Heterogeneous jamming of binary mixture of small and large particles

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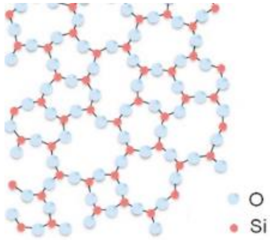
Jammed Particles

Colloids

Emulsion

Grains

- **Dense, disordered, structurally arrested particles**
- **A pile of interesting prop.:** Elasticity, Vibrations, Rheology
- **Relation to the glass physics**



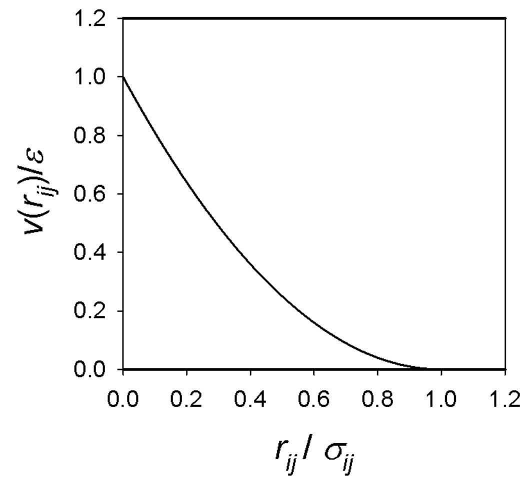
Ideal jamming

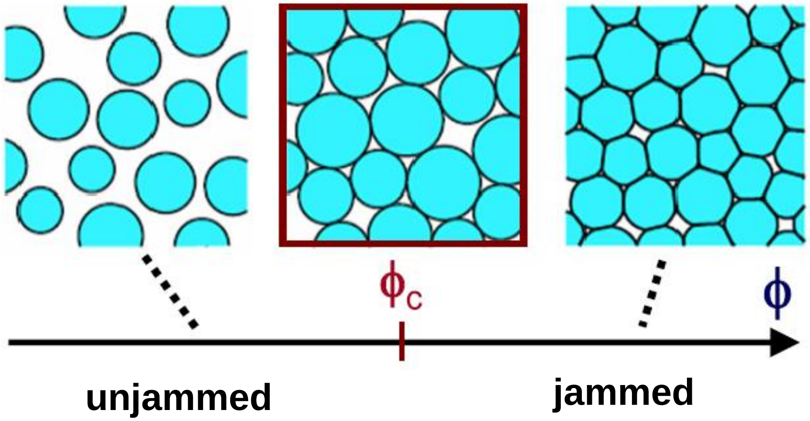
- **Friction-less, nearly monodisperse, repulsive spheres**

$$v(r) = \begin{cases} \epsilon(1 - r/\sigma)^2 & (r \leq \sigma) \\ 0 & (r > \sigma) \end{cases}$$

- Put particles randomly in a box.
- Minimize the potential to find a mechanical equilibrium state
- Jamming point is defined as the density at which the system has non-zero pressure/energy.

Particle interaction

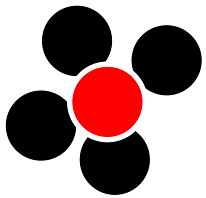




[van Hecke 2009 etc]

Ideal jamming

- **Particles get jammed simultaneously at the jamming point.**
- **Maxwell criteria works at the jamming point.**
  - Number of particles: *N*
  - Number of contacts per particle: *Z*
  - Spatial dimension: *d*



Degree of freedom

$$N \times d$$

Constraint due to contact

$$\frac{N \times Z}{2}$$

These balance when

$$Z = 2d$$

MF type argument which assumes no redundant contact.
But, this equality works precisely for packings at the jamming.

[O'Hern 2003 etc]

- **Shear modulus becomes linear to the excess contact number.**

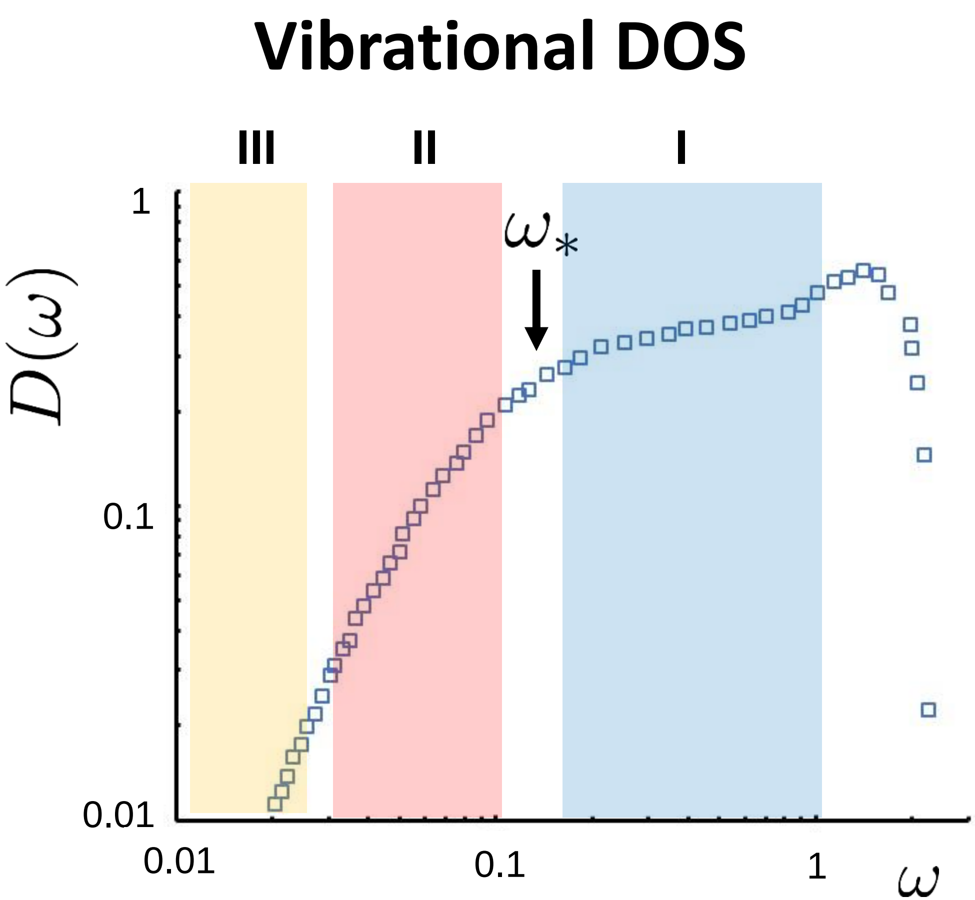
$$G \propto \Delta Z = Z - 2d$$

from MF theory

[Wyart 2005 etc]

- **Too many low frequency vibrations.**

Ideal jamming: Vibrations



- **Region I "Anomalous modes"**

$$D(\omega) \sim \text{const.}$$

  - Criticality of jamming

$$\omega_* \propto \Delta Z$$ from MF theory

- **Region II "Boson-peak"**

$$D(\omega) \propto \omega^2$$

  - Marginal stability of amorphous solids from MF theory

- **Region III "QLV"**

Phonon + Quasi-Localized modes

[Silbert 2005, Wyart 2005, DeGiuli 2014, Charbonneau 2016, Lerner 2016, Mizuno 2017 etc]

Question

- Friction between grains matters in granular materials
- Shape of particles can alter the low frequency vibrations
- **Polydispersity of particles' sizes**
  - **Many "natural" jammed particles are highly polydisperse (cements, emulsions, grains etc)**
  - **Binary mixture is the simplest case**
    - **Size ratio ~ 1**: Jamming of mixtures is similar to jamming of monodisperse particles
    - **Size ratio >>1**: Jamming density changes dramatically. Jamming of small/large particles seems to decouple.

[Xu 2010, Koeze 2016, Prasad 2017, Slivastava 2021 etc]

    - **MF understanding of ideal jamming can be transferred?**

Outline

- **Setting**
- **Jamming phase diagram of binary mixtures**
- **Near the critical point**

Setting

- **Binary mixture of large and small harmonic spheres**

$$v_{ij}(r_{ij}) = \frac{1}{2}(r_{ij} - \sigma_{ij})^2\theta(\sigma_{ij} - r_{ij})$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \qquad \sigma_i = \begin{cases} 6 & i \in \{\text{Large}\} \\ 1 & i \in \{\text{Small}\} \end{cases}$$

  - Size ratio is fixed to be 6.

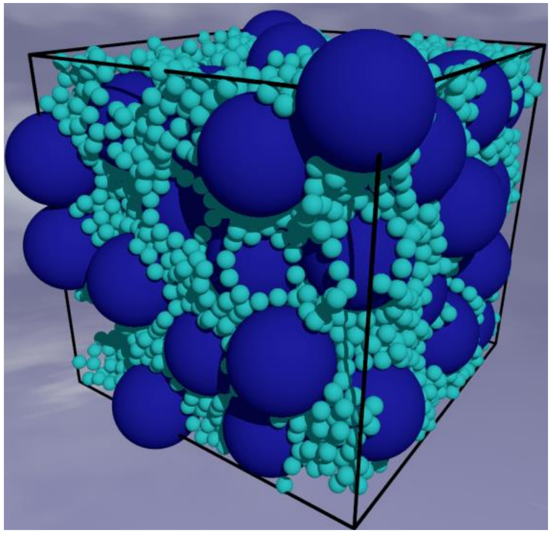
- **Put N_L large and N_S small particles randomly in a box V**
  - Fraction of small particles (in volume)

$$X_S = \frac{N_{\text{Small}}}{N_{\text{Small}} + 6^3 N_{\text{Large}}}$$

Setting

- **Repeatedly minimize the potential energy (using FIRE) and decompress/compress the system, in order to obtain a mechanically stable packing at a fixed pressure**

$$P = -\frac{1}{V}\sum_{\langle ij\rangle} r_{ij} v'_{ij}(r_{ij})$$



- **Our control parameters:**
  - Pressure P
  - Fraction of small particles X_S
  - System size N_S, N_L

- **We generate many (>=200) packings at the same (P,X_s) and analyze the observables averaged over these packings**

Outline

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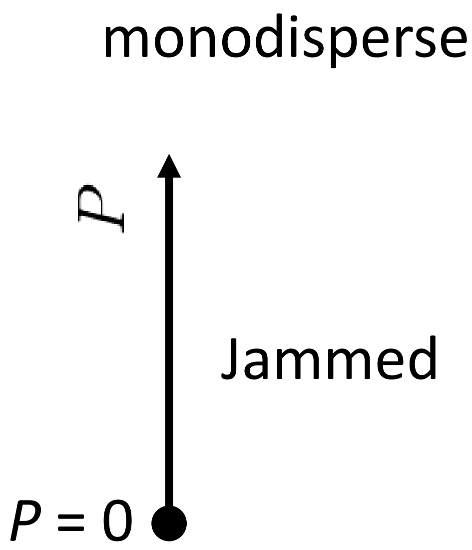
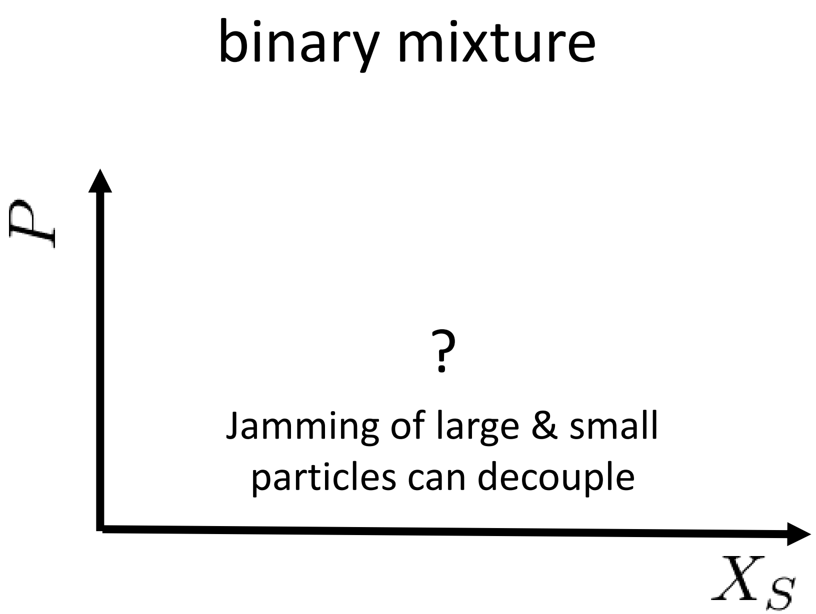
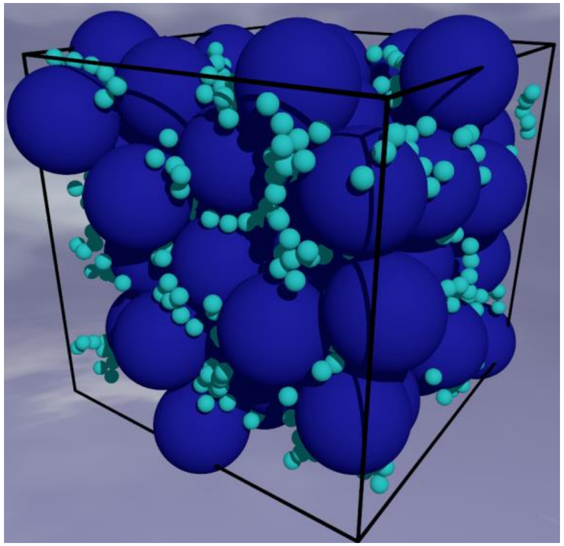
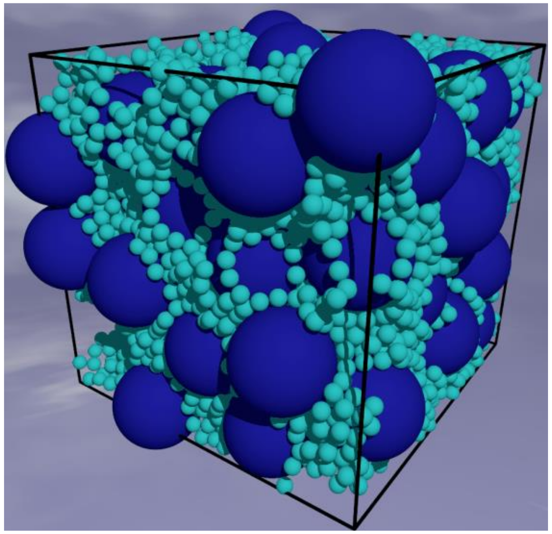




- Near the critical point

Jammed small particles



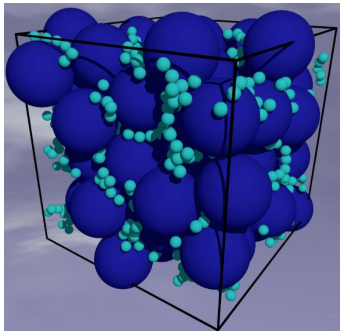


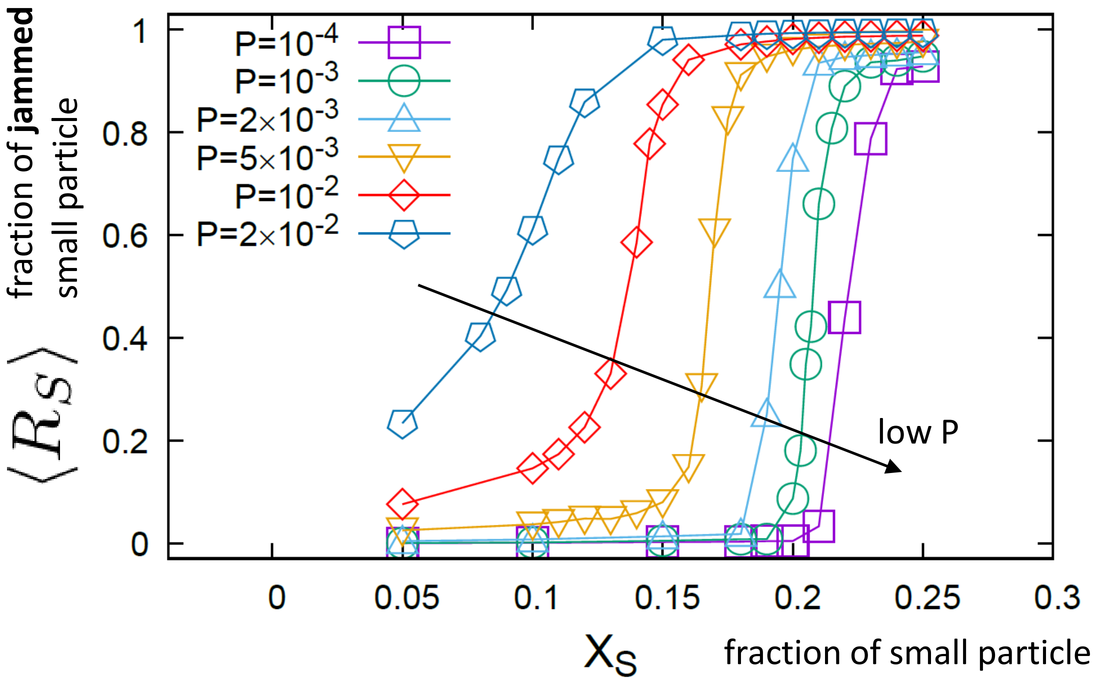
- Jamming of small ones may decouple from jamming of large ones
- **Focus on the *fraction of jammed small particles***

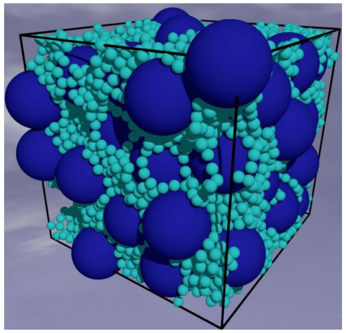
$$R_S = \frac{N_{S,\mathrm{jam}}}{N_S} = \frac{N_S - N_{S,\mathrm{rattler}}}{N_S}$$

  - Rattler: Particles whose contact number is less than 4

1^{st} order transition



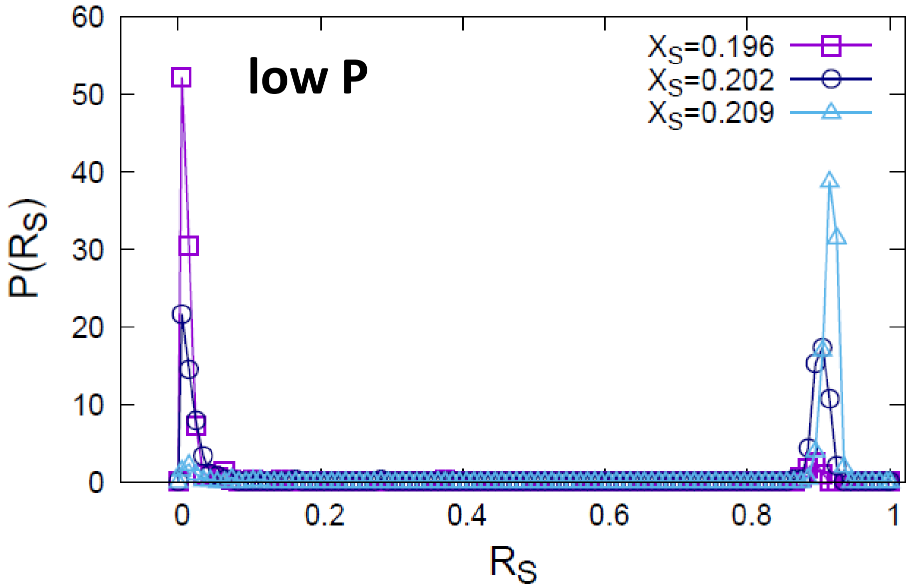


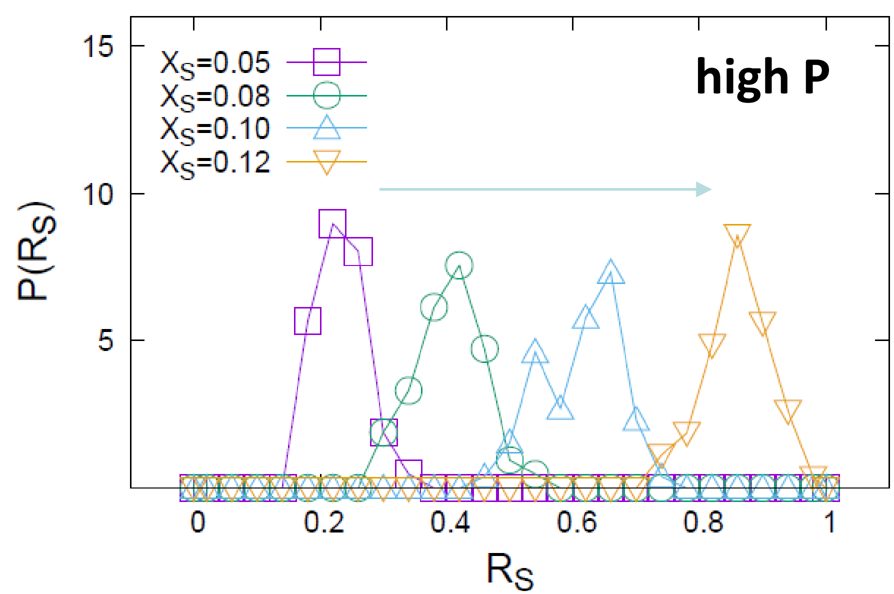


- <*Rs*> increases with *Xs*
  - With increasing the small particles in the system, they tend to get jammed more.
- Discontinuous change in <*Rs*> at low pressure

1^{st} order transition

Probability distribution of *Rs*

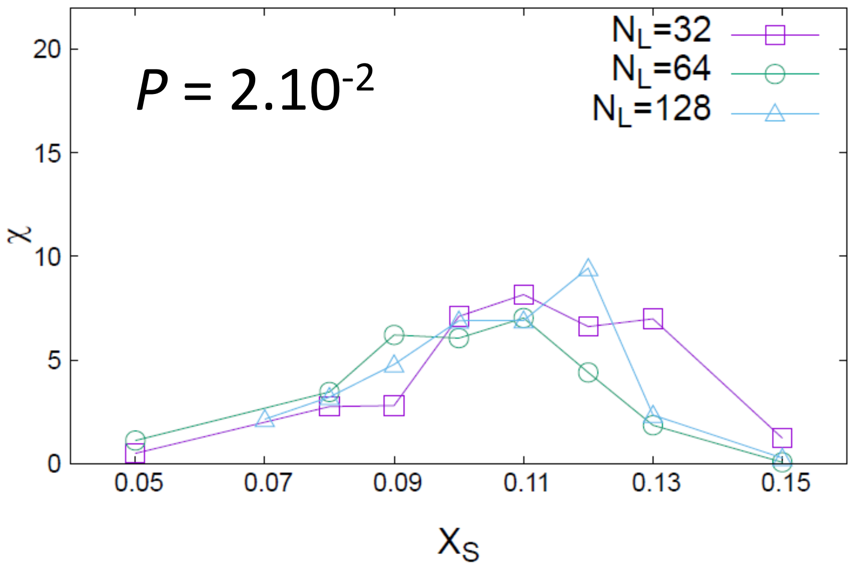




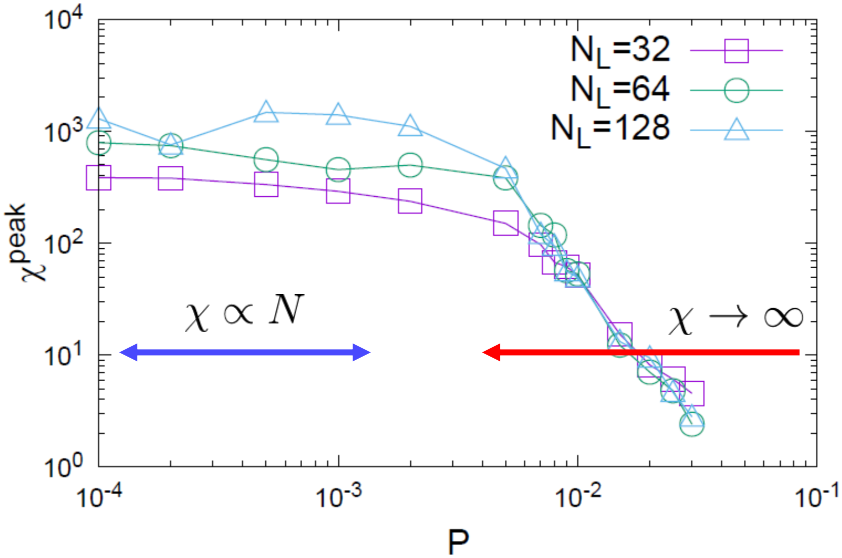
- Low P: 1^{st} order transition
  - Analysis of the binder parameter supports this (not shown)
- High P: Continuous

Critical point

Susceptibility $\chi = N_S(\langle R_S^2 \rangle - \langle R_S \rangle^2)$

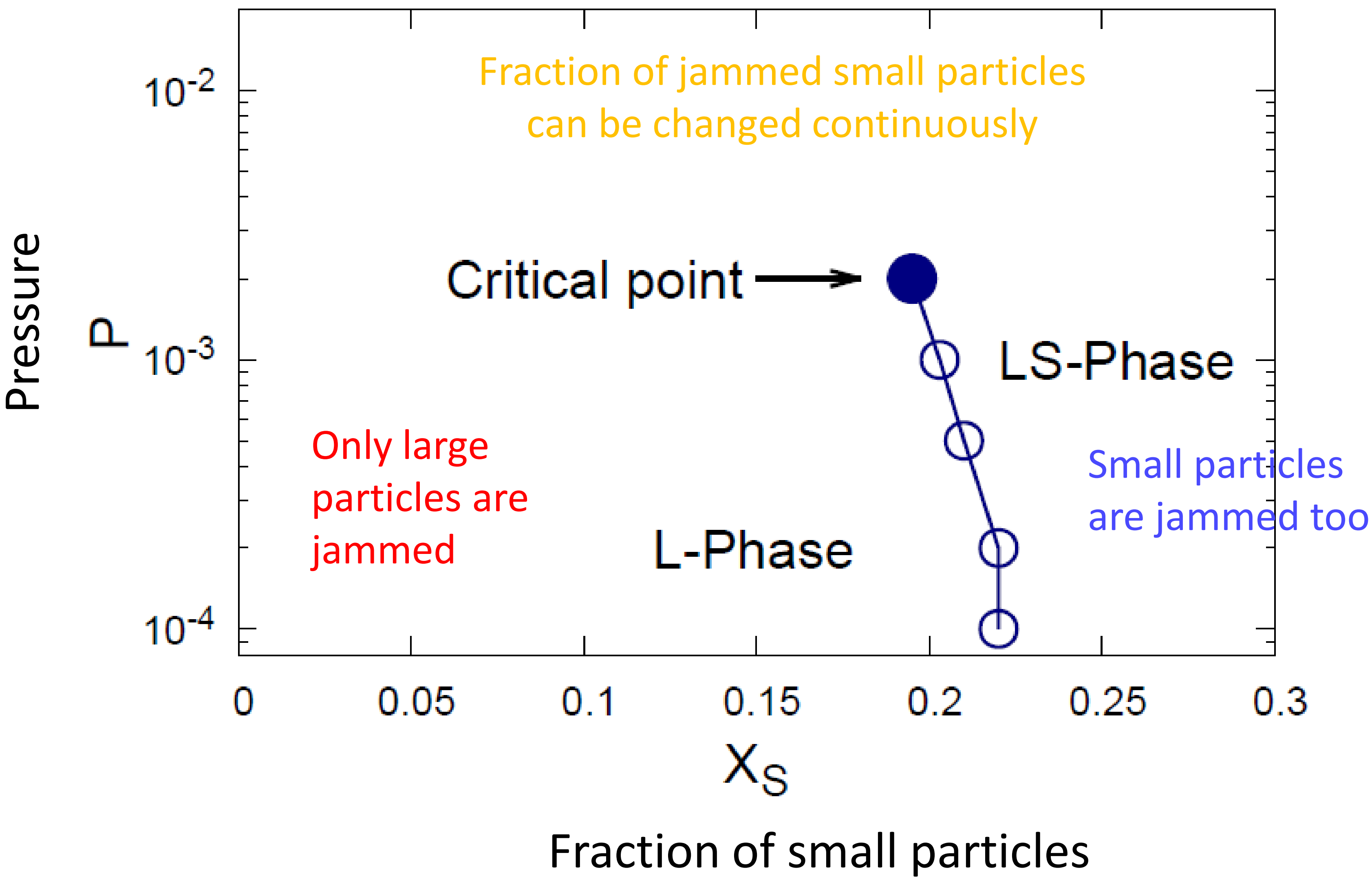


Peak height of χ

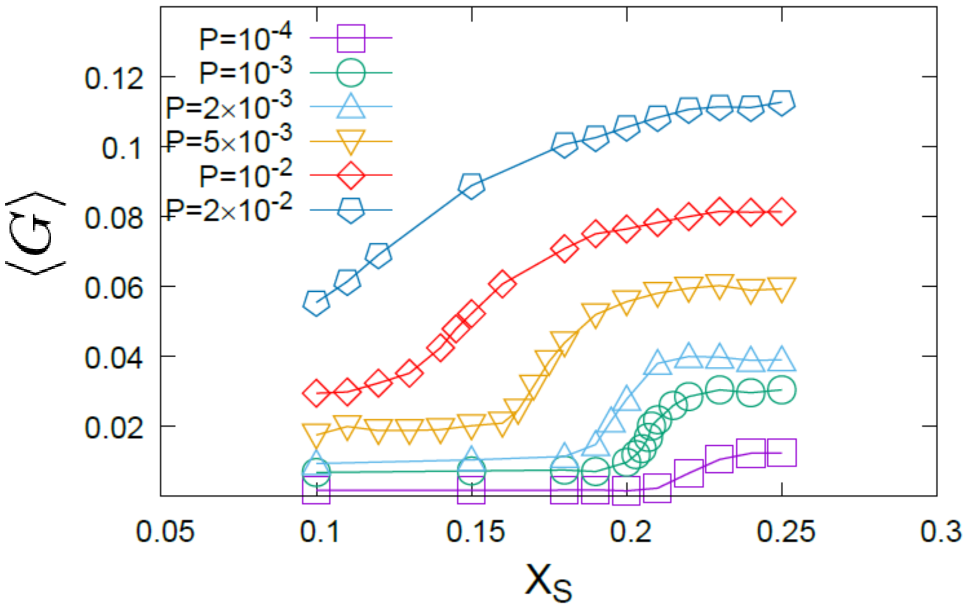


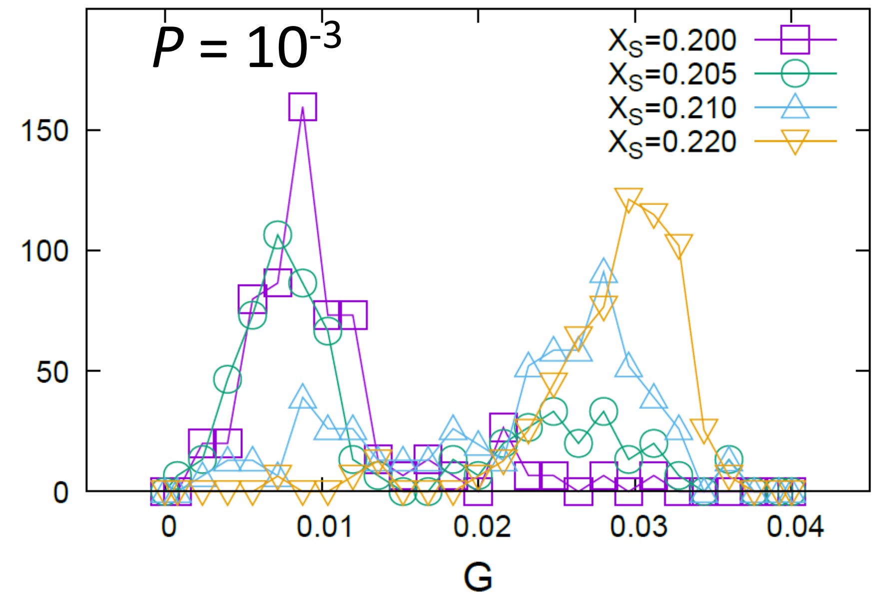
There is a critical point (P^*, X_S^*) at which the susceptibility diverges

Phase diagram



Shear modulus





- Shear modulus discontinuously jumps when the phase boundary crossed.
- Away from the CP, the scaling known for monodisperse packing works:

L-phase: $G \sim A_L \Delta Z$ **LS-phase:** $G \sim A_{LS} \Delta Z$ $A_L \neq A_{LS}$

Outline

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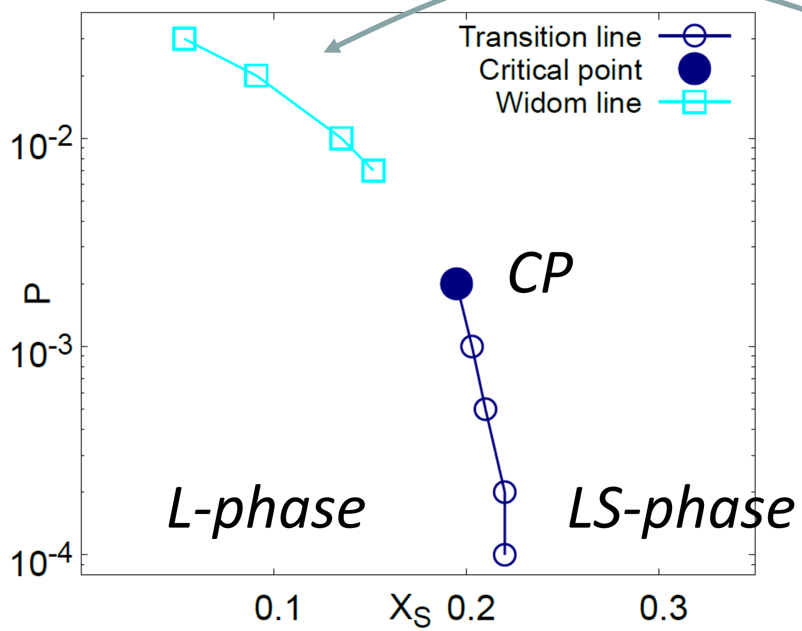
- **Near the critical point**



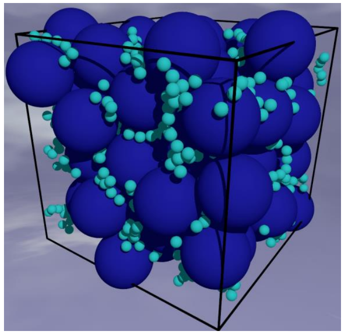
Focus on packings on the "Widom-line"

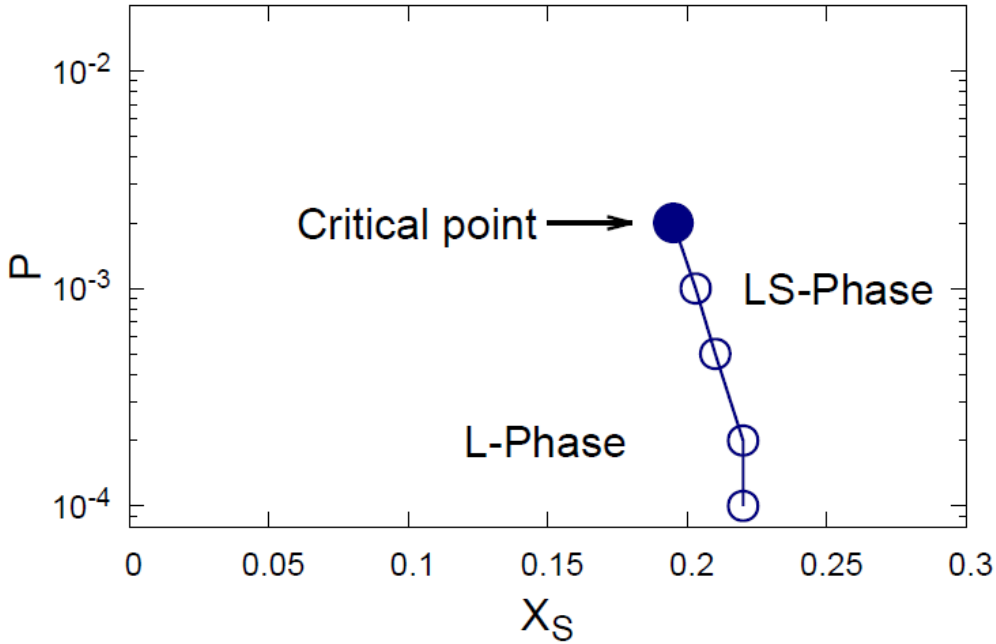
$$\langle R_S \rangle \sim 0.5$$

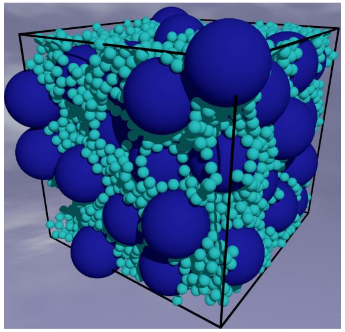
→ Almost half of small particles are jammed

Conclusion 1

- **L-phase and LS-phase exist in the jamming phase diagram**
  - Two phases are separated by the 1st order transition
  - There is a critical point. Above the critical pressure, the two phases are connected smoothly.







Hara Mizuno, Ikeda PRR 2020