^{\alpha-2}$$

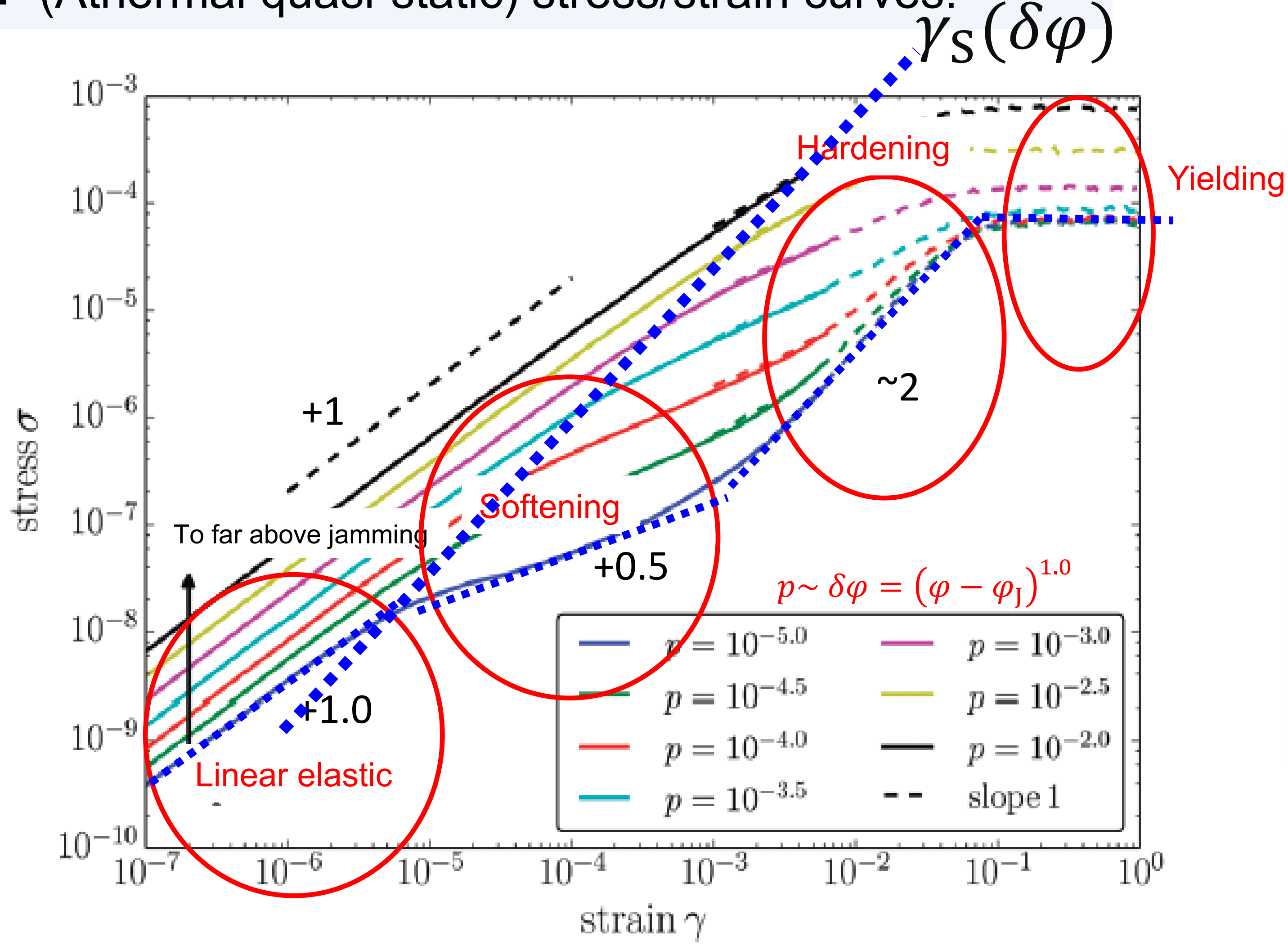
➢ all particles sustain the solidity

$$G \sim N\Delta z\, \Delta^{\alpha-2} \propto \delta\varphi^{\frac{1}{2}}\delta\varphi^{\alpha-2} = \delta\varphi^{\alpha-\frac{3}{2}}$$

M. van Hecke, J. Phys.: Condens. Matter **22**, 033101 (2010).

Intro: Nonlinear rheology near the jamming transition point

- (Athermal quasi-static) stress/strain curves:



J. Boschan, et al., Soft Matter **12**, 5450 (2016).

- Becomes extremely complicated near the jamming transition point.
- The curves vary systematically with distance with $\delta\varphi$.
- Critical scaling relations

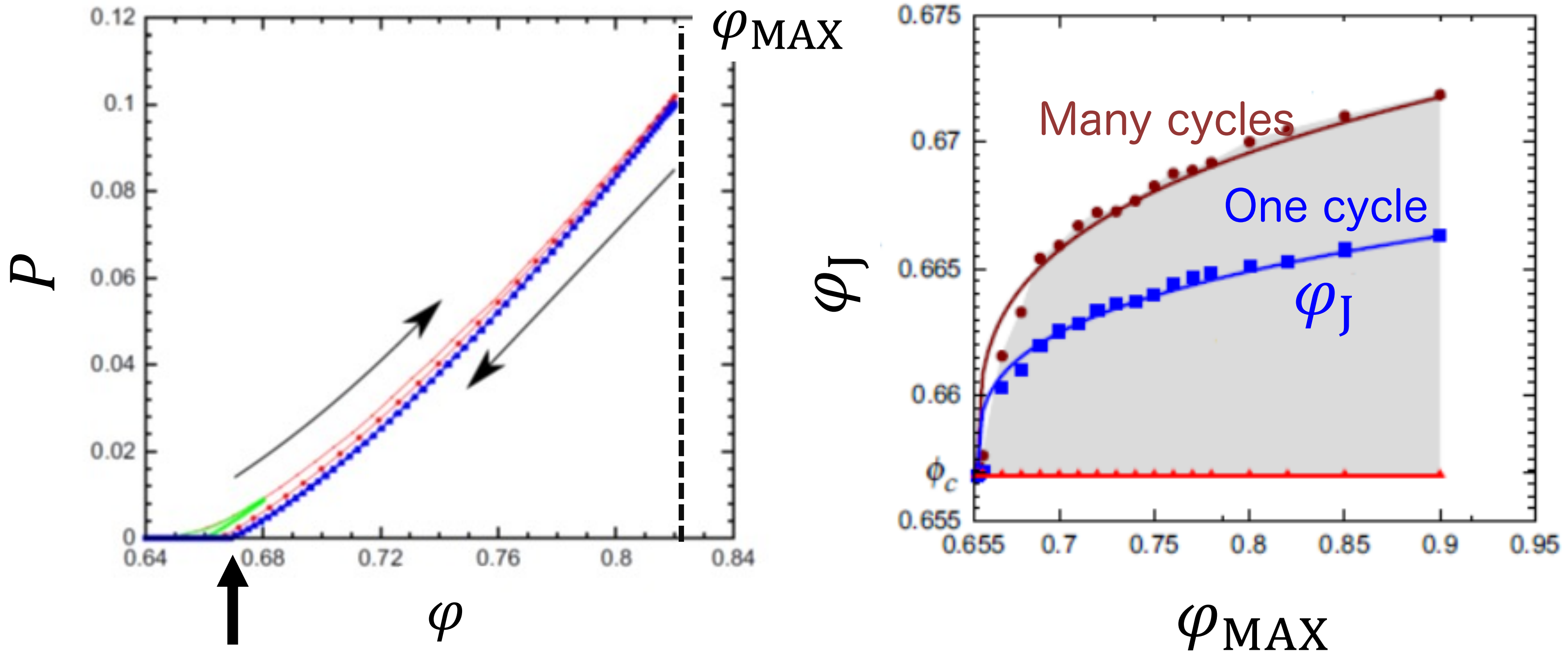
$$\sigma=\delta\varphi^x\,\mathcal{F}\left(\frac{\gamma}{\delta\varphi^y}\right),$$

have been studied intensively but they are still controversial.

Intro: φ_J depends on the "history" of the preparations

- Jamming configuration undergoing mechanical training

- φ_J strongly depends on history



φ_J (Jamming transition point for the particle configurations experiencing the training)

N. Kumar and S. Luding, Granular Matter **18**, 58 (2016).

➢ Scaling of non-linear rheology with respect to $\delta\varphi (= \varphi\text{-}\varphi_J)$ needs special attentions, because under large deformation, <u>φ_J should change</u>.

Objectives

■ Establishment of jamming critical scaling under large deformations.

Finding:

■ Nonlinear rheology contains a protocol-dependent and a protocol-independent part.

■ By their disentanglement, we establish a precise critical scaling law.

T. Kawasaki and K. Miyazaki, Phys. Rev. Lett. **132**, 268201 (2024)

Methods

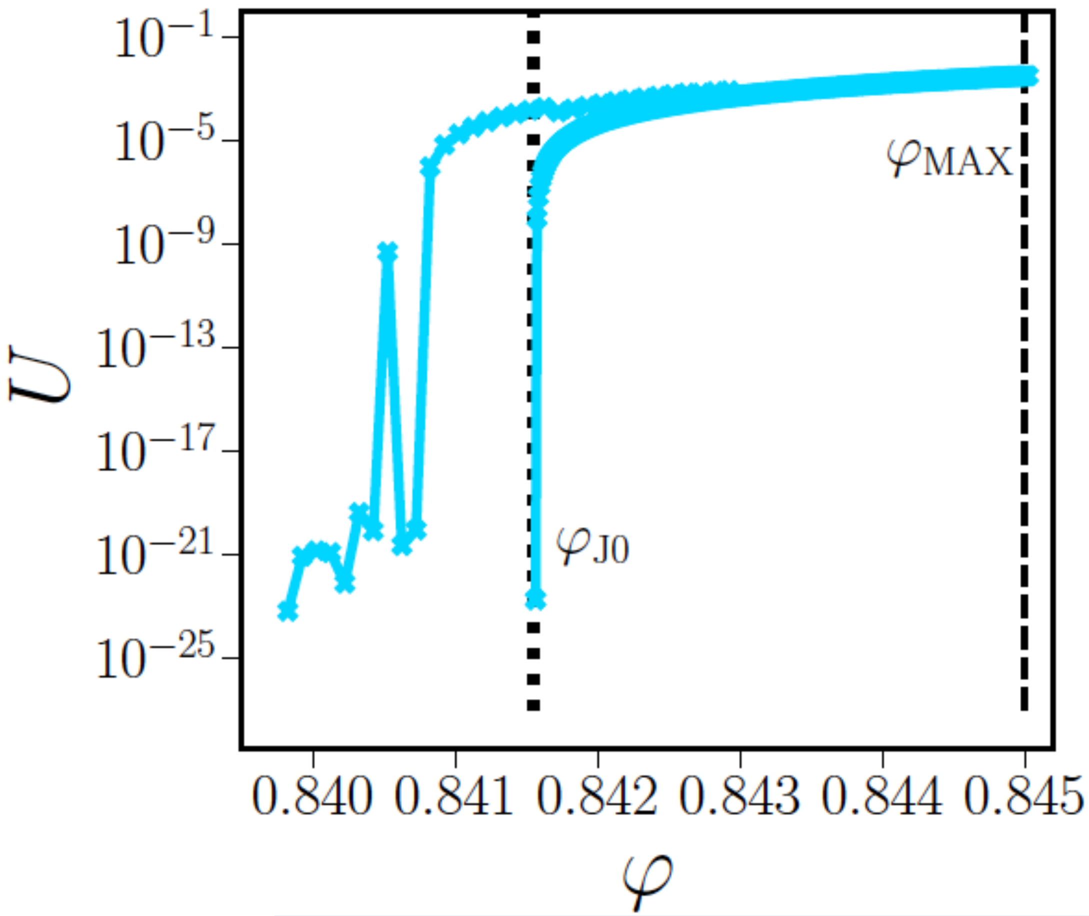
- **Athermal quasi-static (AQS) simulation**:
  - FIRE method [E. Bitzek,et al., Phys. Rev. Lett. 97, 170201 (2006)]: minimize energy at each step.
  - Mainly two-dimensional systems (equivalent for three-dimensional systems)
- **Interaction potential:**
  - Mainly harmonic potential:

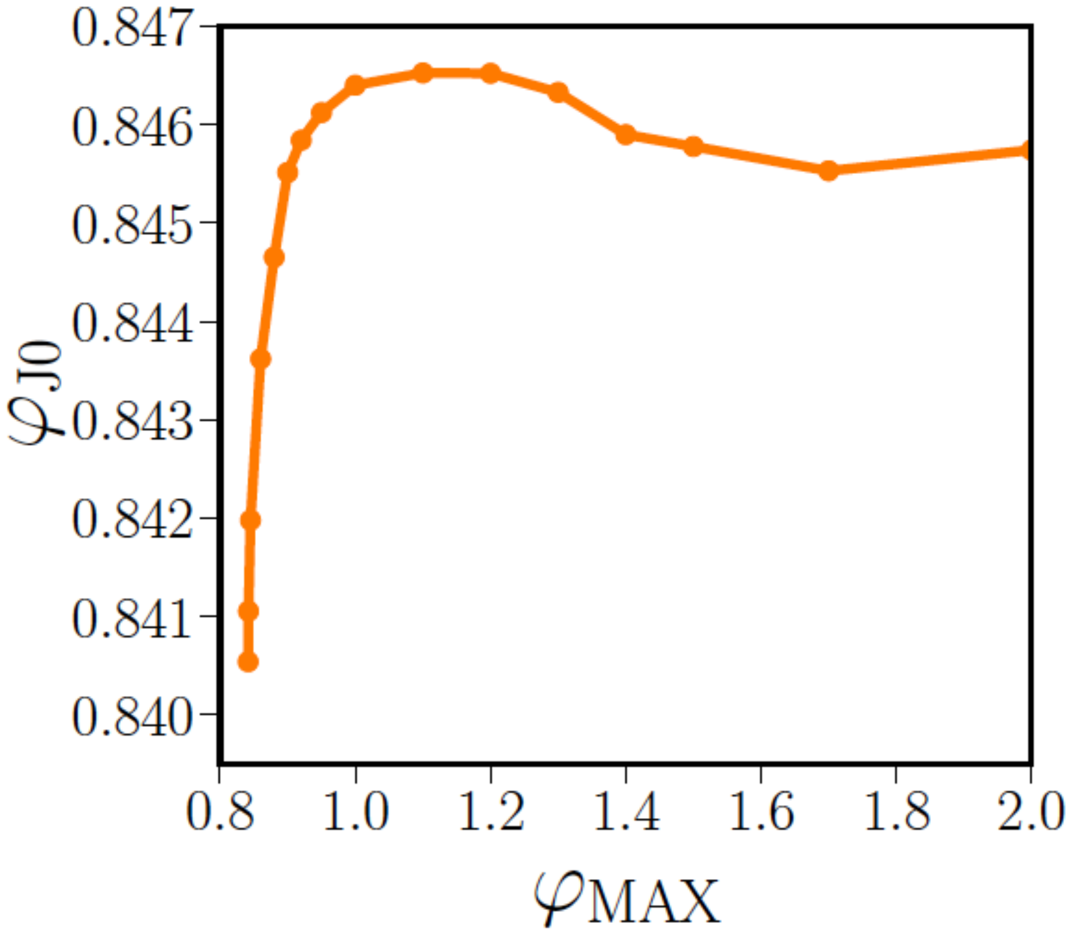
$$U = \sum_{i<j} \frac{\epsilon}{2}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 .$$

- **Particle size dispersion**:
  - Binary mixtures (size ratio 1.0:1.4, particle number ratio 1:1)
- **Frictionless particles**

Result: Generation of jamming configuration

- For the test of protocol dependence:
  - ➢ Generate varieties of initial conditions by the systematic mechanical training.

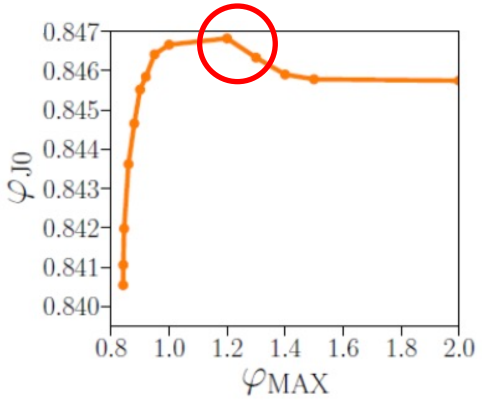


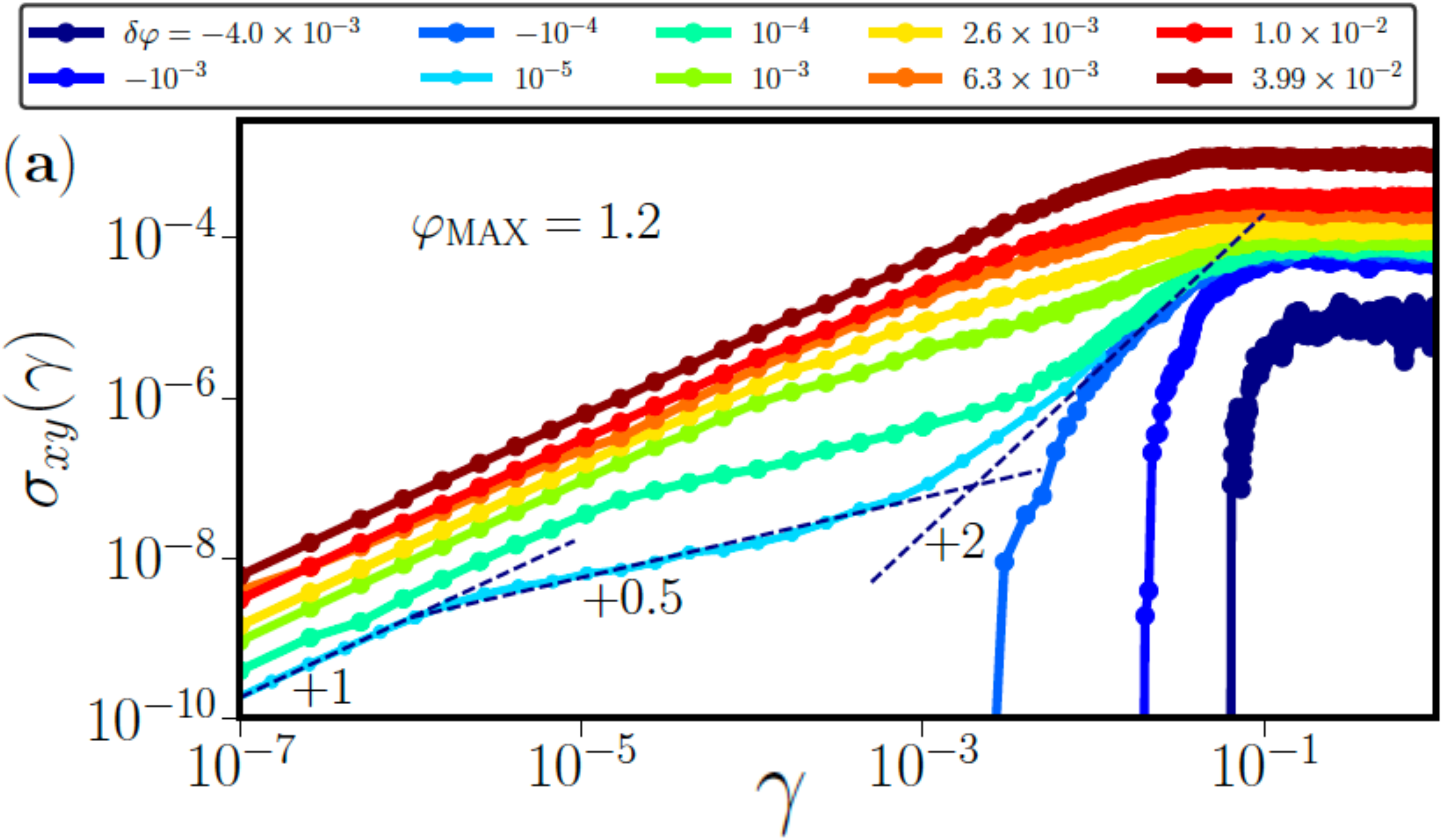


- ➢ Changing the density of each jamming configuration.
- ➢ Applying AQS shear flow.

Result: Stress-strain curve under constant volume

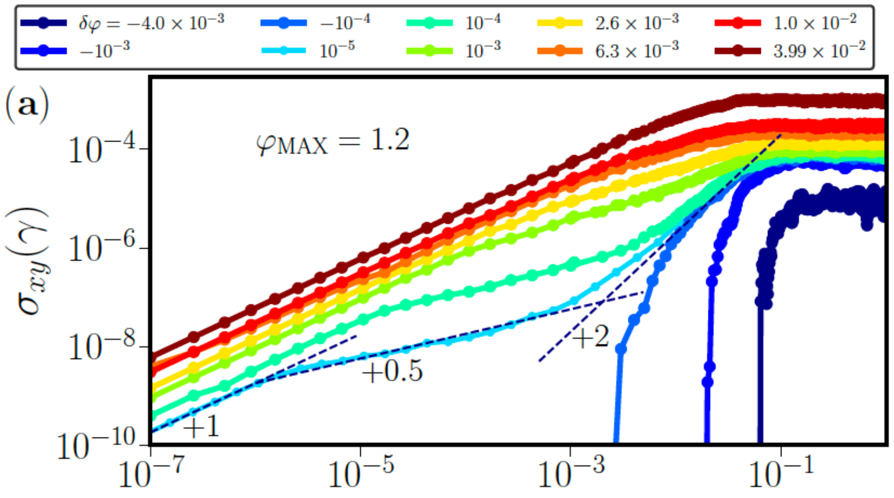
■ φ-dependence of stress/strain curves under constant volume (at well−trained system $\varphi_{\mathrm{MAX}} = 1.2$)

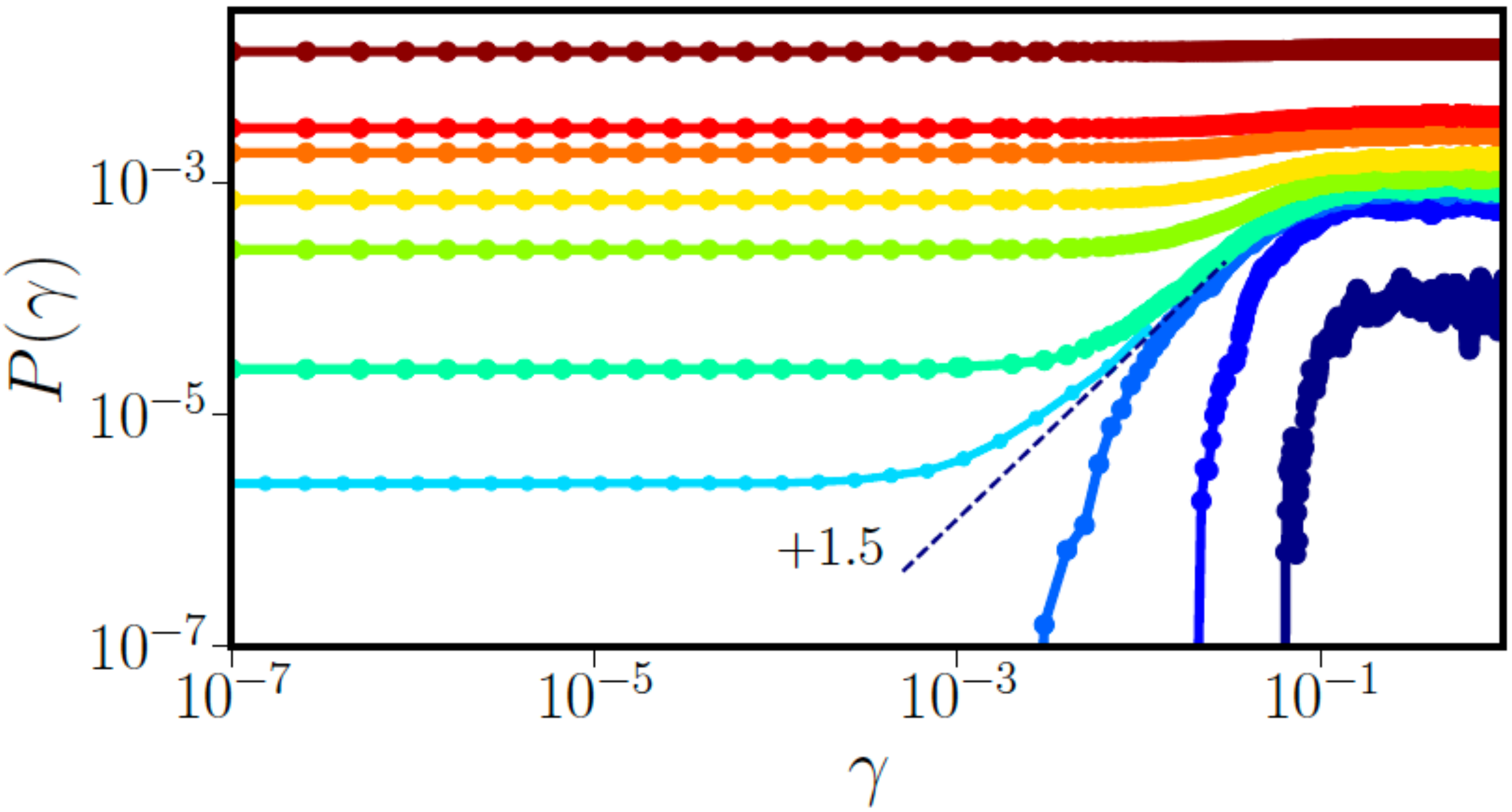




➢ Elastic, softening, hardening, shear jamming, and yielding are observed.

Result：Pressure-strain curve under constant volume ($\varphi_{\mathrm{MAX}} = 1.2$)





$$P(\gamma) \sim \left(\varphi - \varphi_J(\gamma)\right)$$

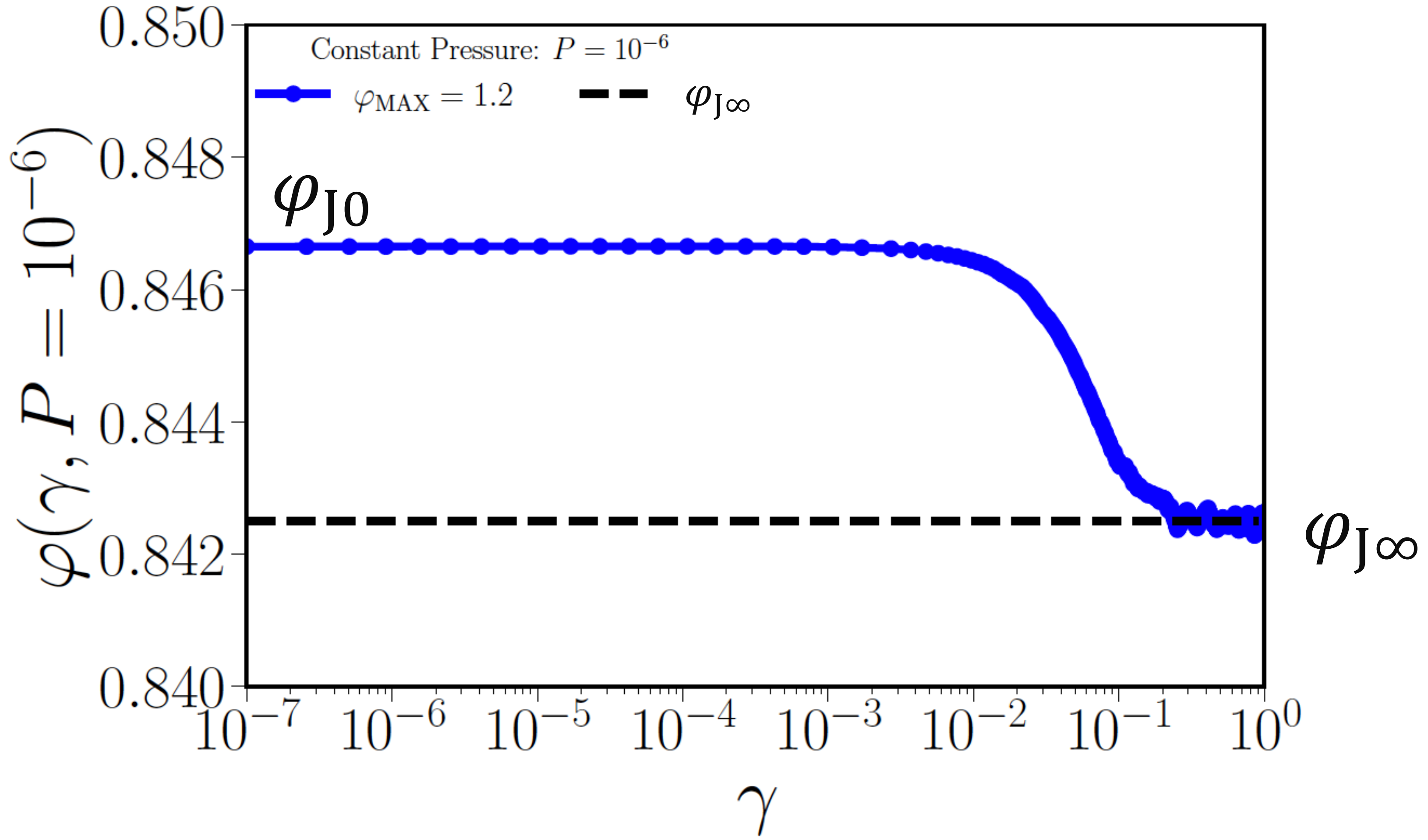
Pressure change = Change in jamming point

Result: Change in jamming point while shearing

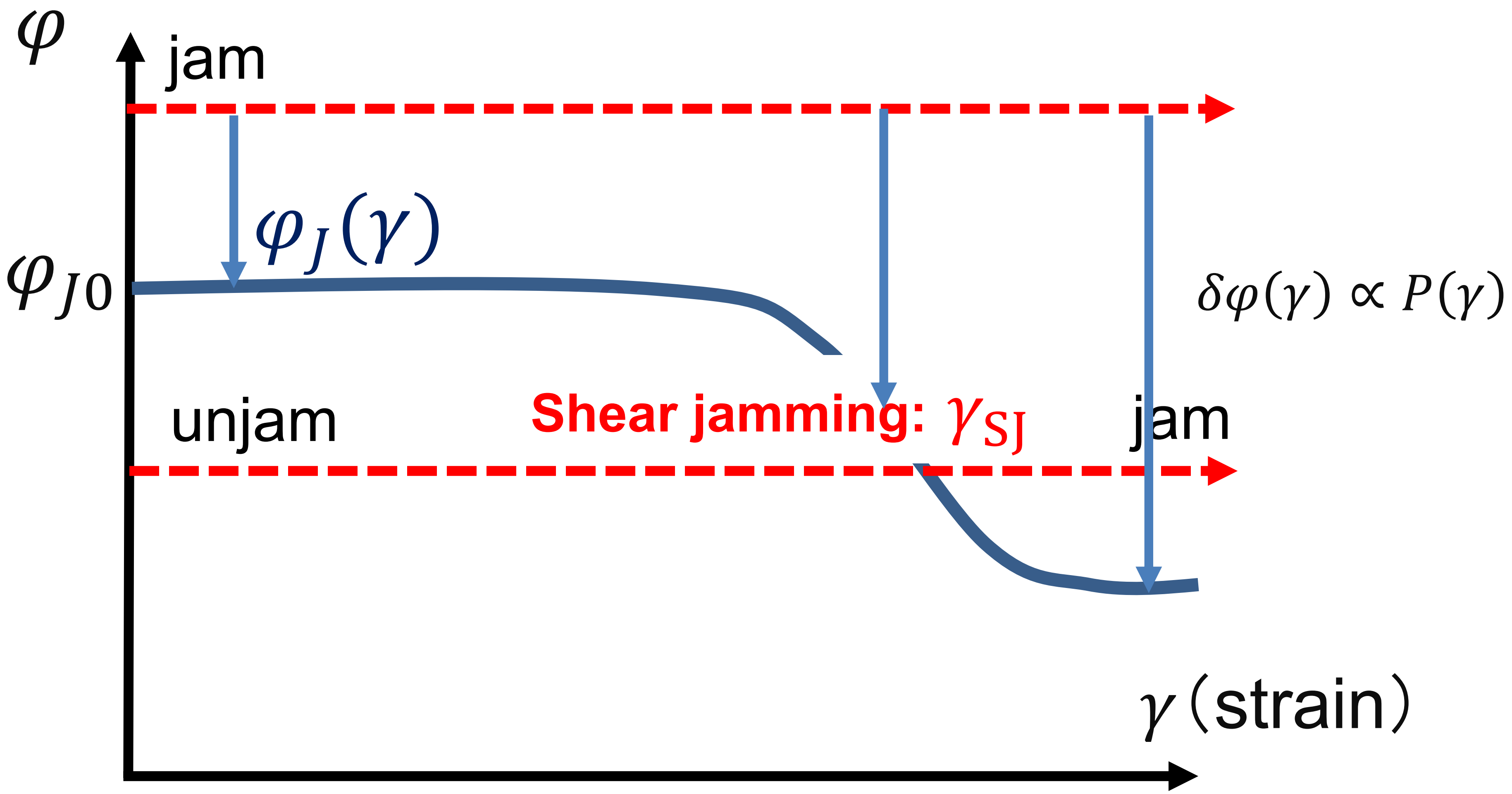
- Computing φ_J under shear deformation:
  - Fixing at a very small pressure and tracking density

$$P(\gamma) \propto \delta\varphi(\gamma) = \varphi(\gamma) - \varphi_J(\gamma) \ll 1$$

$$\therefore \varphi(\gamma) \sim \varphi_J(\gamma)$$

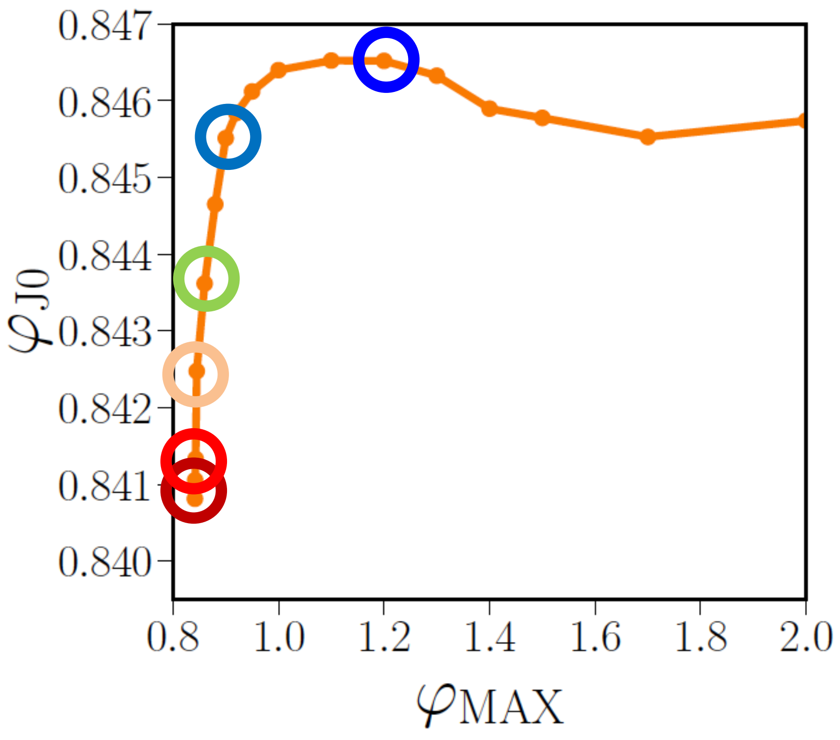


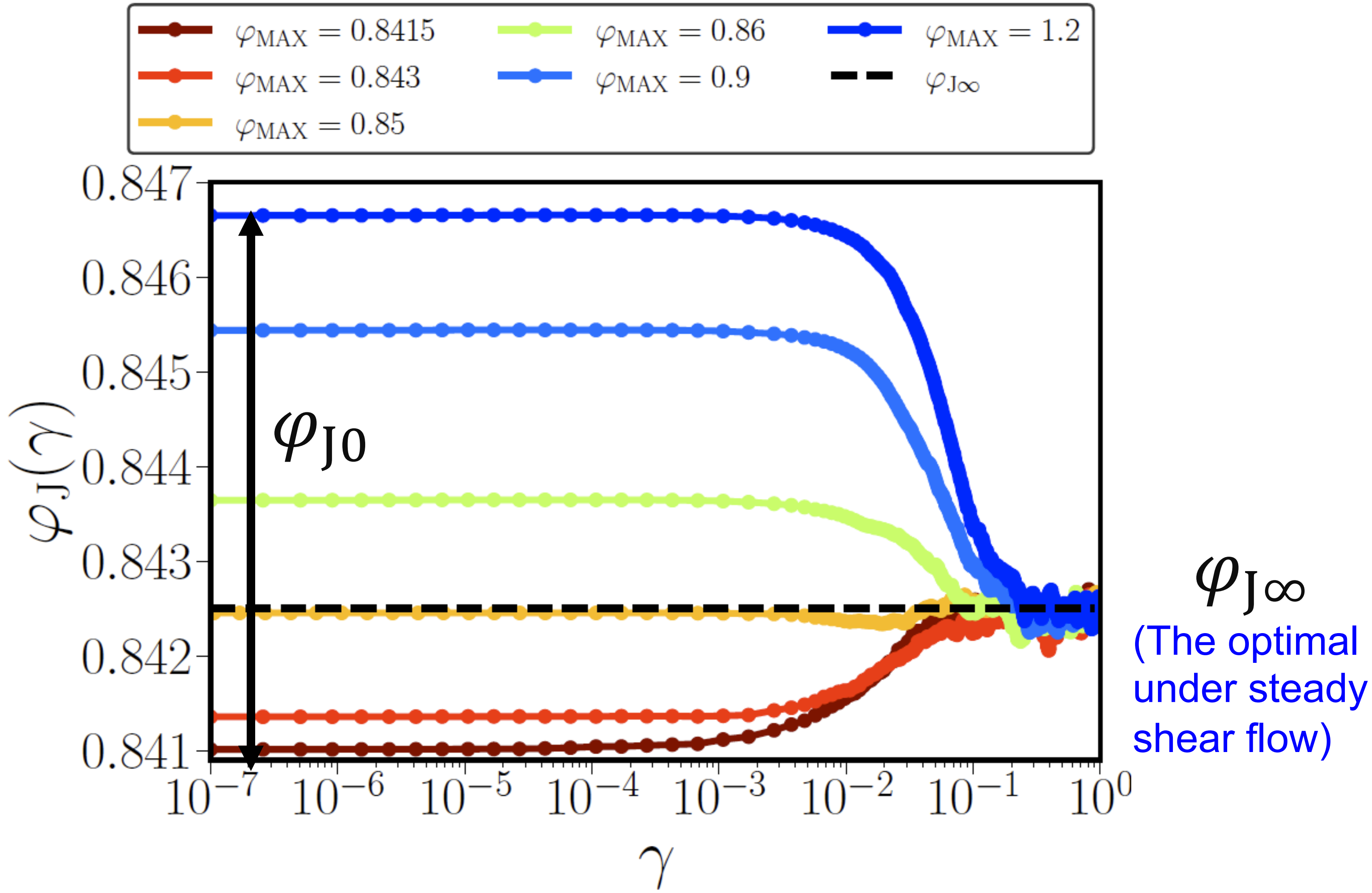
Discussion: Origin of shear hardening and shear jamming



Result: Change of the jamming transition density by steady shear

■ Estimating the $\varphi_J(\gamma)$, for various annealing intensities φ_{MAX}.

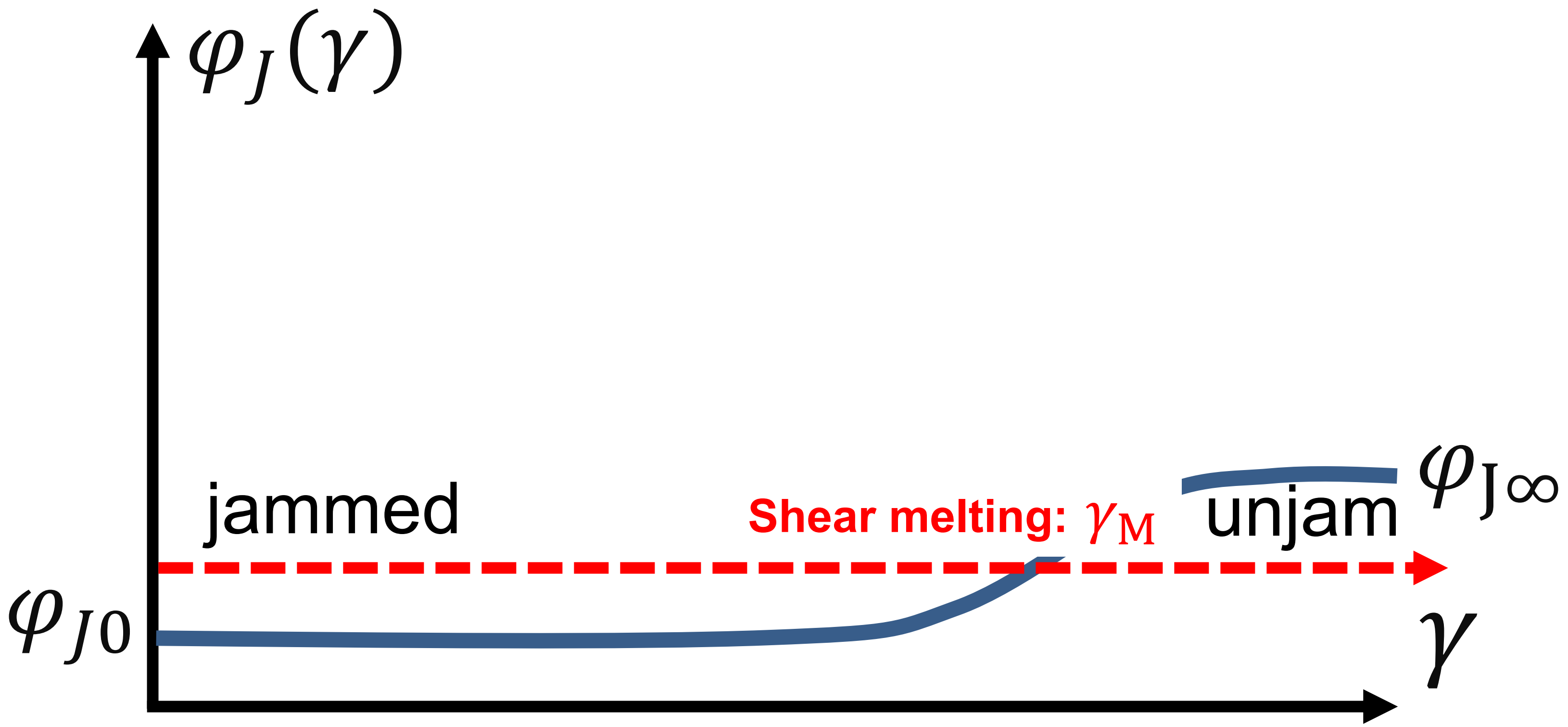




➢ ill-trained configurations: φ_J increases by applying γ.

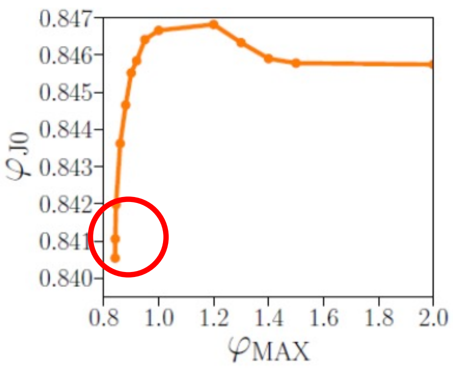
Discussion: Shear melting

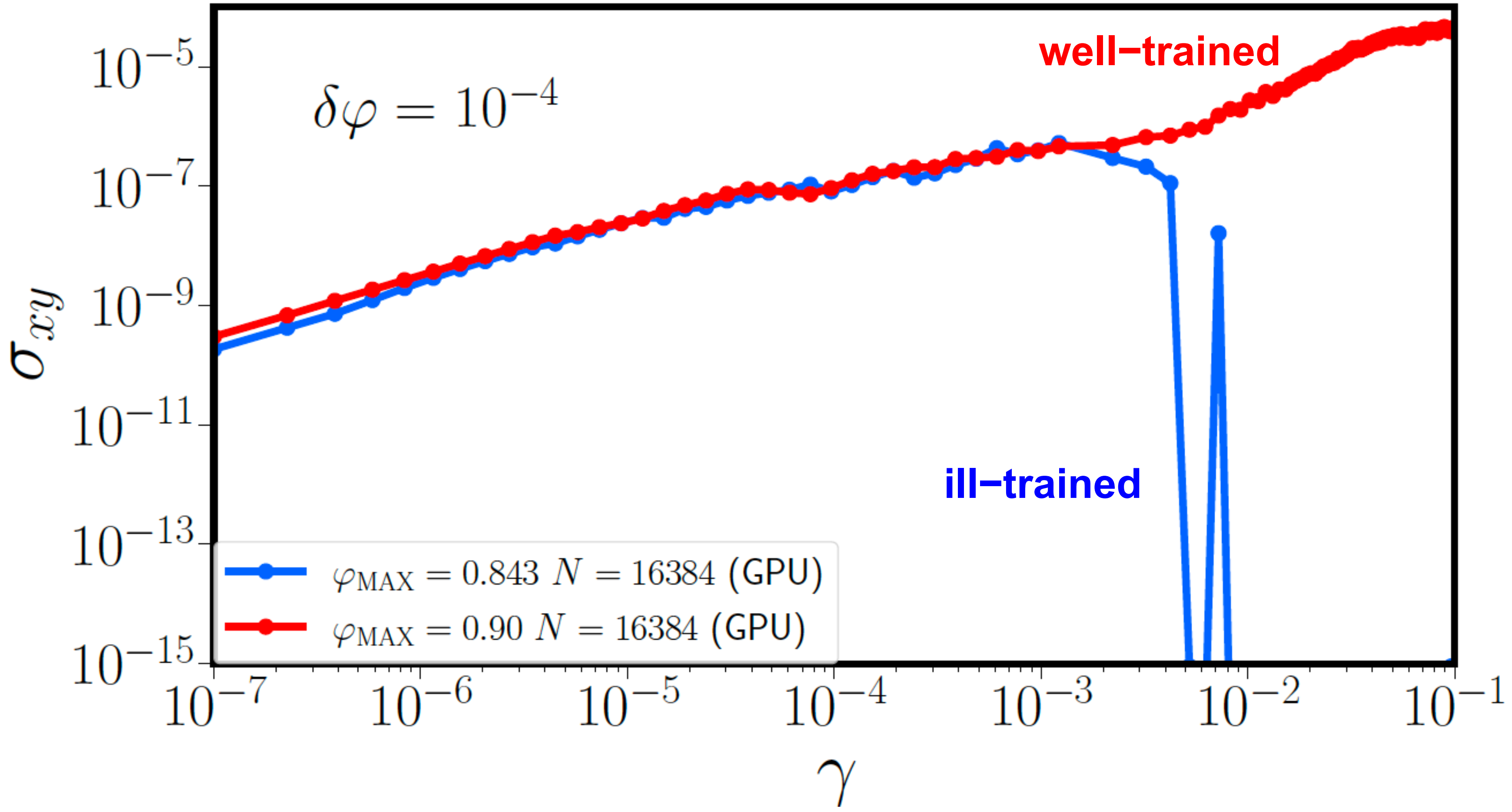
- An ill-trained case: shear melting takes place.



The mechanical responses of an ill-trained system

- Constant volume stress-strain curves near jamming at $\varphi_{\mathrm{MAX}} = 0.843$(**ill−trained system**).



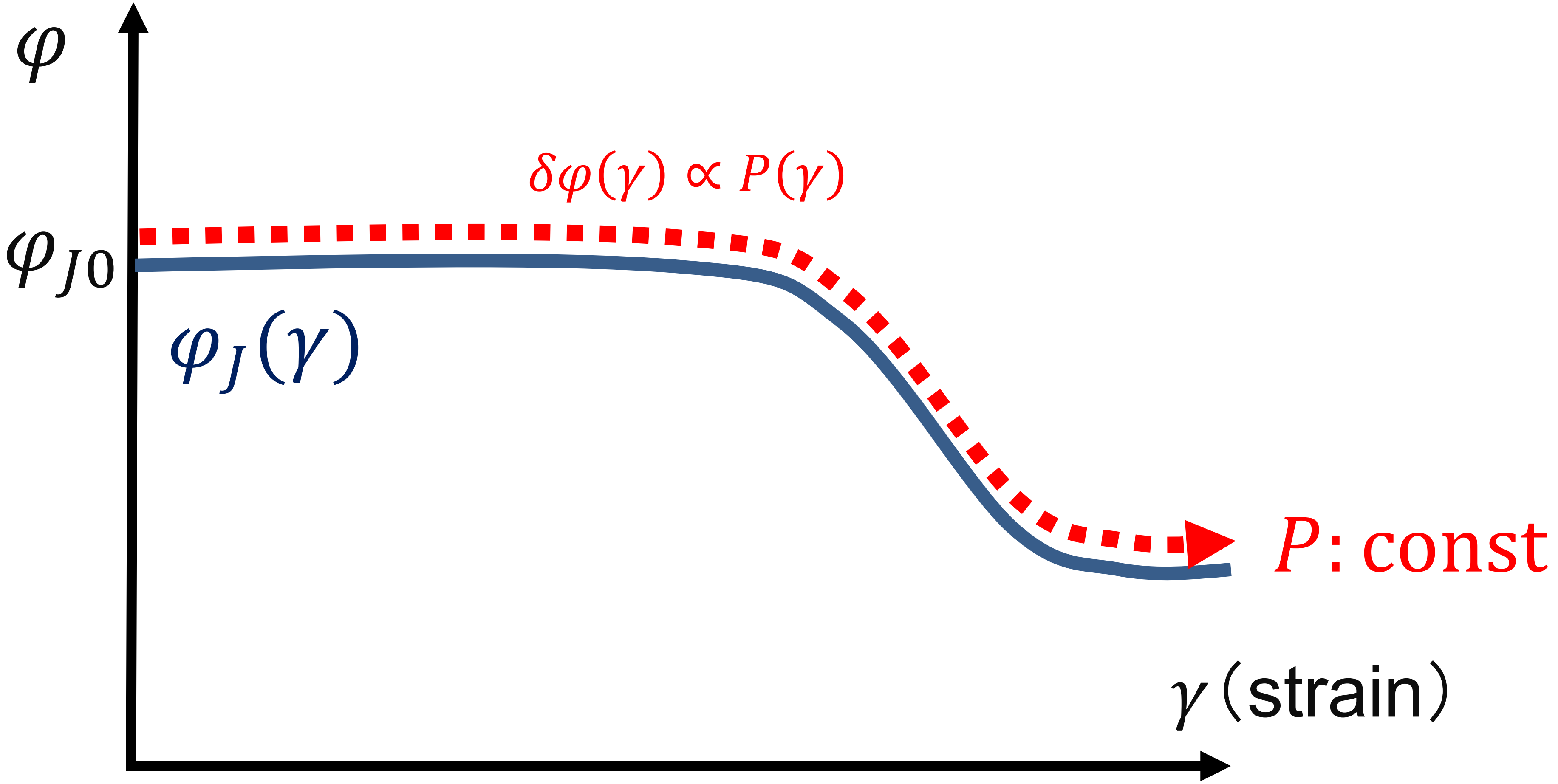


➢ The system melts under shear flow -- shear melting takes place.

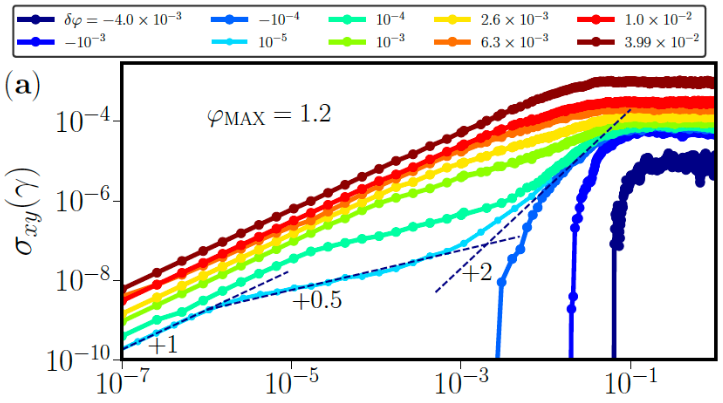
Discussion: Constant pressure makes $\delta\varphi$ keep constant

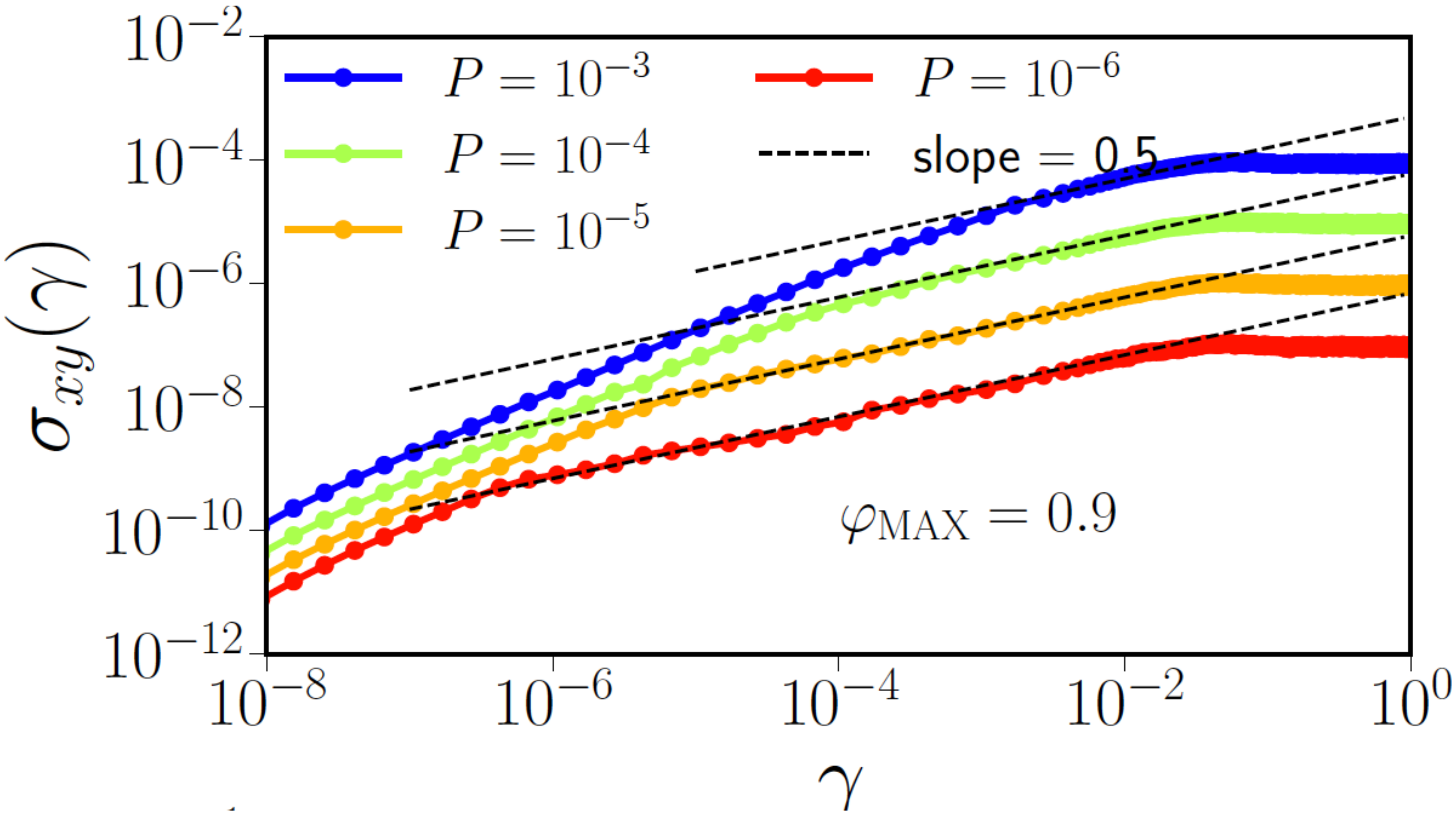
- The change in $\delta\varphi$ at constant volume is protocol-dependent, and inconvenient for critical scaling.

  - Constant pressure makes $\delta\varphi$ keep constant.



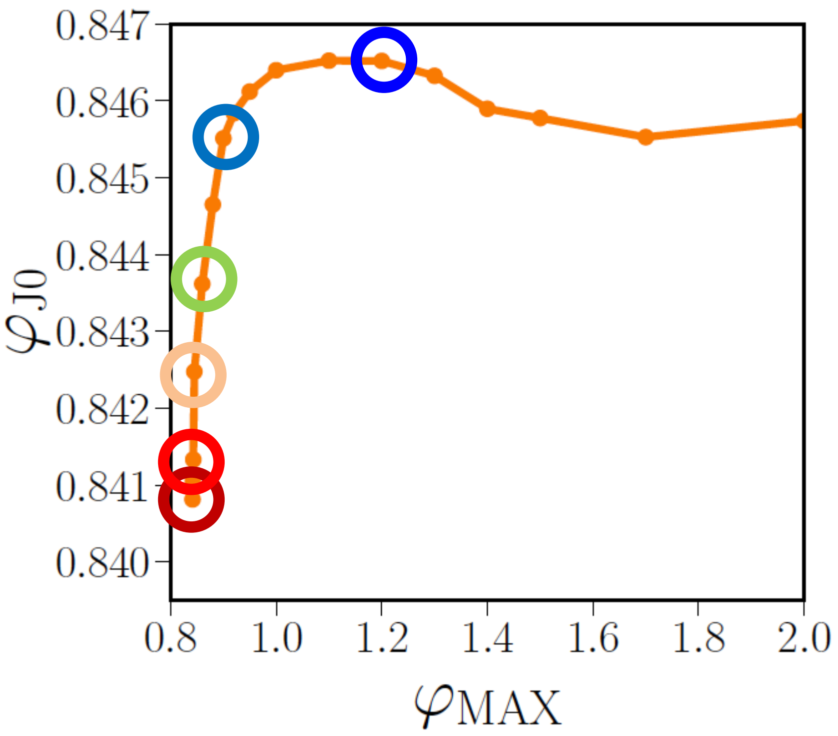
Result: Stress-strain curves under constant pressure

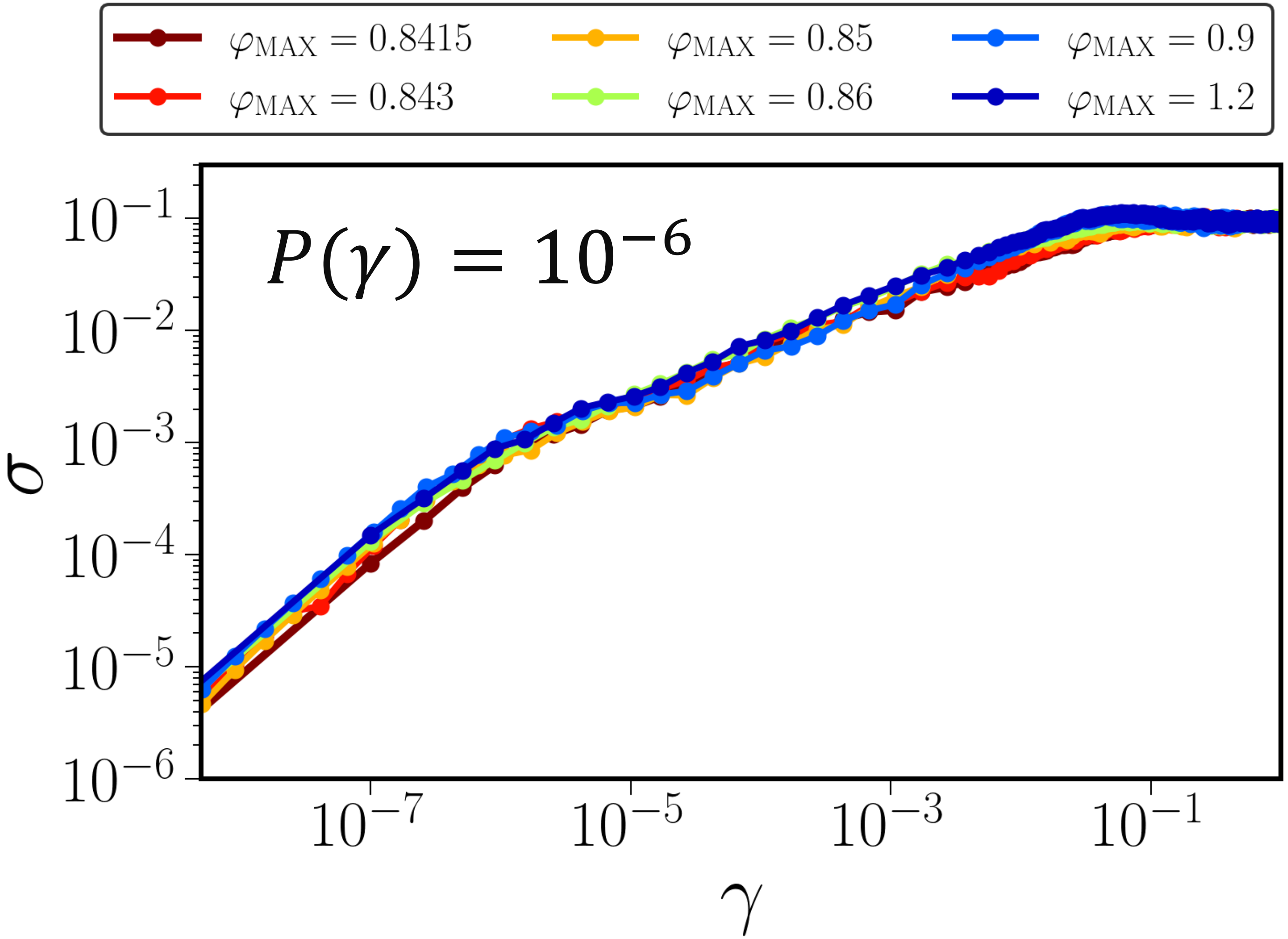




- ➢ A hardening disappears.
- ➢ Finding the connection between softening and yielding.

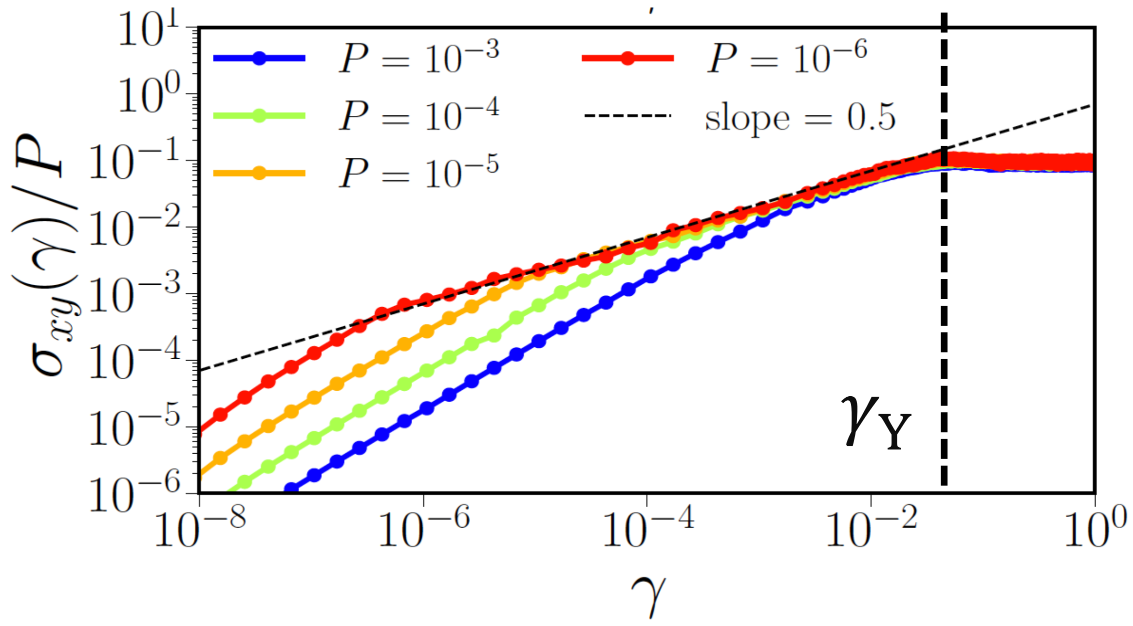
Result: The protocol dependence on the non-linear rheology

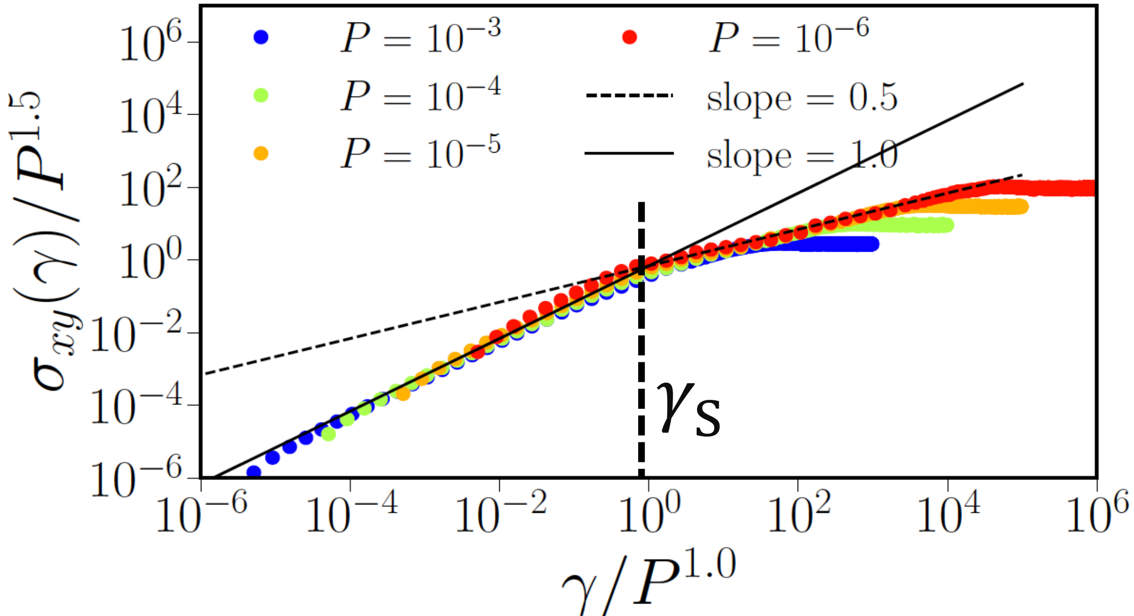




- ➢ We get protocol independent mechanical response!
- ➢ Expect reliable scaling relationships.

Result: Scaling relations (at constant pressure)





- **Yielding:**
  - $\sigma_{xy}(\gamma \to \infty) \sim P_{\gamma\to\infty} \sim \varphi - \varphi_{J\infty}$

  Softening onset:
  - $\gamma_{\rm Y} \sim 0.1$

- **Softening:**
  - $\sigma(\gamma) \sim (\delta\varphi)^{1.0}\gamma^{0.5} = P(\gamma)\,\gamma^{0.5}$

  Elastic onset:
  - $\gamma_{\rm S} \sim \delta\varphi^{1.0} \sim P$

Cf: M. Otsuki and H. Hayakawa, Phys. Rev. E 90, 042202 (2014)

➢ Explain why such scaling is established from a microscopic view point.

Discussion: Microscopic dynamics and structure (under constant pressure)

(Assume) Softening is attributed to the reconnection of interparticle overlap.

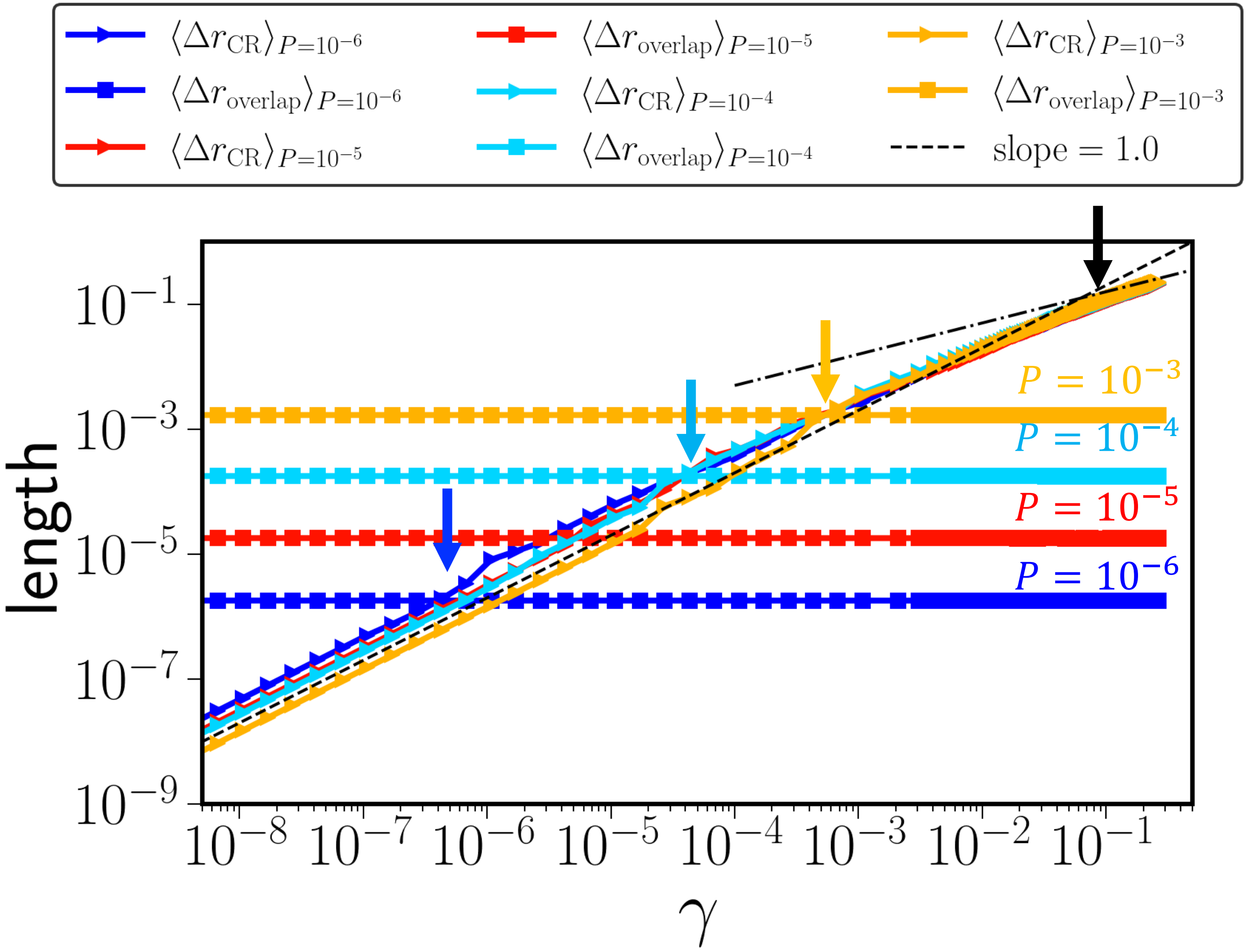
- Interparticle overlap
  $\langle \Delta r_{\mathrm{overlap}} \rangle \sim \delta\varphi \sim P$

- Cage relative (CR) displacement
  $\langle \Delta r_{\mathrm{CR}} \rangle \sim \gamma$

➢ Softening conditions:
$\langle \Delta r_{\mathrm{CR}} \rangle > \langle \Delta r_{\mathrm{overlap}} \rangle$
$\therefore \ \gamma_{\mathrm{S}} \sim \delta\varphi$

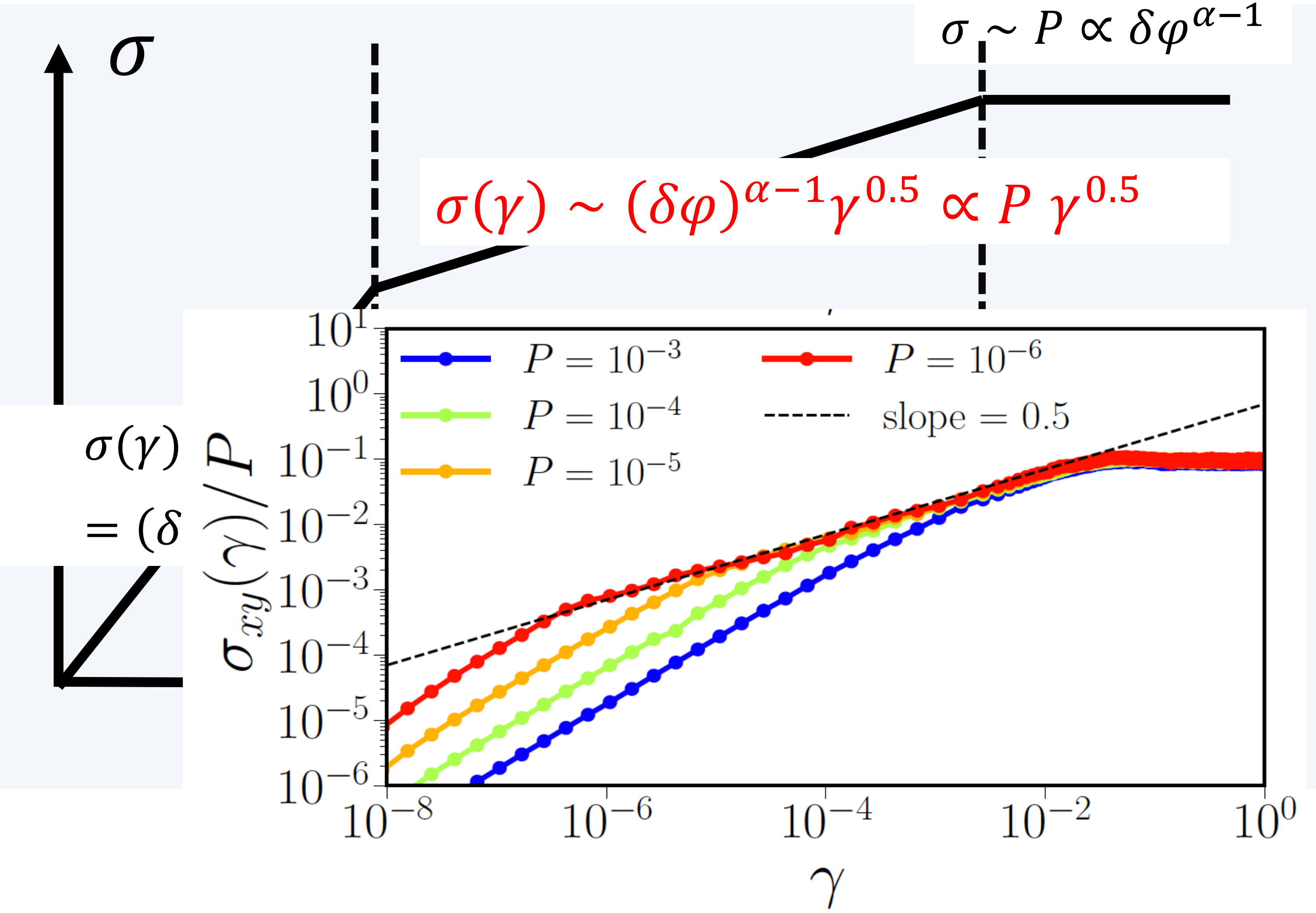
Yielding occurs when the cages are broken.

- Yielding condition:
  $\langle \Delta r_{\mathrm{CR}} \rangle \sim 0.1\sigma$
  $\therefore \ \gamma_{\mathrm{Y}} \sim 0.1$



Conclusion: Scaling relations near the jamming transition

Derivation of scaling functions for softening regions



- Intersection of the Softening and Yielding:

$$(\delta\varphi)^{a}\gamma_{\mathrm{Y}}^{b} \propto \delta\varphi^{\alpha-1}$$

$$\therefore \quad a = \alpha - 1$$

- Intersection of the elastic and softening

$$(\delta\varphi)^{\alpha-\frac{3}{2}}\gamma_{s} \propto (\delta\varphi)^{\alpha-1}\gamma_{s}^{b}$$

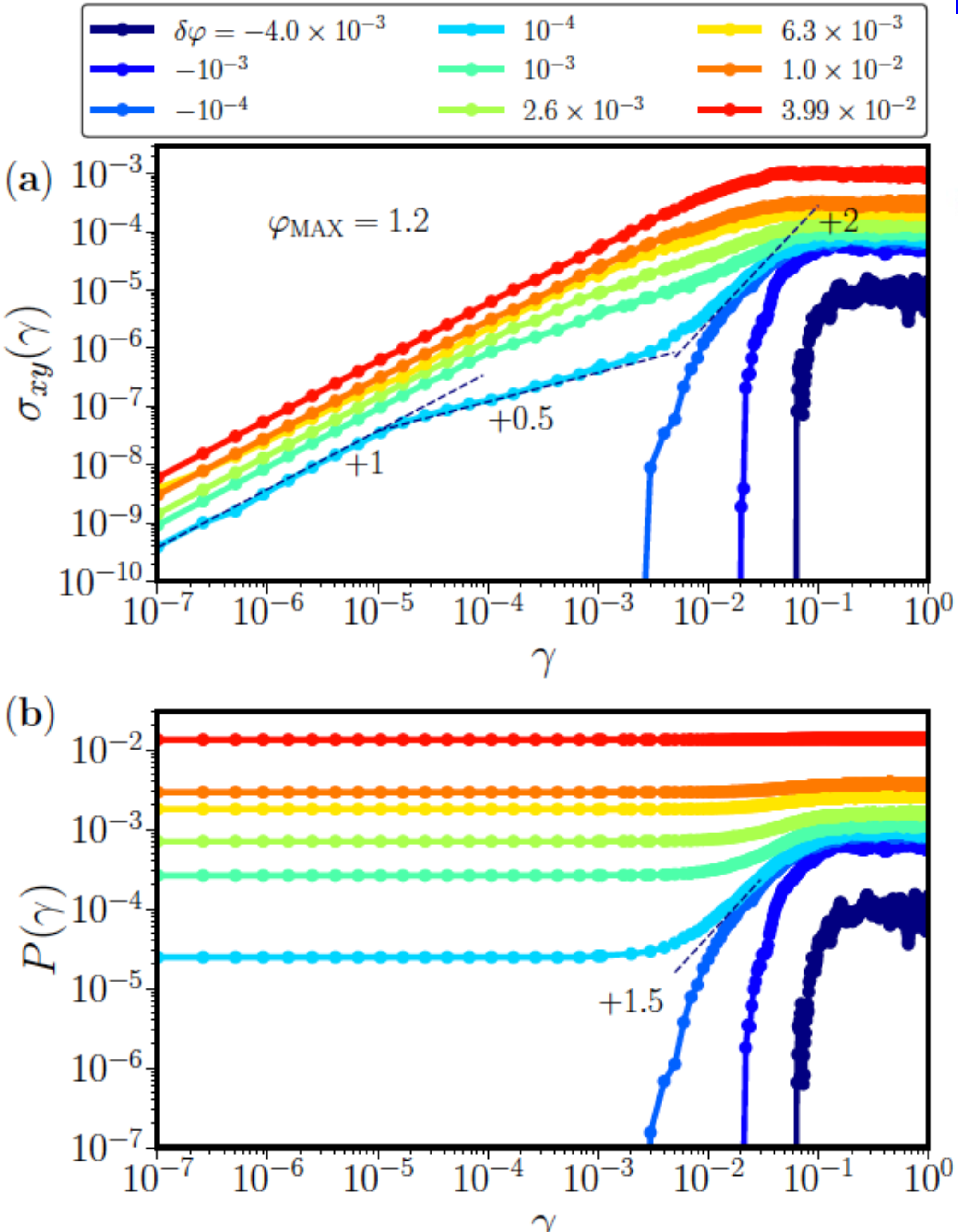
$$\therefore \quad b = \frac{1}{2}$$

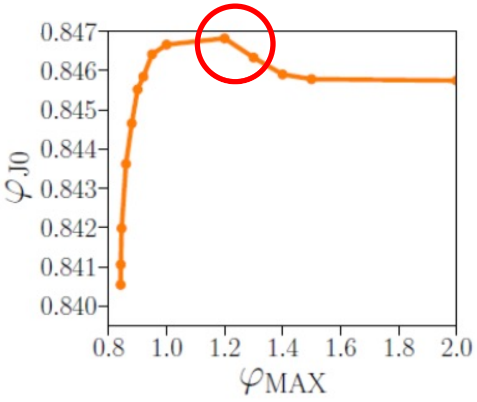
Results: Revisit constant volume simulations

In constant pressure:

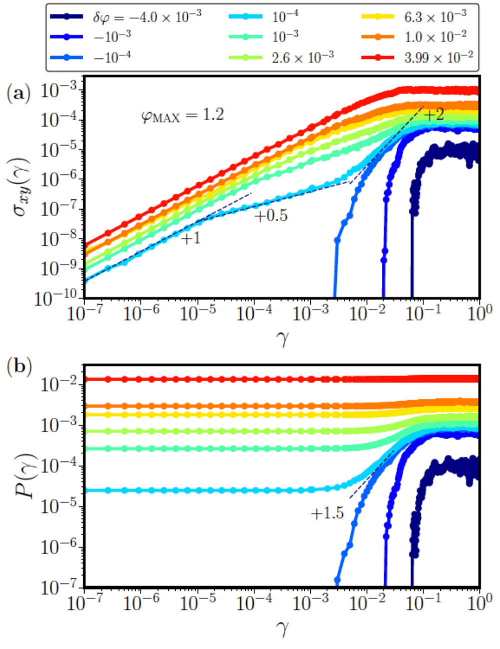
- Softening: $\sigma(\gamma) \sim P(\gamma)\,\gamma^{0.5}$
- Yielding: $\sigma(\gamma) \sim P(\gamma)$

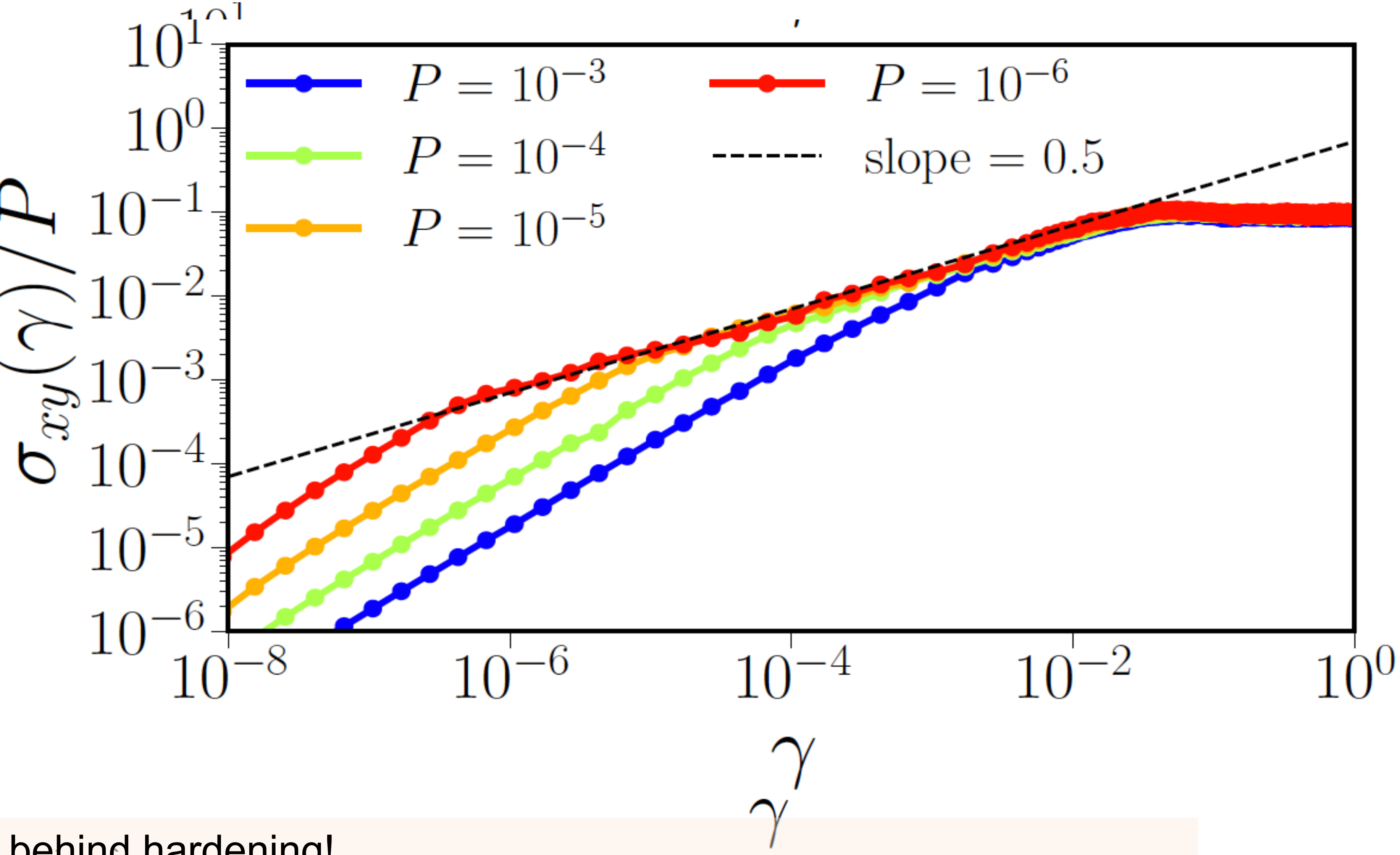
How about constant volume??





Results: Disentangling of shear hardening, shear jamming and softening in constant volume simulations





Softening:

$\sigma(\gamma)/P(\gamma) \sim \gamma^{0.5}$

Yielding:

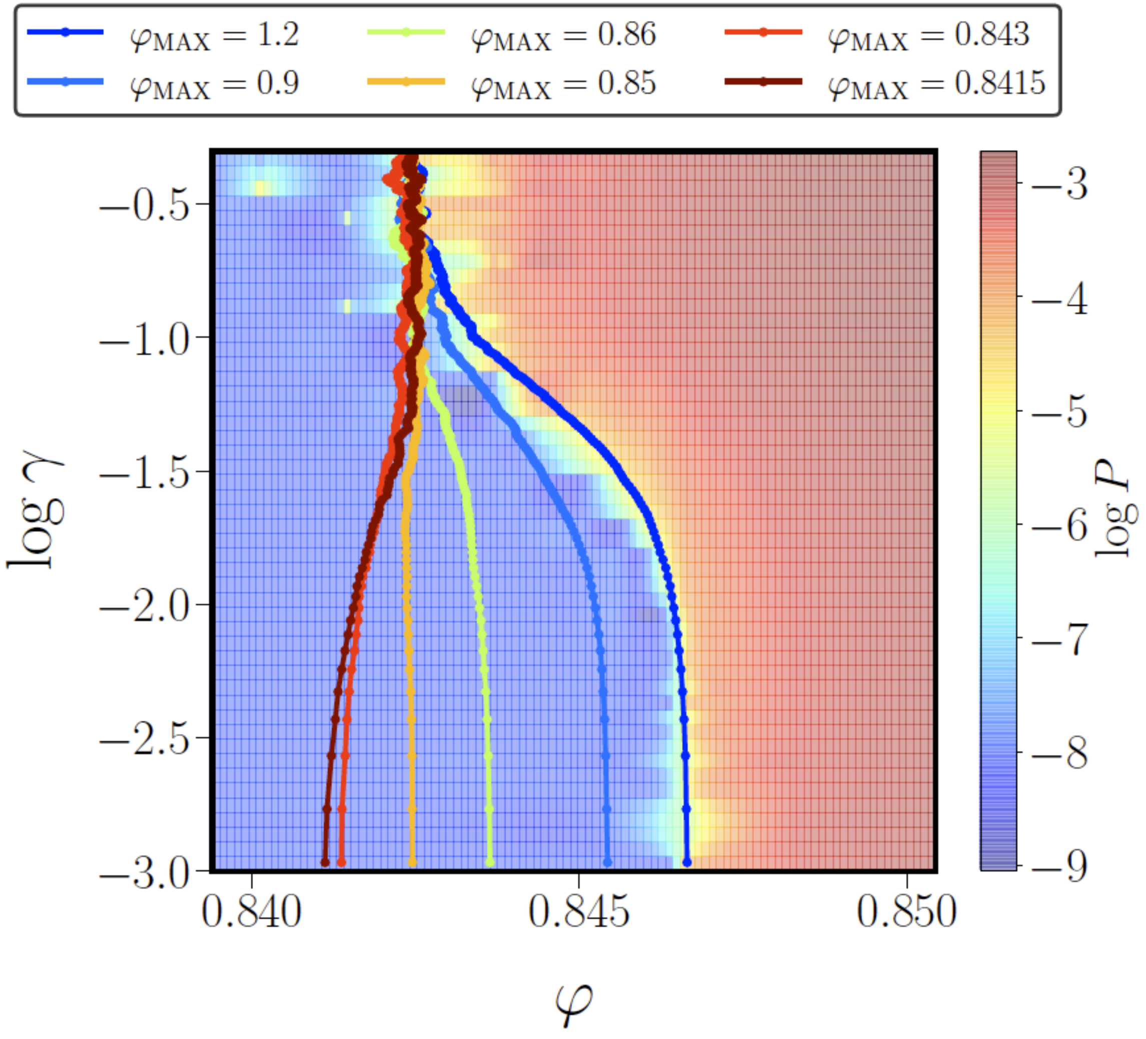
$\sigma(\gamma)/P(\gamma) \sim$ const

- ➢ Softening exists behind hardening!
- ➢ Protocol-independent mechanical response equivalent to constant pressure is obtained.

Conclusions

- Shear jamming / shear hardening/ shear melting are attributed to the change of φ_J.

- Constant pressure simulations are not contaminated by change of φ_J.
  - Wide-range of critical scaling has been obtained regardless of generation protocols of the jamming configurations.
  - Even constant volume, σ/P shows protocol independent scaling relations.



T. Kawasaki and K. Miyazaki, Phys. Rev. Lett. **132**, 268201 (2024).

Open questions

- Softening and yielding
  - for frictional particle system?
  - at finite shear rate?
  - at unjammed state?
  - with microscopic theoretical arguments?

Thank you for your attention.