

Numerical analysis of compressive deformation process of aggregates with bi-modal fine particles

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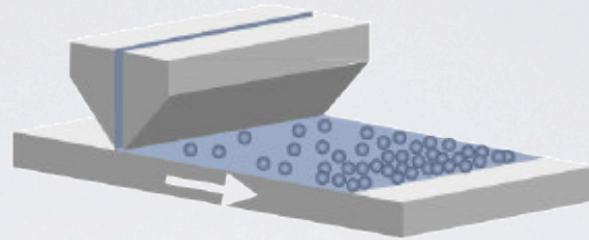
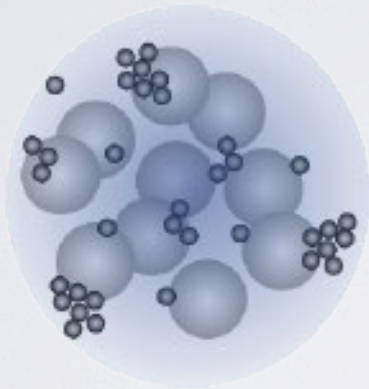
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二峰性微粒子凝集体の
圧縮変形過程の数値解析

小池 修^{*}・辰巳 怜[†]・山口 由岐夫^{*}

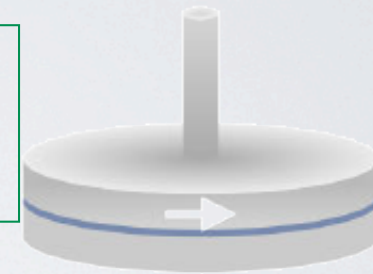
Colloidal Suspensions in Industrial Use

Kneading
Dispersing



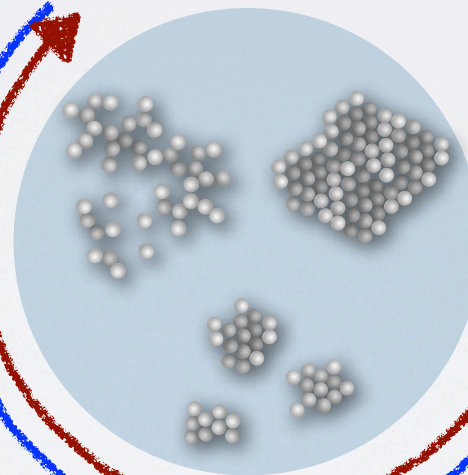
Coating

Chemical
Mechanical
Polishing



Flow field (applied field)
→ Particle structures

Contact Network
Orientation
Size Distribution



Method X

Strength /Viscosity

correlation

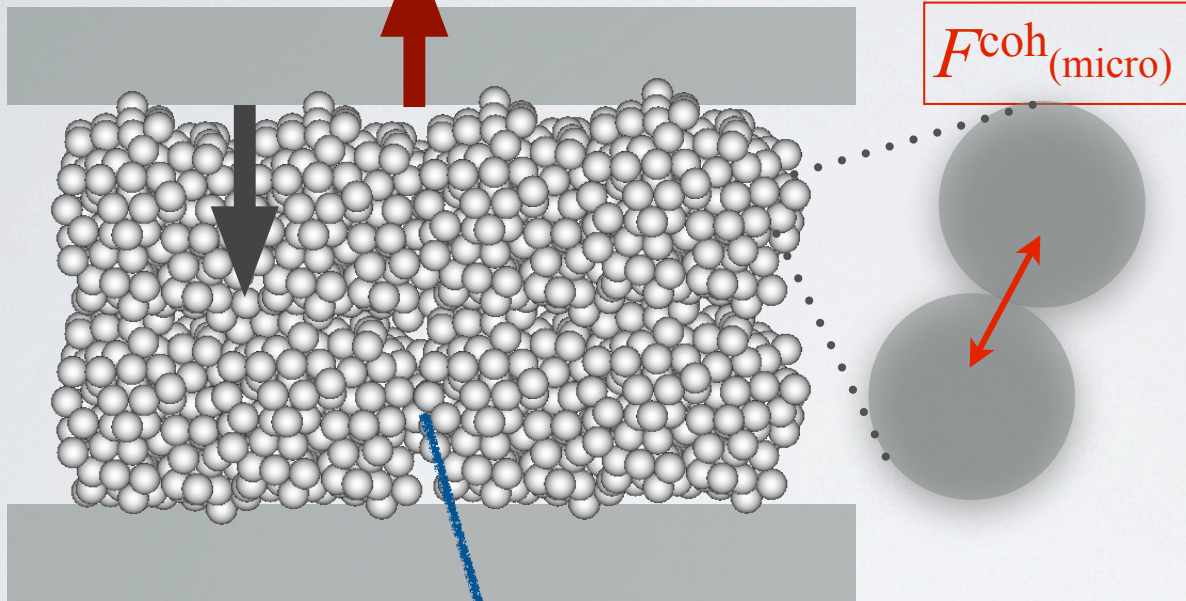
Thermal /Electrical
Conductivity
Optical Property
Mass Diffusivity

DNS

Tensile Strength of Granular Bed

directly observable :

$\sigma_{\text{(macro)}}$



Rumpf's formula

$$\sigma = \frac{\varphi_p n_c F^{\text{coh}}}{\pi d^2}$$

$$\sigma \propto d^{-1} \quad \text{if } F^{\text{coh}} \propto d.$$

For $d = 1.0 \mu\text{m}$,
 $F^{\text{coh}} \sim 0.1 \mu\text{N}$

Conditions

valid for Rumpf's formula:

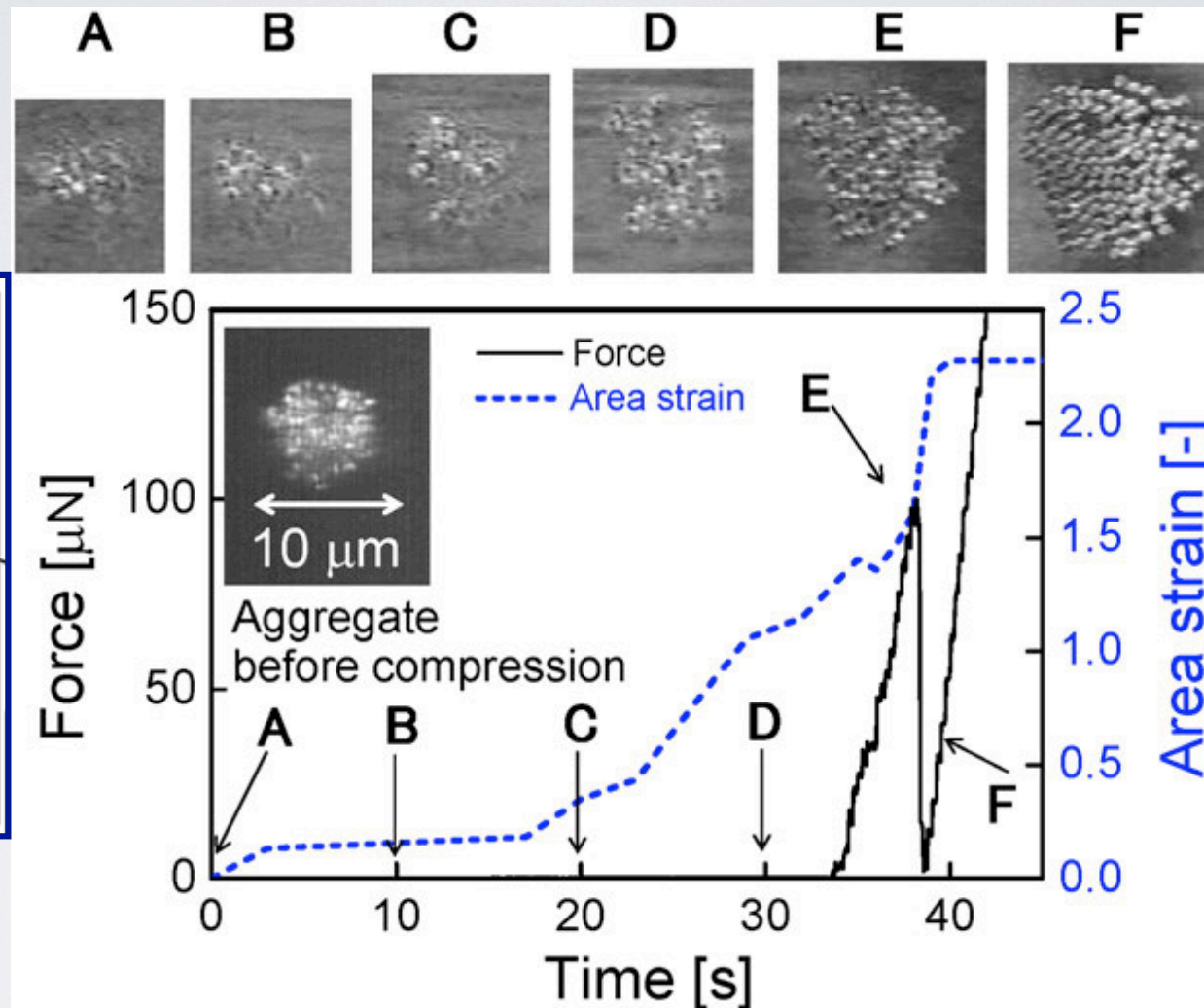
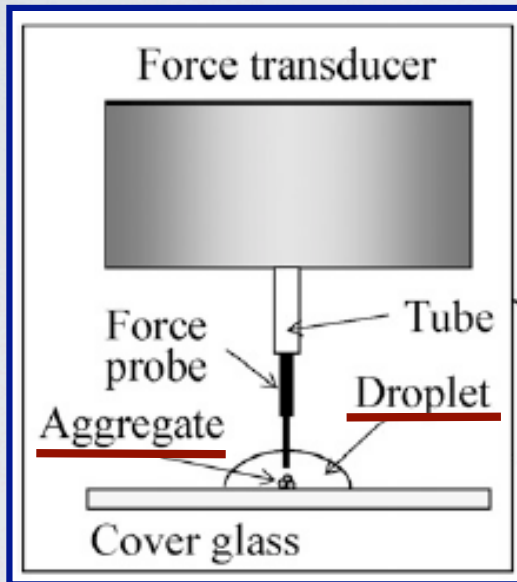
Uniform sphere,

Random packing (isotropic)

Previous Study I

- monomodal particles in liquid -

Exp.



$$d_p = 1 \mu\text{m}$$

Kubo et al.,
Powder Technology 287 (2016) 431

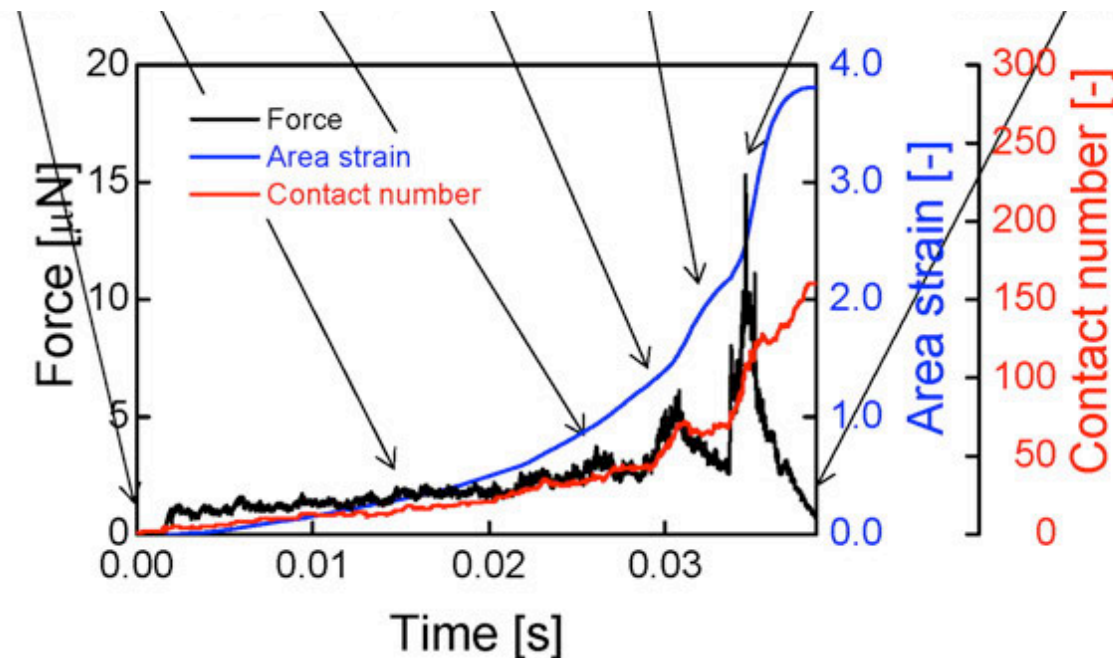
Previous Study I

- monomodal particles in liquid -

Sim.

Strength

$$d_p = 1 \mu\text{m}$$



Kubo et al.,
Powder Technology 287 (2016) 431

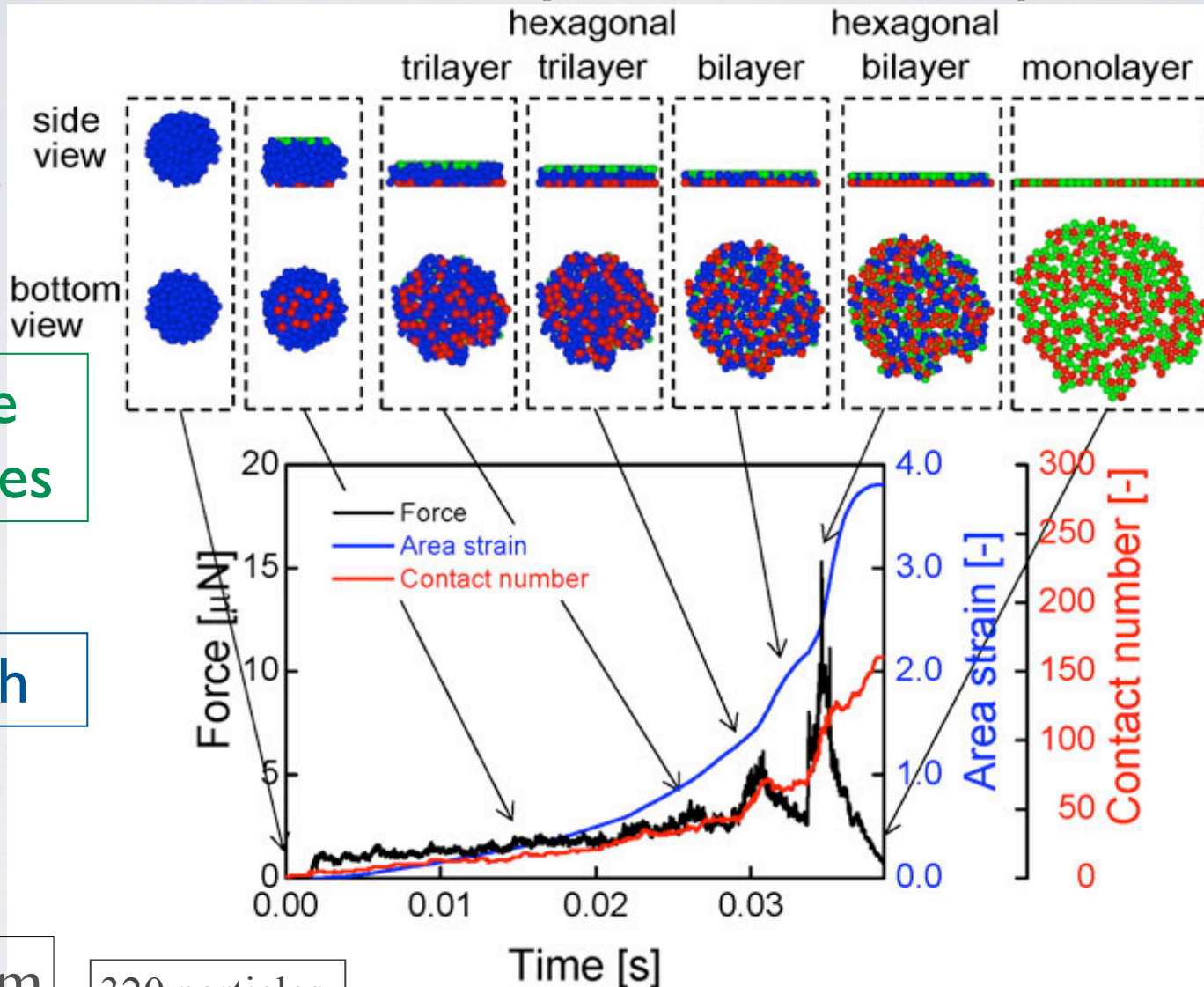
Previous Study I

- monomodal particles in liquid -

Sim.

Particle
structures

Strength



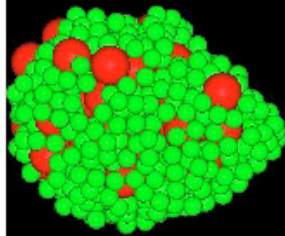
$$d_p = 1 \mu\text{m}$$

320 particles

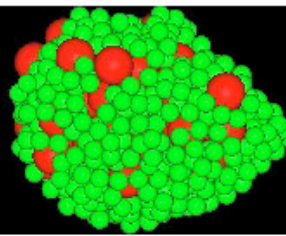
Kubo et al.,
Powder Technology 287 (2016) 431

Previous Study II

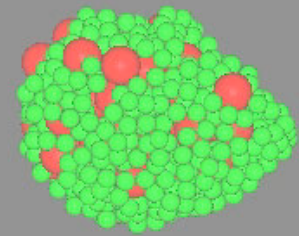
- bimodal particles in gas -



Wall - x



Wall - y



Wall - z

$$d_L = 1.0 \mu\text{m}$$
$$d_L / d_S = 2.0, \quad X_s = 0.5$$

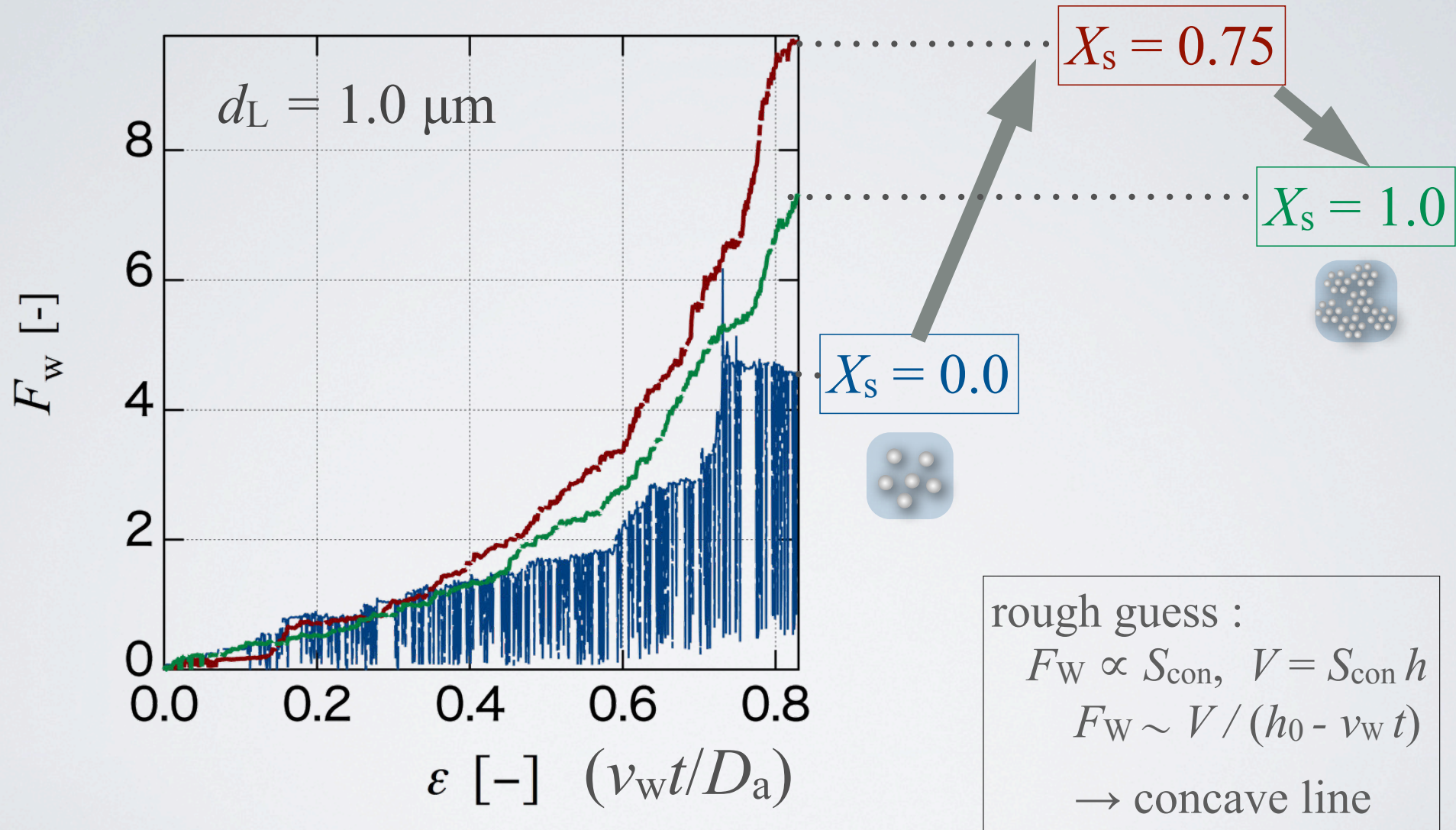
1000 particles
for $X_s = 1.0$

$$Da \sim 6d_L$$

Koike et al.,
2017 SCEJ 82th Annual Meeting

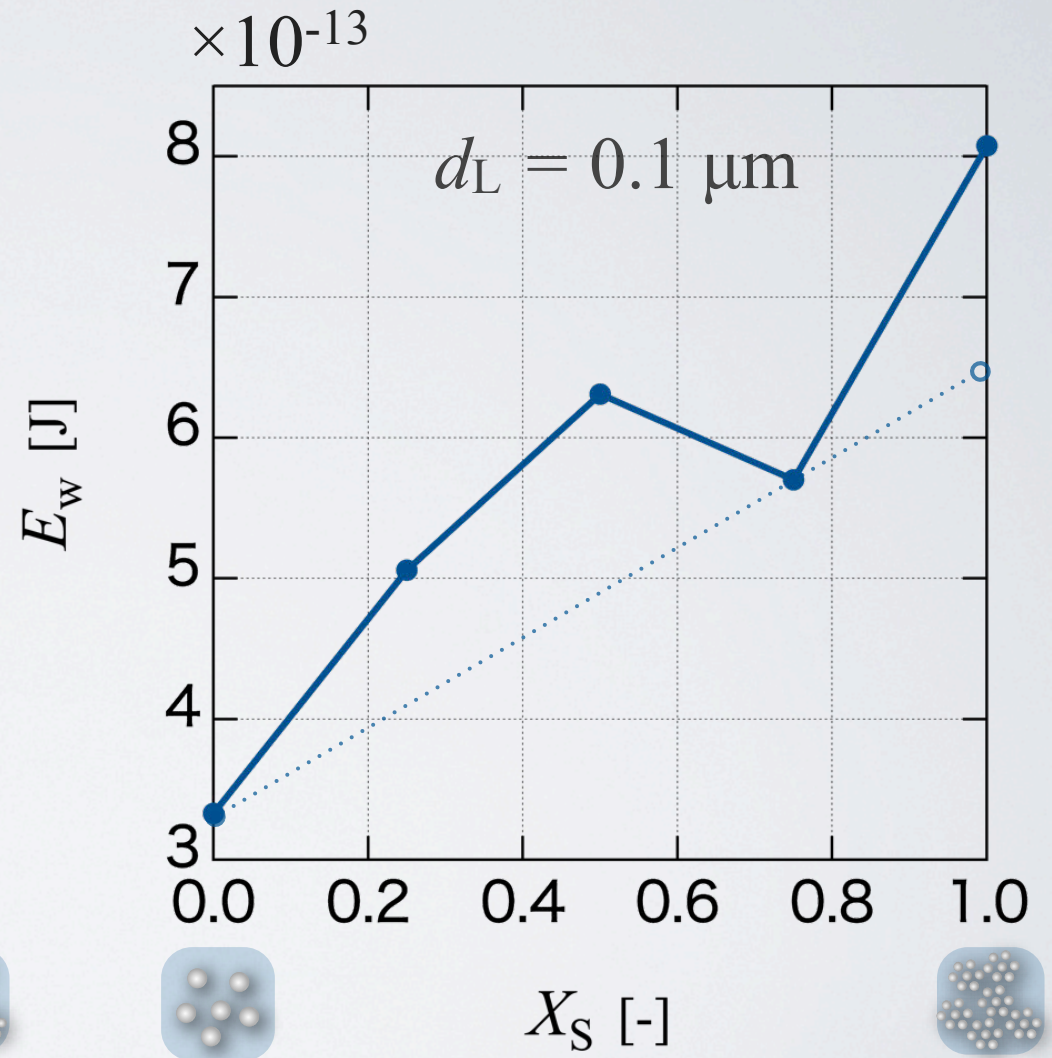
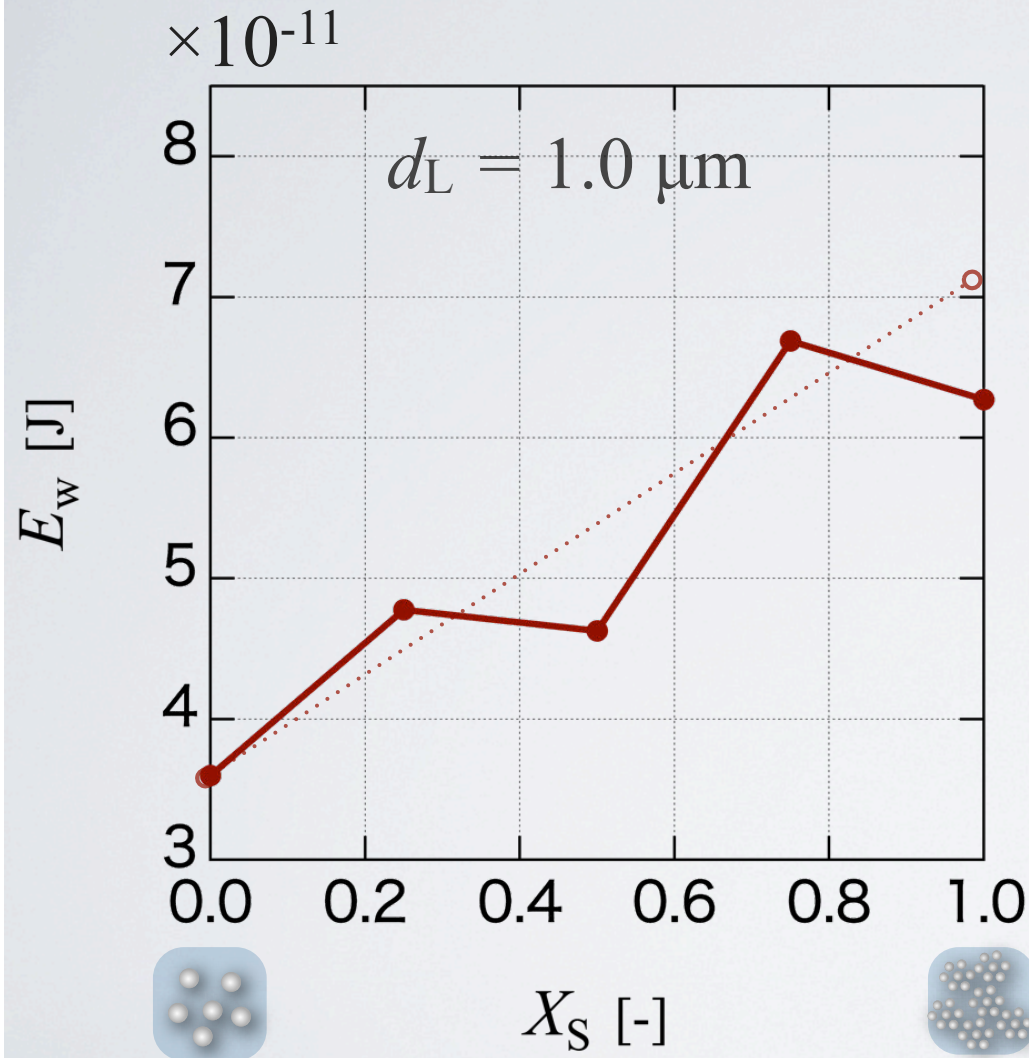
Previous Study II

- bimodal particles in gas -



Previous Study II

- bimodal particles in gas -



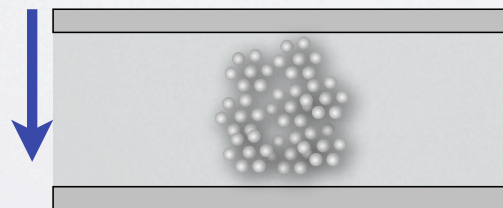
E_w : average work done by wall,
 $\varepsilon : 0 \rightarrow 0.83$; $\delta \sim 5d_L$

Objective

- Analyse deformation process of aggregates composed of bimodal fine particles by DEM (numerical simulation)

Method

- Based on Discrete Element Method (SNAP-L)
- Compress aggregates by moving plane-parallel walls



Equation of Motion for Particle

D.O.F



$$m \frac{d\mathbf{v}_p}{dt} = \mathbf{F}^{\text{co}} + \mathbf{F}^{\text{v}} + \mathbf{F}^{\text{cb}}$$

Cohesive force:
van der Waals force
capillary bridge force

$$F^{\text{coh}} \propto d$$

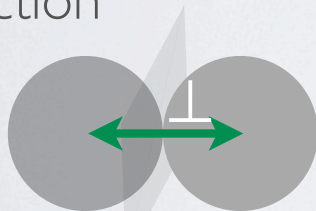


$$I \frac{d\omega_p}{dt} = \mathbf{T}^{\text{co}}$$

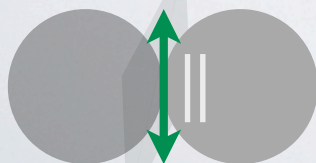
Contact force:
Visco-elastic type
Coulomb's friction

$$|\mathbf{F}_t^{\text{co}}| = \min(|\mathbf{F}_t^{\text{co}}|, \mu |\mathbf{F}_n^{\text{co}}|)$$

Direction



$$: F_n^{\text{co}} \quad F_n^{\text{v}} \quad F_n^{\text{cb}}$$



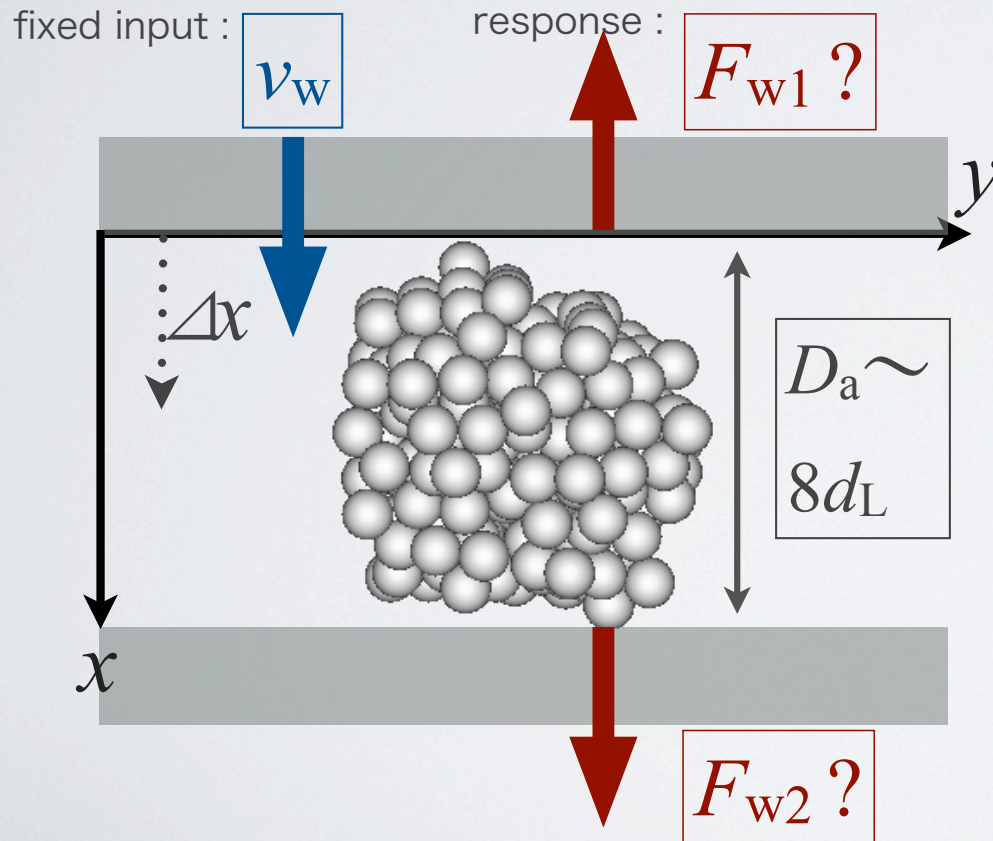
$$: F_t^{\text{co}}$$

Simulation Condition

Wall

$$v_w \text{ [m/s]} : 2.5 \times 10^{-3}$$

$$\Delta x, \Delta y, \Delta z = 7d_L = \delta$$



Particle

$$d_L \text{ [}\mu\text{m]} : \begin{matrix} \xrightarrow{\quad} 1/10 \\ 1.0 & 0.1 \end{matrix}$$

$$d_s \text{ [}\mu\text{m]} : \begin{matrix} 0.5 & 0.05 \\ \downarrow 1/2 \end{matrix}$$

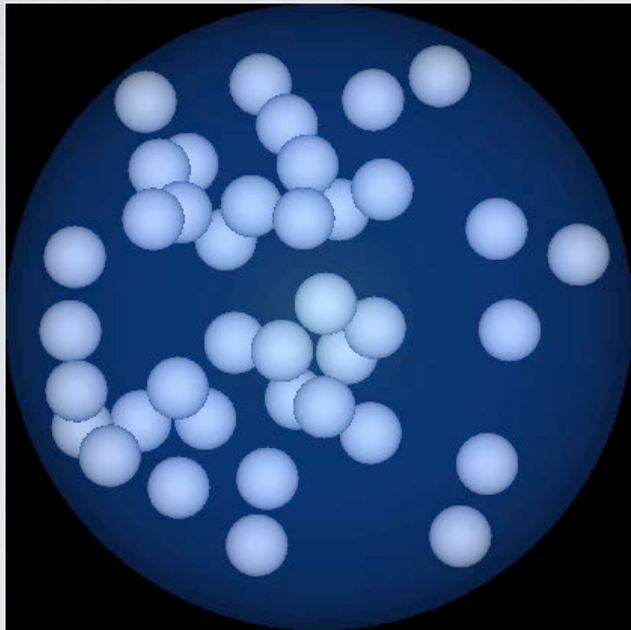
$$X_s = V_s/V : 0.0 - 1.0$$

For $X_s = 1.0$,
 2.0×10^3 small particles

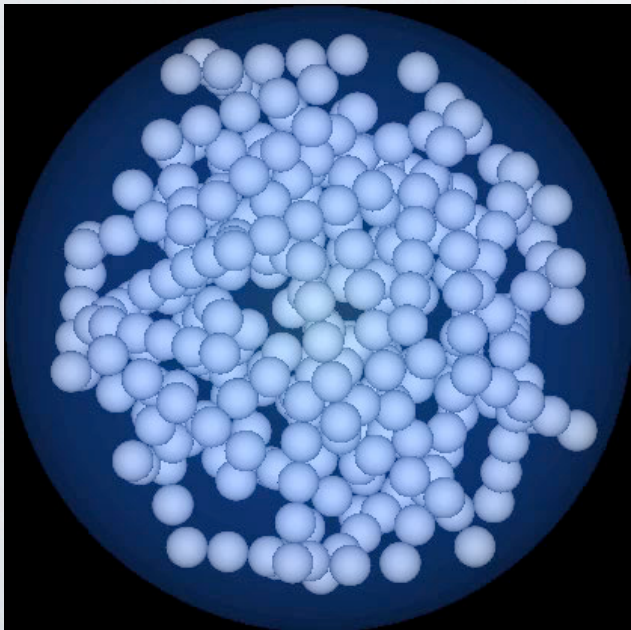
$$A \text{ [J]} : 3.0 \times 10^{-20}$$

Particle is same as wall
 in mechanical properties

How to Make Single Aggregate



- Confine particles in a droplet
- Shrink the droplet during drying
- Push particles into the center of droplet by capillary force



- Simple and efficient method
- It is hard to control the fractal dimension as in DLCA

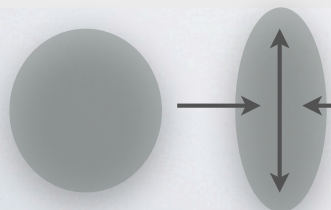
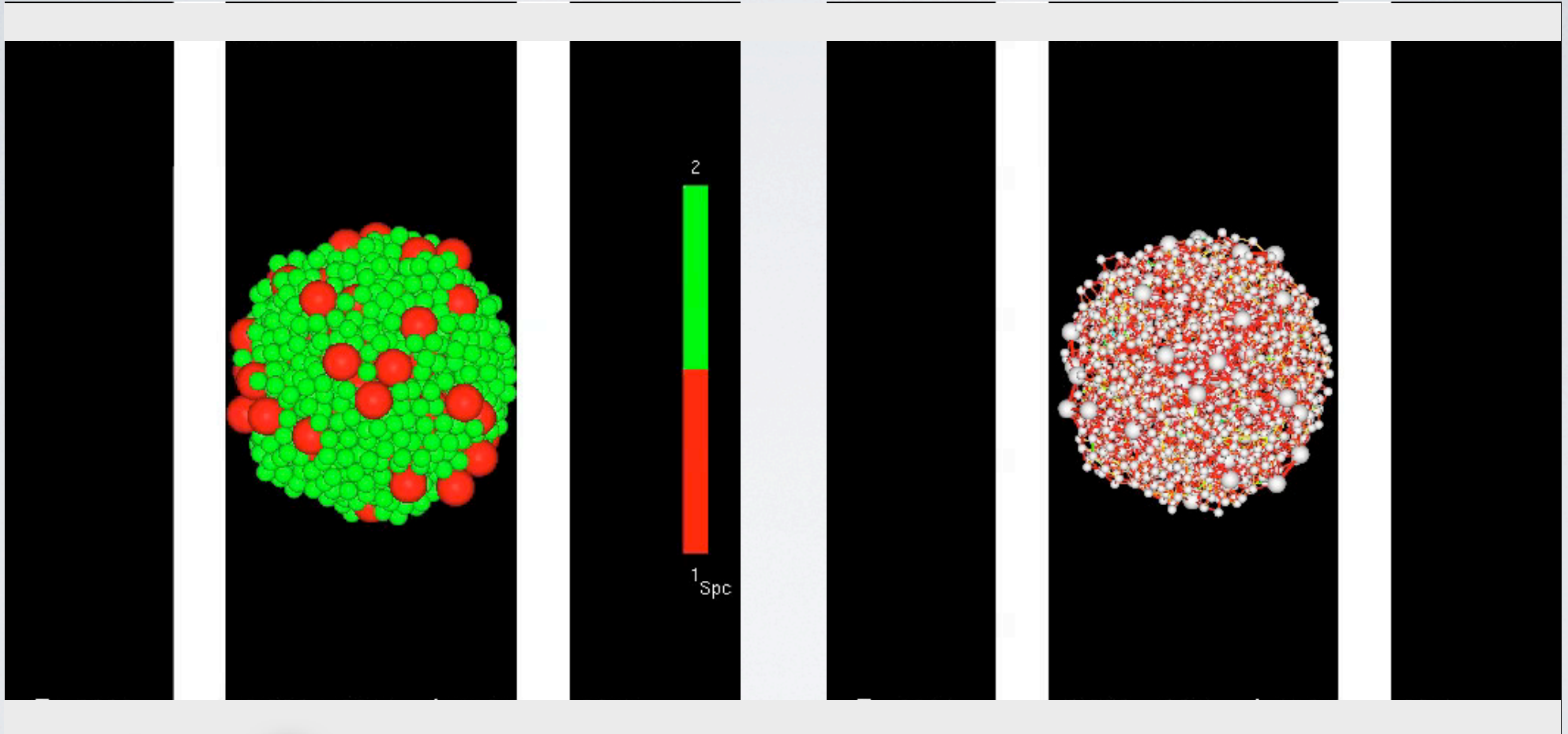
Gyration radius of an aggregate

$$\left(\frac{R_g}{a} \right) \propto N^{1/d_f} \quad d_f \text{ [-] : 2.89}$$

d_f : fractal dimension

Particle Motion & Force Chain

$$d_L = 1.0 \mu\text{m}, \quad X_s = 0.5$$



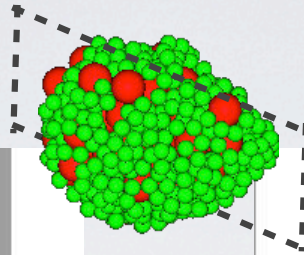
Oblate
deformation

Frequent variation
in contact force

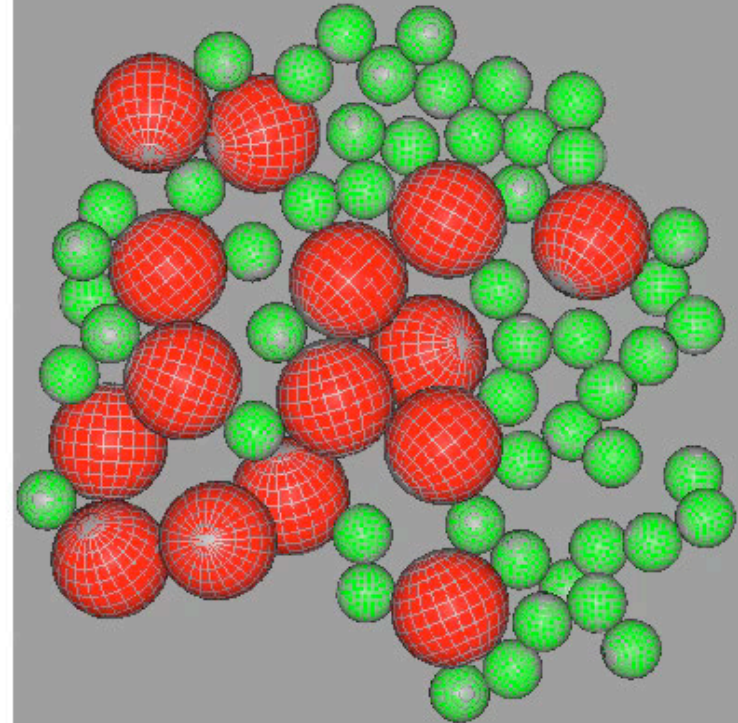
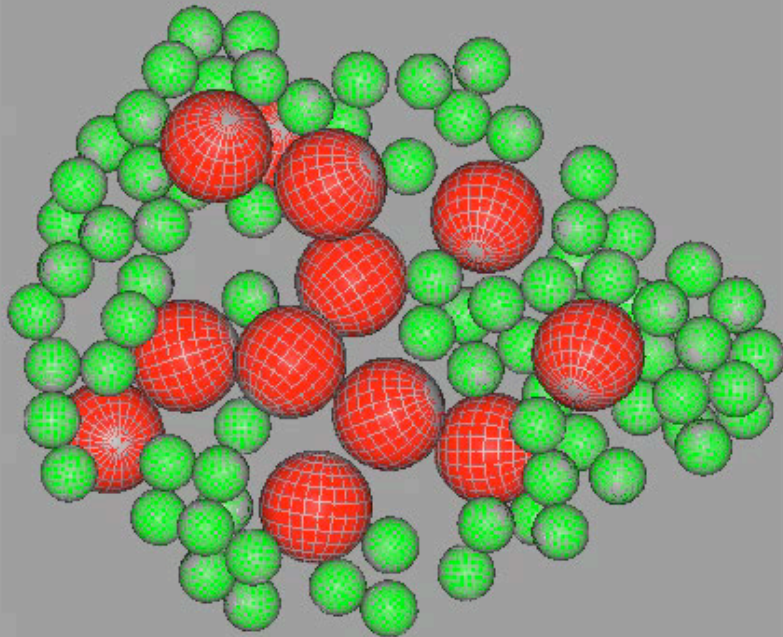
Rotation of Particle

$$X_s = 0.5$$

$$d_L = 1.0 \mu\text{m}$$



$$d_L = 0.1 \mu\text{m}$$

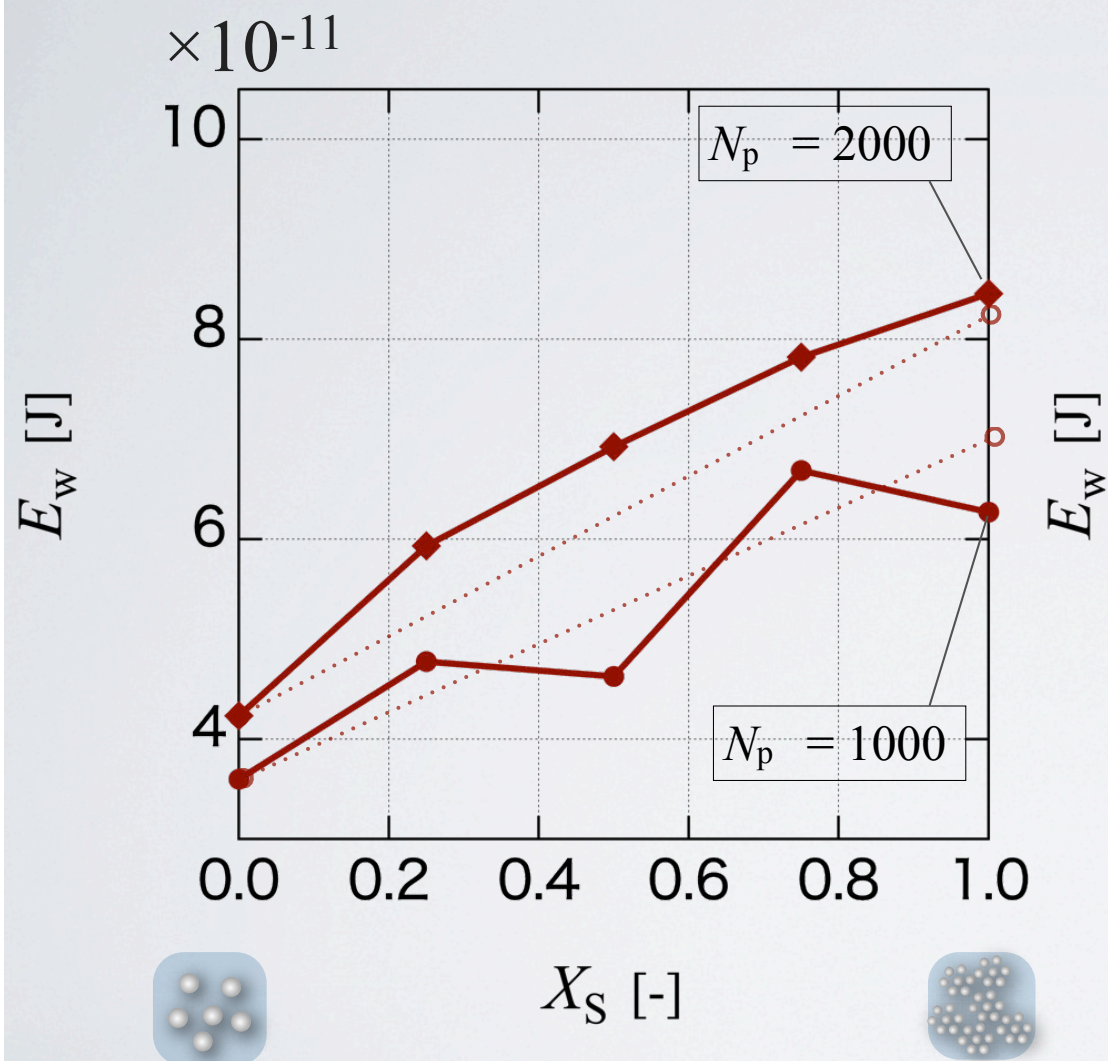


Frequent rotation with slip
for smaller particles

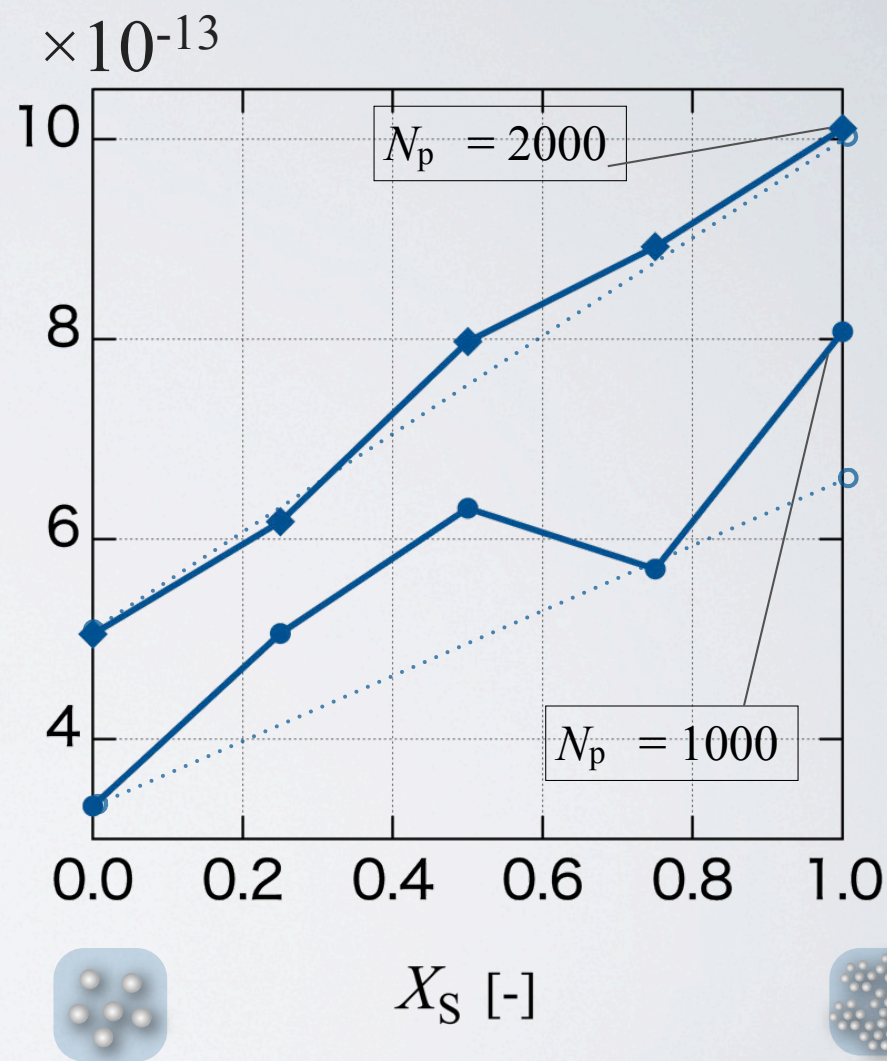
$$I = \frac{2}{5}ma^2 \propto a^5$$

Work vs. X_s

$d_L = 1.0 \mu\text{m}$



$d_L = 0.1 \mu\text{m}$



E_w : average work done by wall,
 $\delta \sim 5d_L$

Remarks

- Benefit of DNS -

- Our approach enable us to visualize the detailed breakup process of the aggregate.
- Our approach leads us to catch a key factor / basic concept affecting compression process / strength of an aggregate.