SCEJ 56th Autumn Meeting
Sept. 18, 2025

Particle-scale simulation of drying slurry coated onto a particulate layer

粒子層上でのスラリー塗布膜の乾燥の粒子スケールシミュレーション

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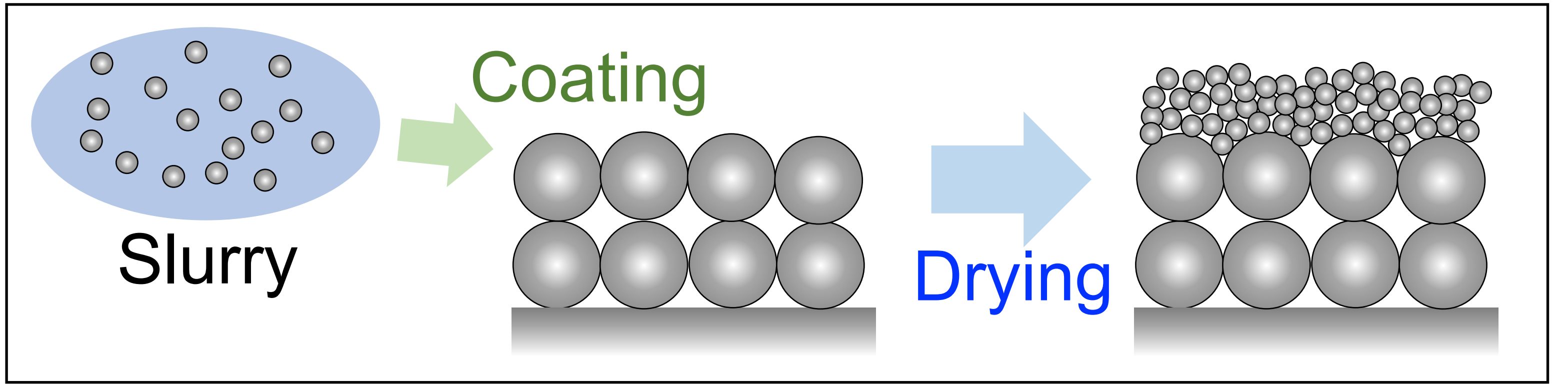
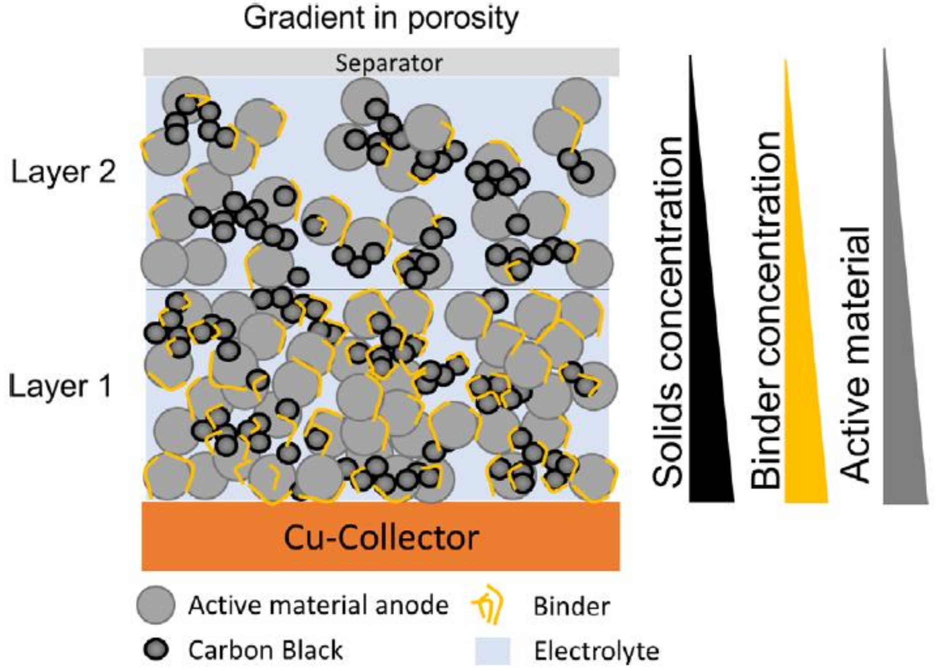
Slurry coating onto particulate layers



Glazed ceramics

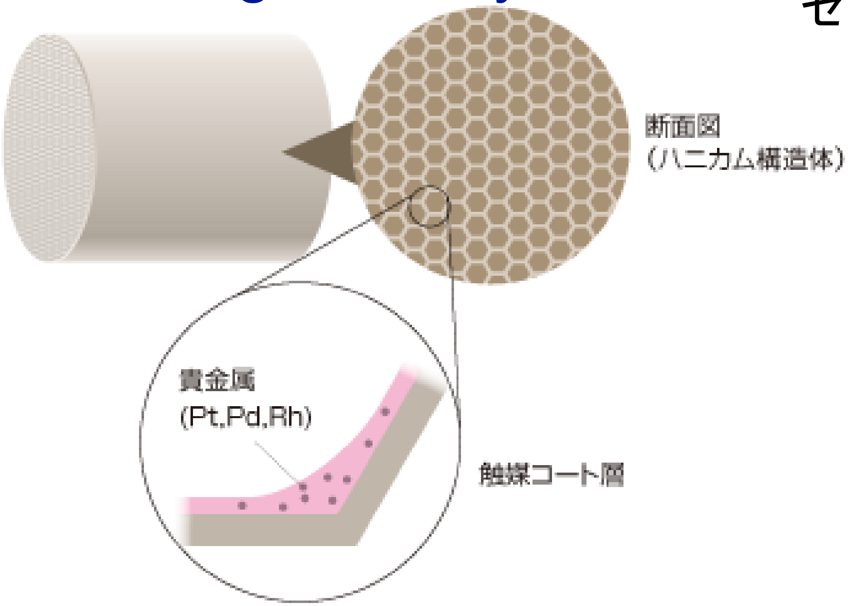
濱崎喜仁,
セラミックス **55** (2020).

Two-layer anode (Lithium-ion battery)



Gottschalk *et al.*, Energy Technol. **11** (2023).

Exhaust gas catalyst



https://www.cataler.co.jp/train/qa/living/03.php

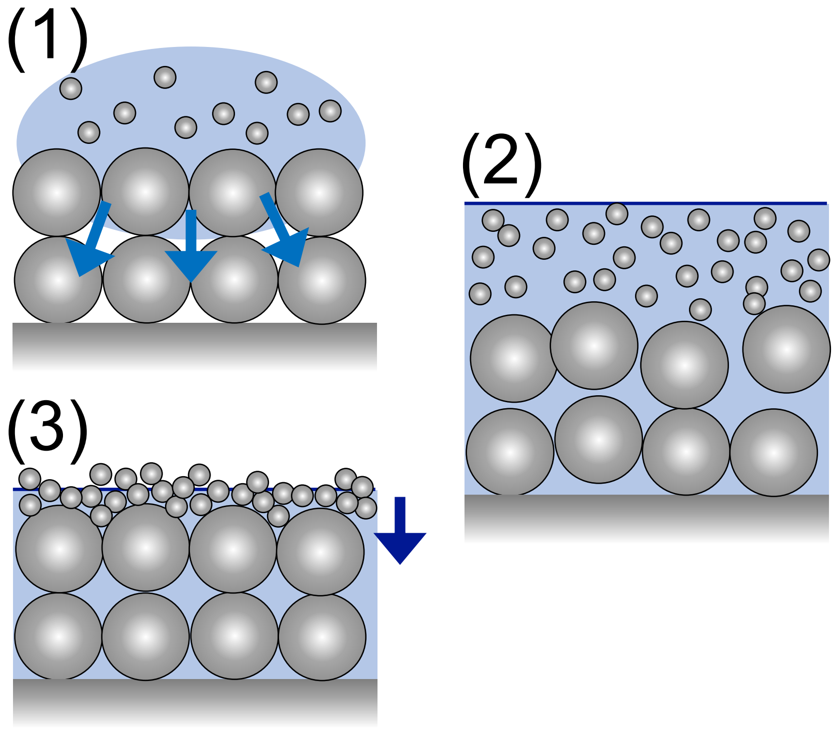
Slurry coating onto particulate layers

Elementary processes

(1) Penetration of solvent

(2) Dispersion and dissolution of particulate layers

(3) Drying of slurry



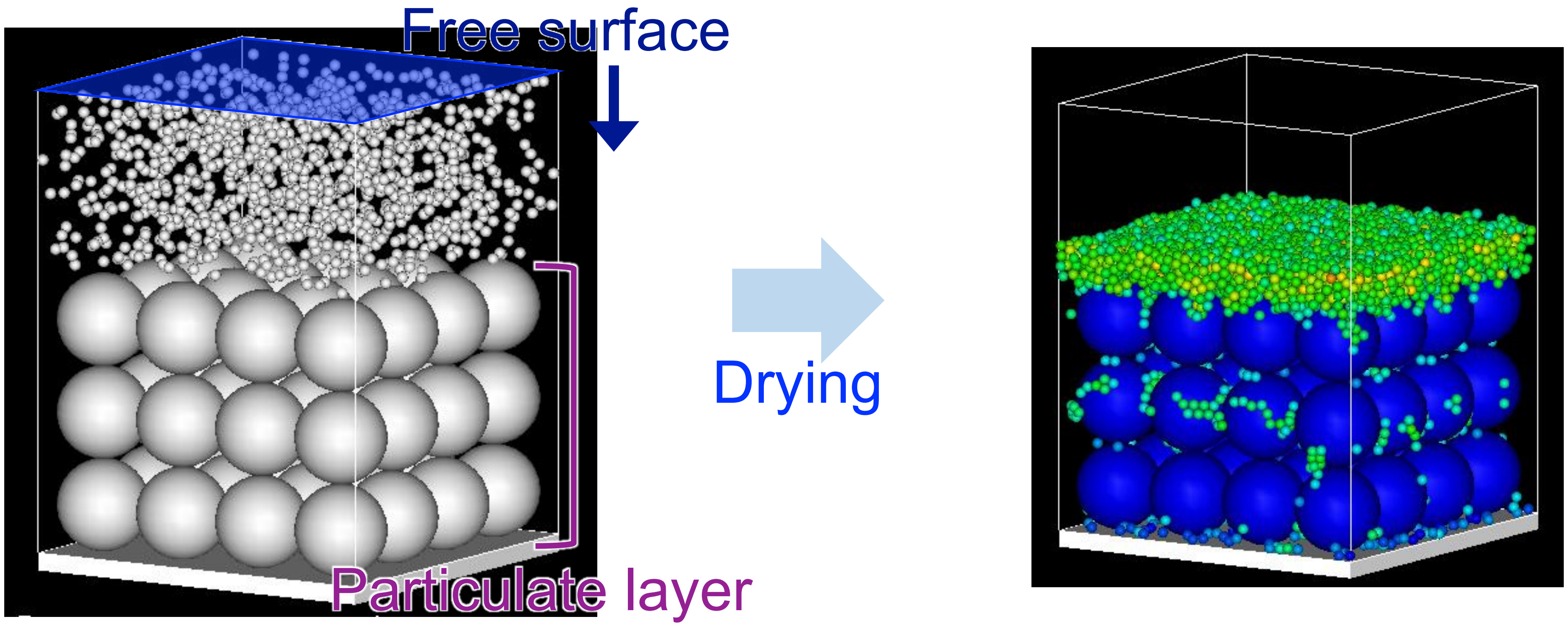
Timescale separation (Thin particulate layer, Rapid drying)

(1) < (3) < (2)

Present study

Objective & Method

Numerical simulation of drying slurry coated onto a particulate layer



- Structure of particulate layer
- Surface tension of solvent
  (vs. particle interactions)

- Particle distribution
- Coated layer thickness
- Surface roughness

Model: Particles' motion

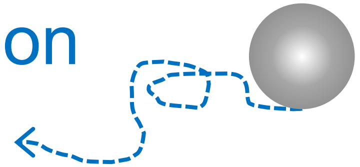
$$m_i \dot{\boldsymbol{v}}_i = -\zeta_i \boldsymbol{v}_i + \boldsymbol{F}_i^{\mathrm{R}} + \boldsymbol{F}_i^{\mathrm{cpl}} + \boldsymbol{F}_i^{\mathrm{cnt}} + \boldsymbol{F}_i^{\mathrm{DLVO}}$$

Fluid Free surface Particles

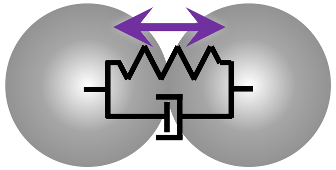
- **Hydrodynamic force**

  Drag: $-\zeta_i \boldsymbol{v}_i$, Fluctuations: $\boldsymbol{F}_i^{\mathrm{R}}$

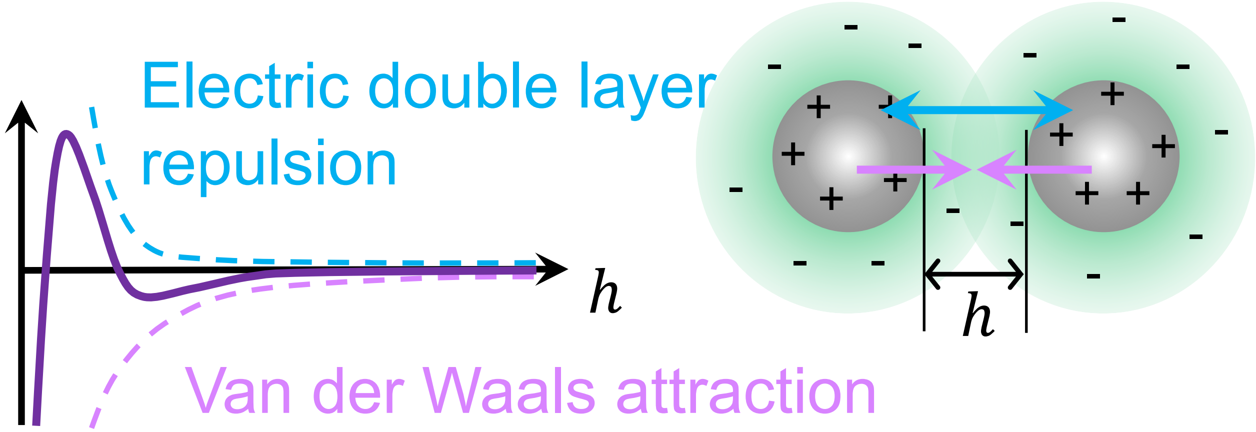
  → Brownian motion



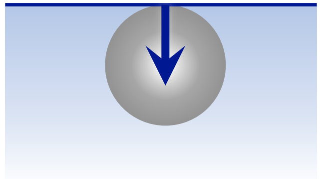
- **Contact force**: $\boldsymbol{F}^{\mathrm{cnt}}$



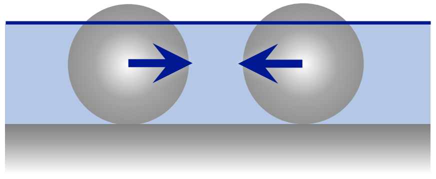
- **DLVO force**: $\boldsymbol{F}^{\mathrm{DLVO}}$



- **Capillary force**: $\boldsymbol{F}^{\mathrm{cpl}}$



Vertical



Lateral

Simulation conditions

Particles

- Diameter: $d = 100\ \mathrm{nm}$
- Initial concentration: $7.5\ \mathrm{vol\%}$
- Zeta potential: $-28\ \mathrm{mV}$

Particulate layer

- Particle diameter: $d_\mathrm{L} = 8d$
- Number of layers: 3
- Structure: sc, fcc

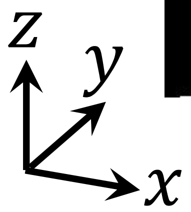
Fluid

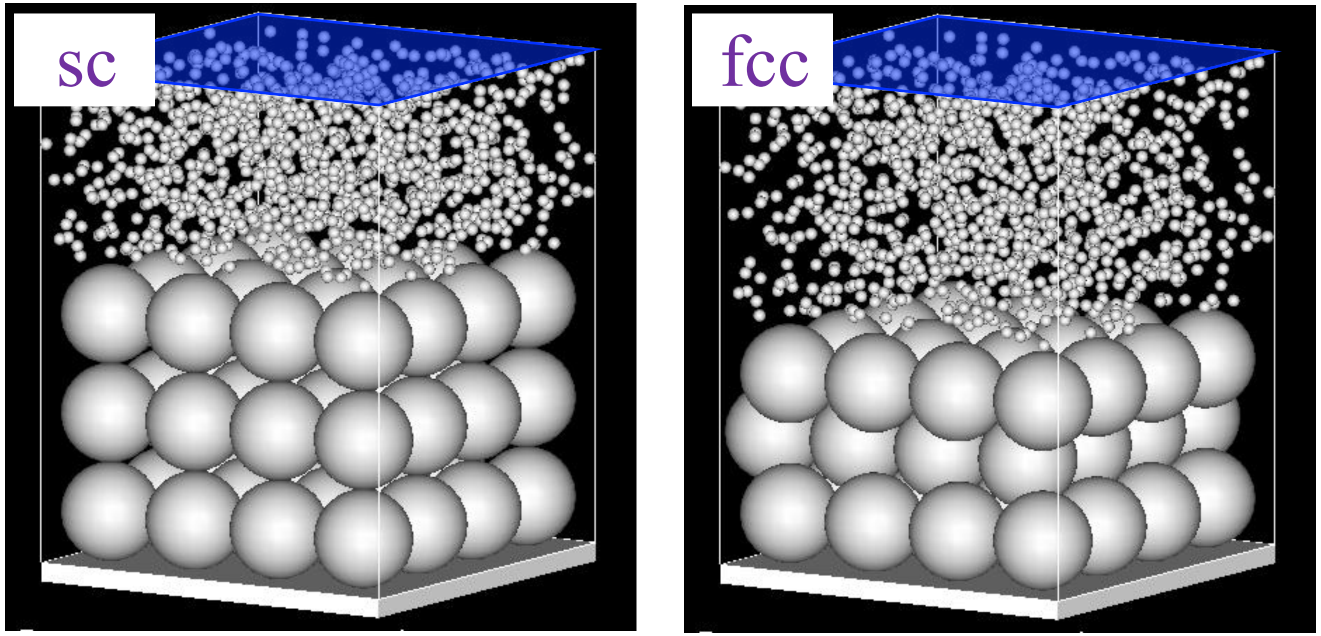
- Surface tension:

$$\alpha = \frac{(\text{Capillary force})}{(\text{Adhesion force})} = \frac{(\pi/2)\gamma d}{Ad/(24\delta^2)} = 0.05, 0.5$$

γ: Surface tension A: Hamaker constant $\delta \sim 1\ \text{Å}$

System size: $4d_\mathrm{L} \times 4d_\mathrm{L} \times 5d_\mathrm{L}$



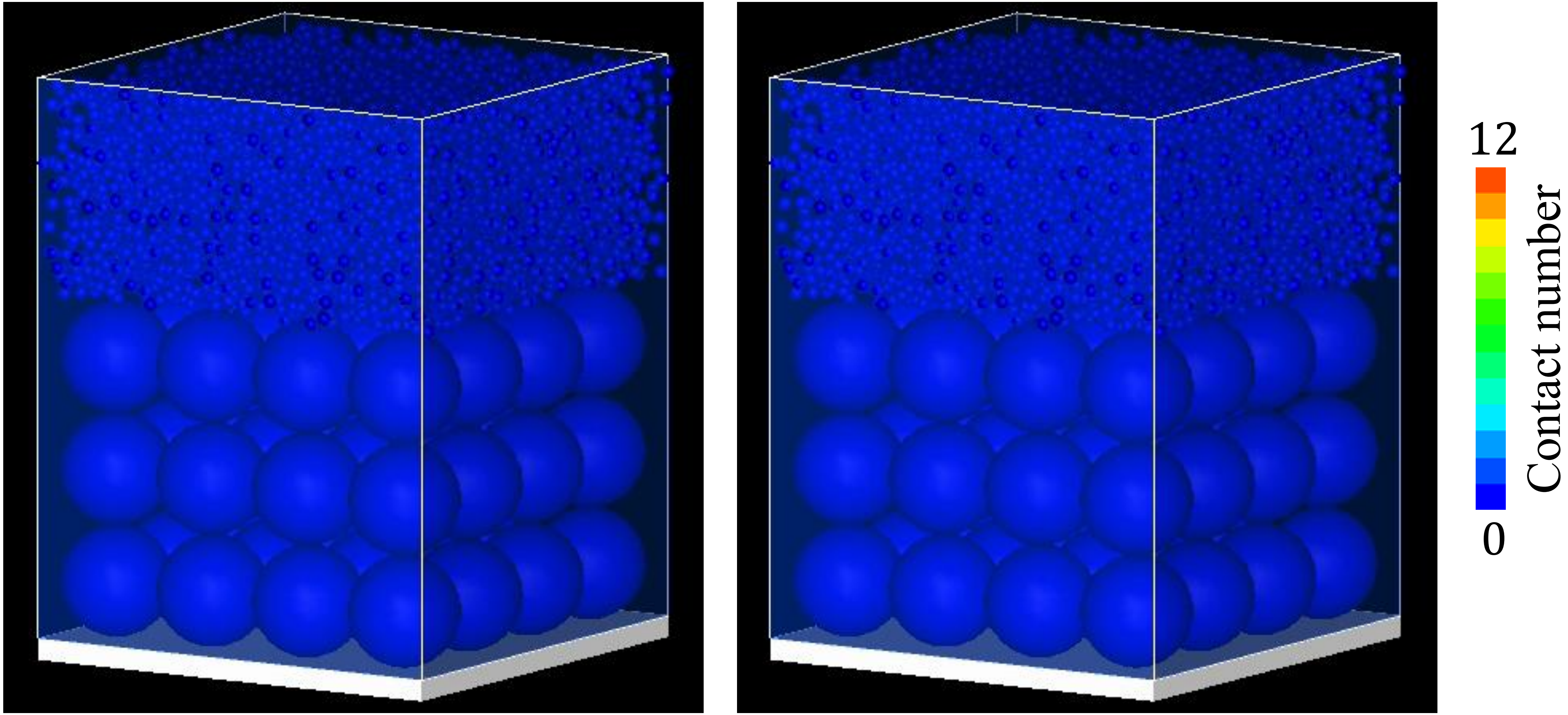


Simple cubic Face-centered cubic

- Particle drying Péclet number

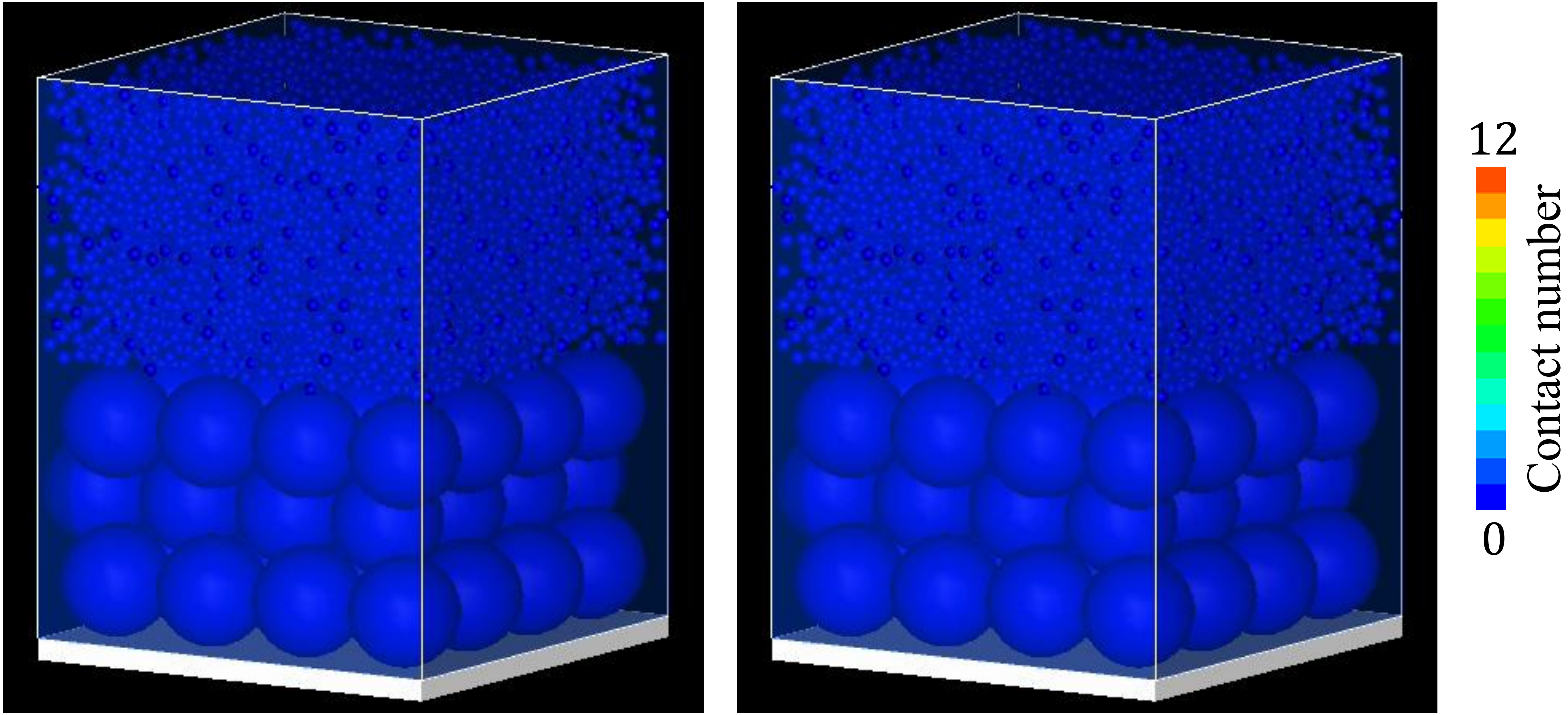
$$\mathrm{Pe} = \frac{(\text{Drying rate})}{(\text{Diffusion rate})} = \frac{U}{D/d} = 10$$

Results (sc)



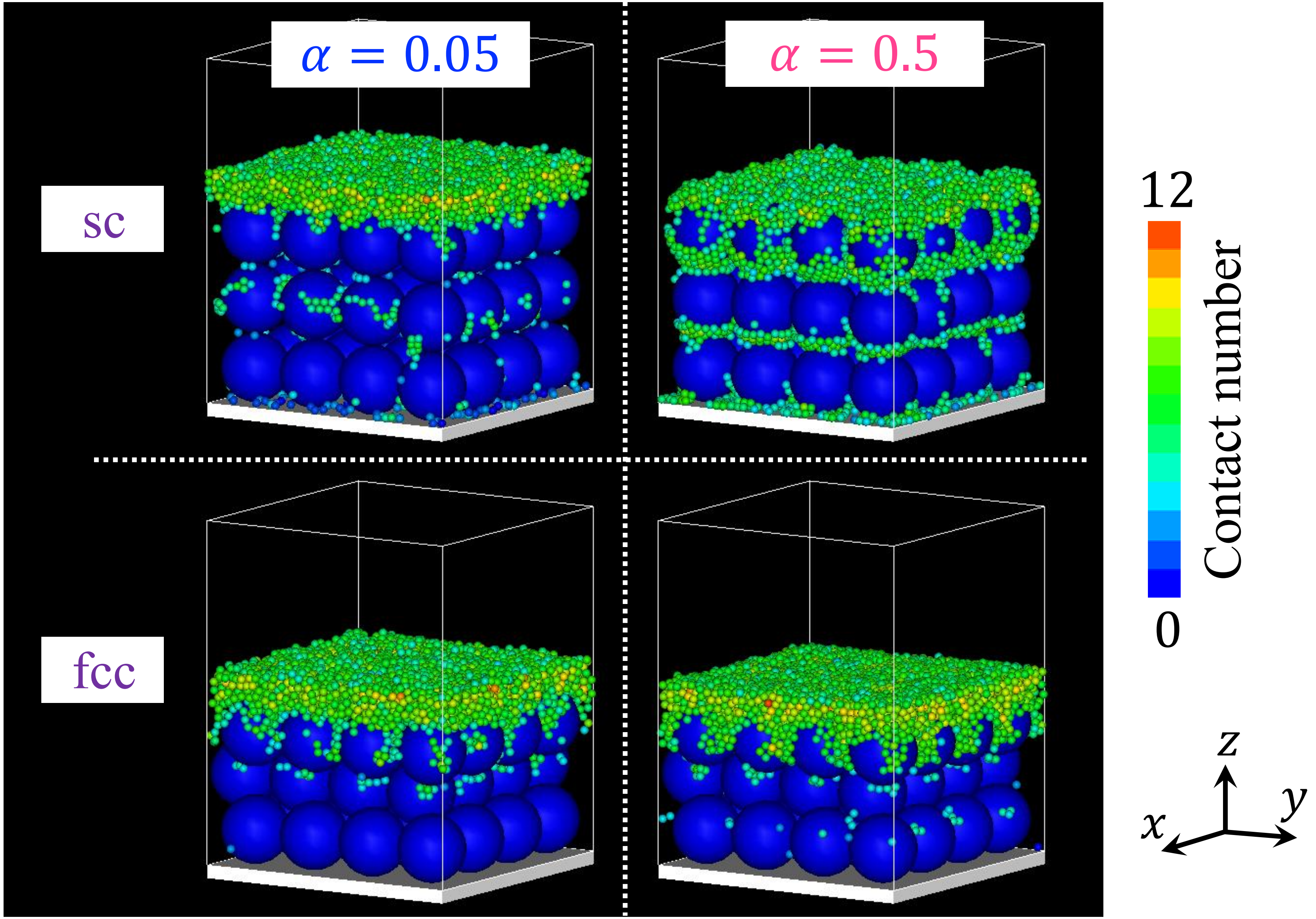
$\alpha = 0.05$ $\alpha = 0.5$

Results (fcc)

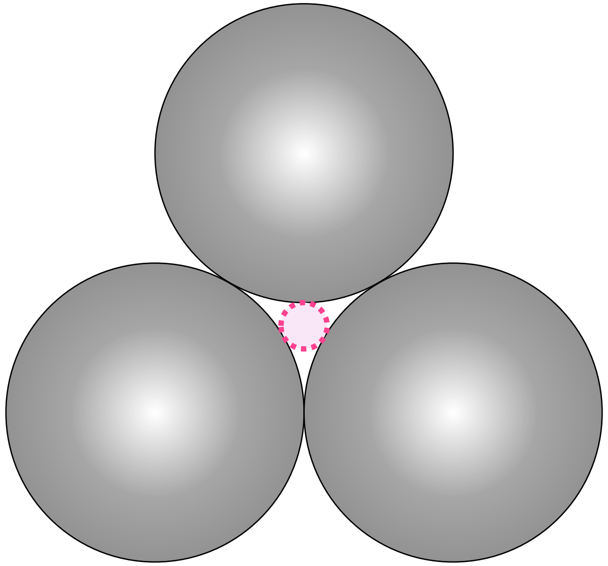


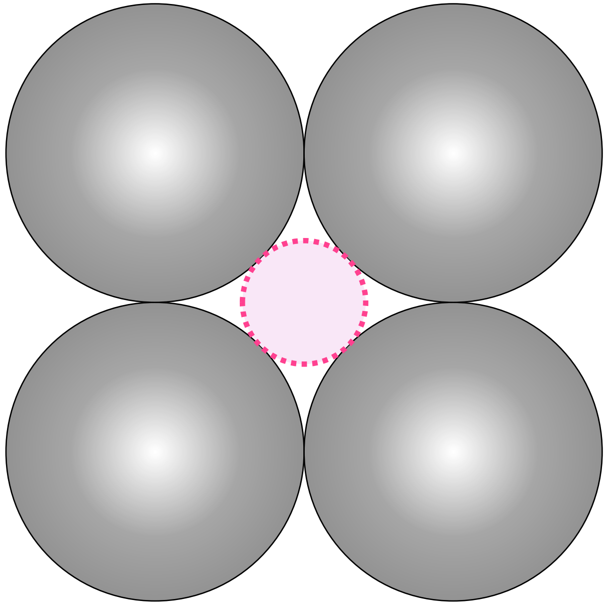
$\alpha = 0.05$ $\alpha = 0.5$

Results



Pore size

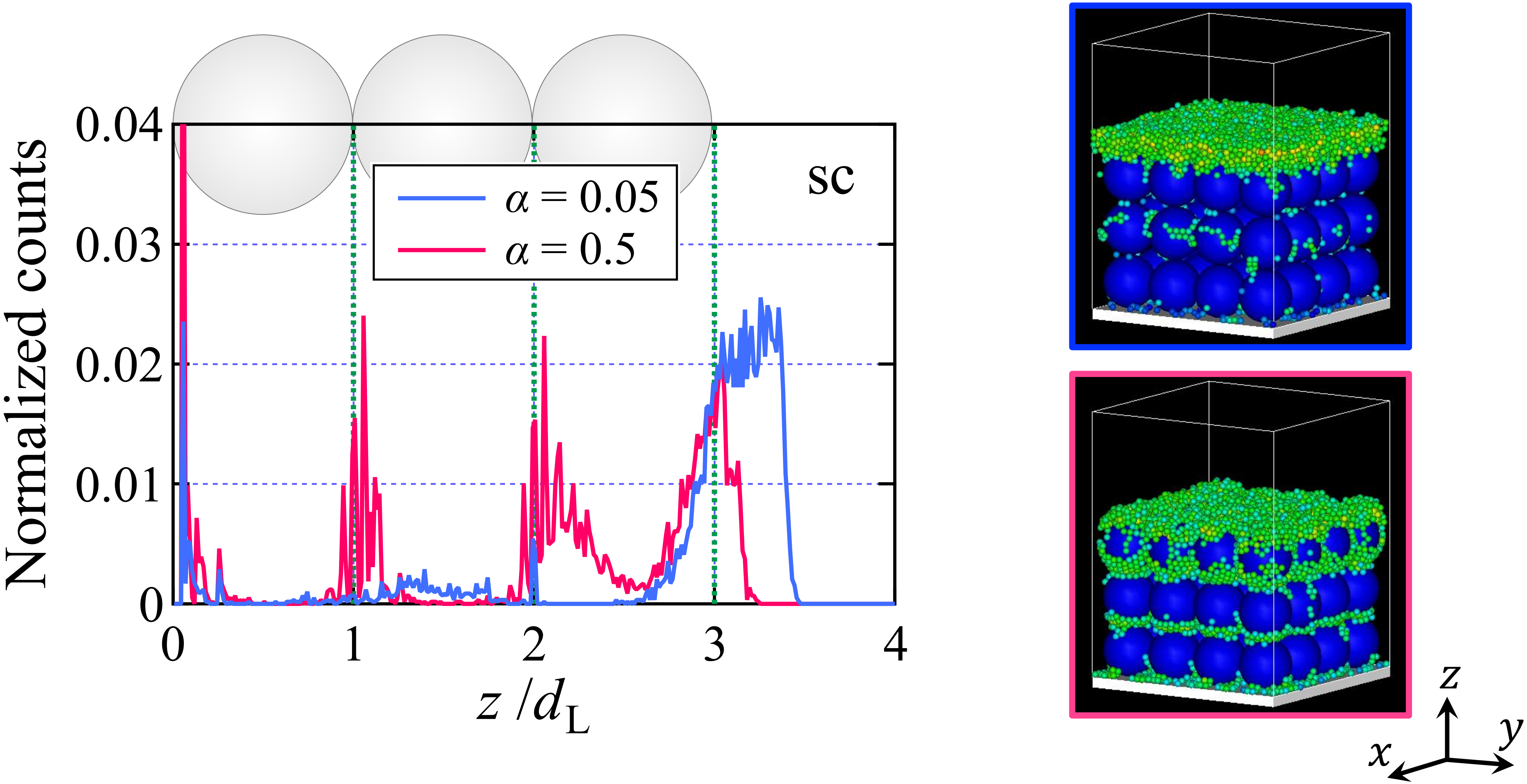




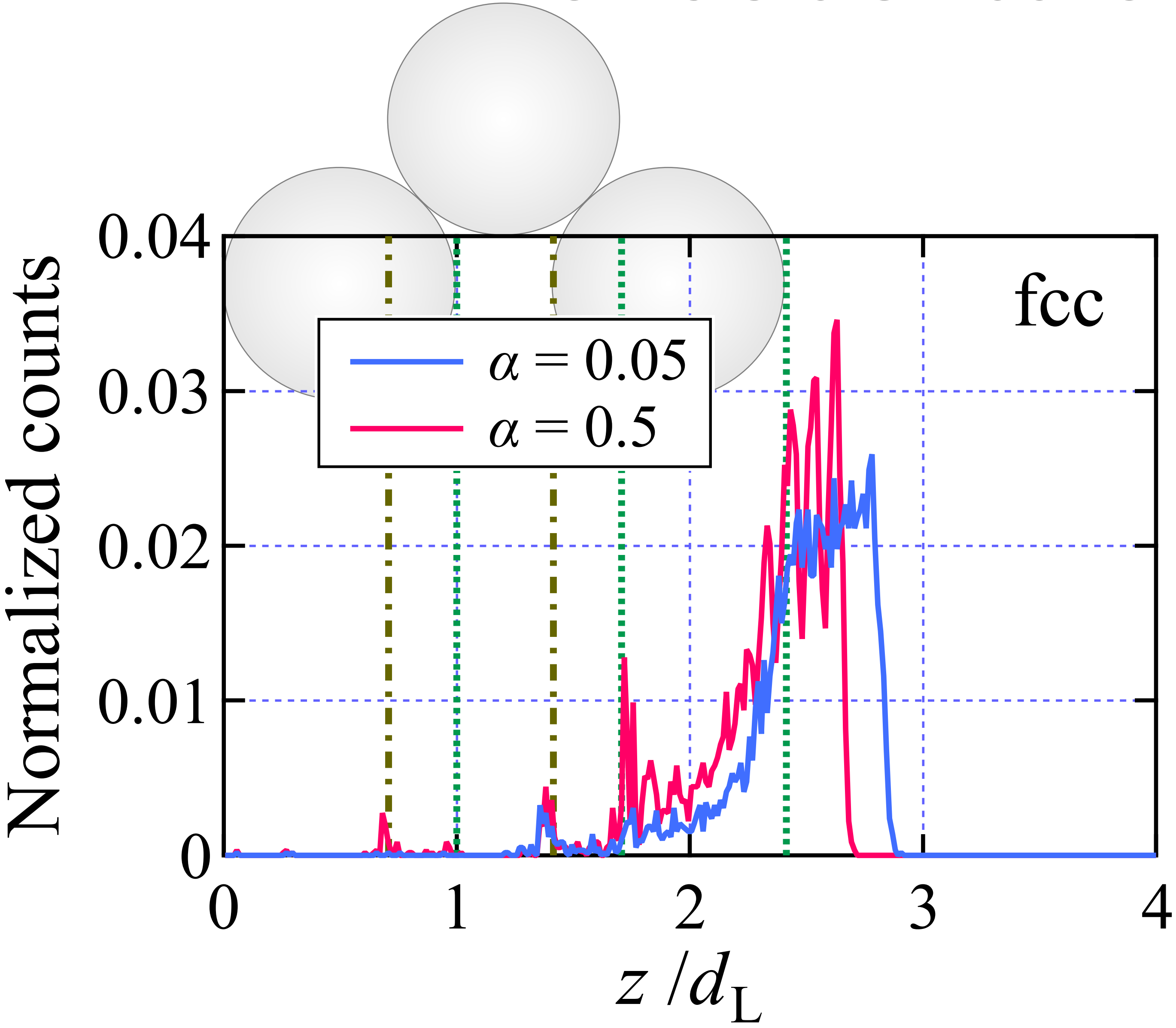
Pore diameter $\frac{\Delta}{d_\mathrm{L}} = \frac{2}{\sqrt{3}} - 1 \approx 0.16$ $\frac{\Delta}{d_\mathrm{L}} = \sqrt{2} - 1 \approx 0.41$

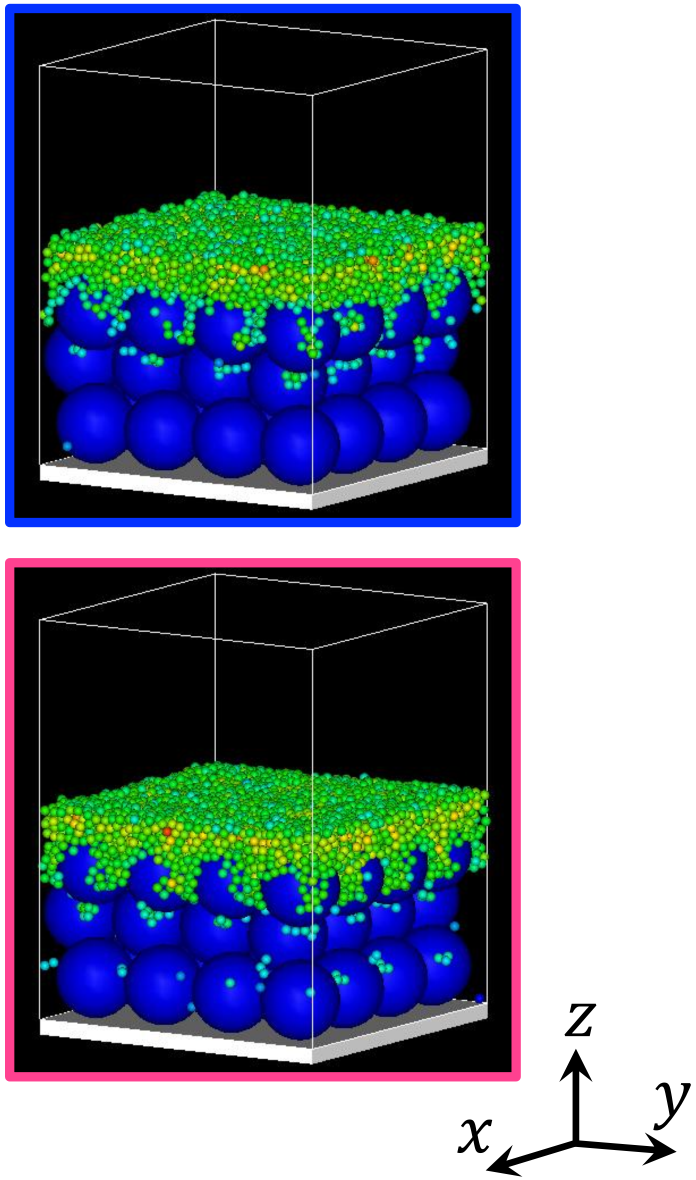
$\frac{d_\mathrm{L}}{\Delta} \approx 6.5$ $\frac{d_\mathrm{L}}{\Delta} \approx 2.4$

Particle distribution (sc)

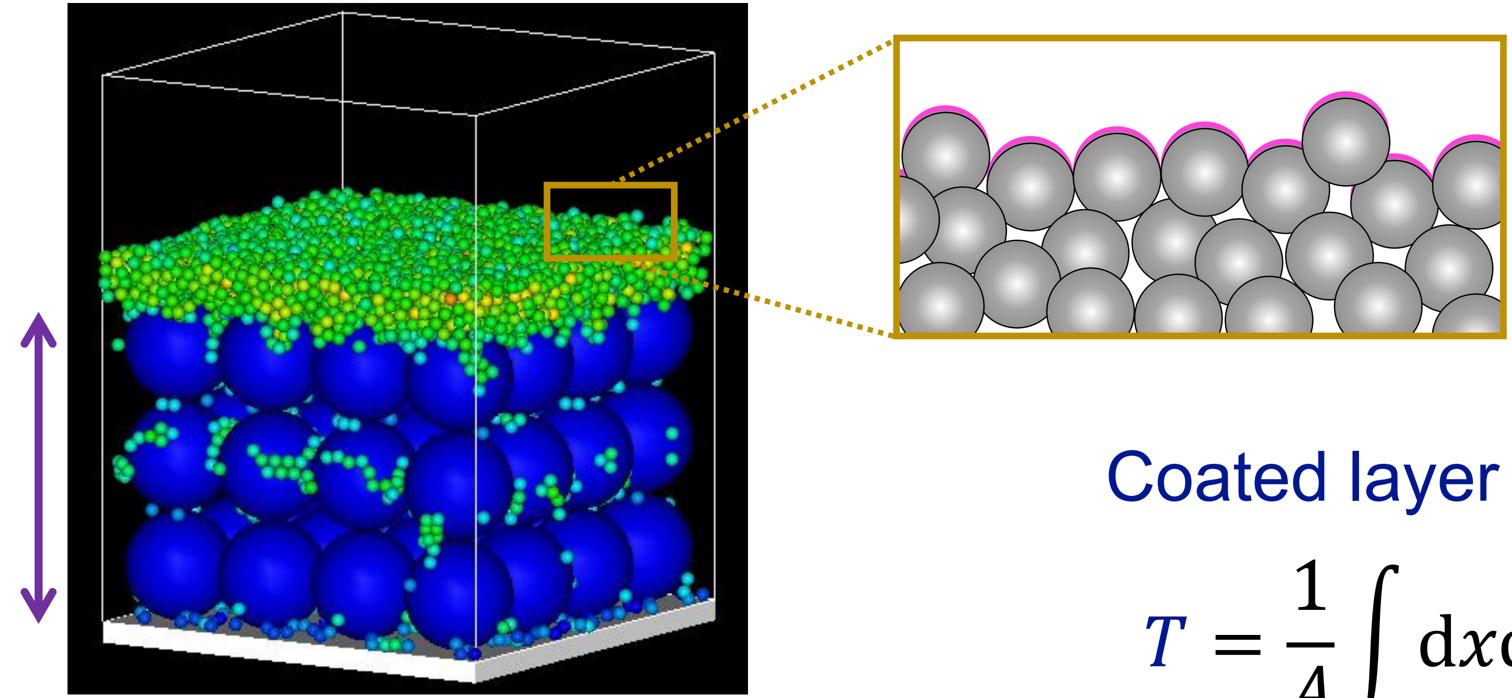


Particle distribution (fcc)





Coated layer thickness/roughness



$z_{\mathrm{max}}(x, y)$

Particulate layer thickness: L

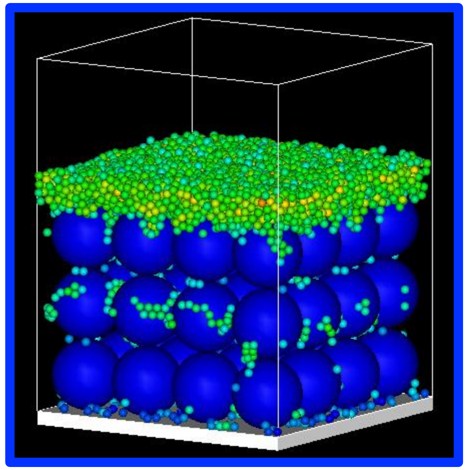
Coated layer thickness

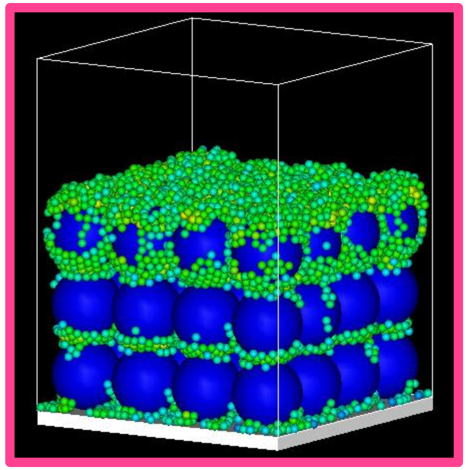
$$T = \frac{1}{A}\int_A \mathrm{d}x\mathrm{d}y\,[z_{\mathrm{max}}(x, y) - L]$$

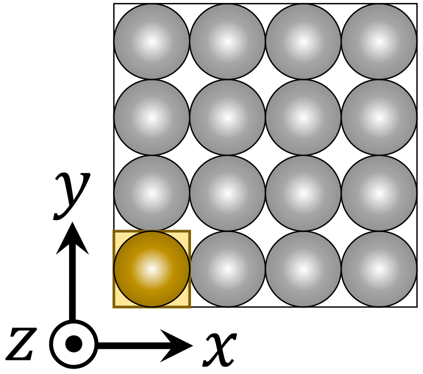
Surface roughness

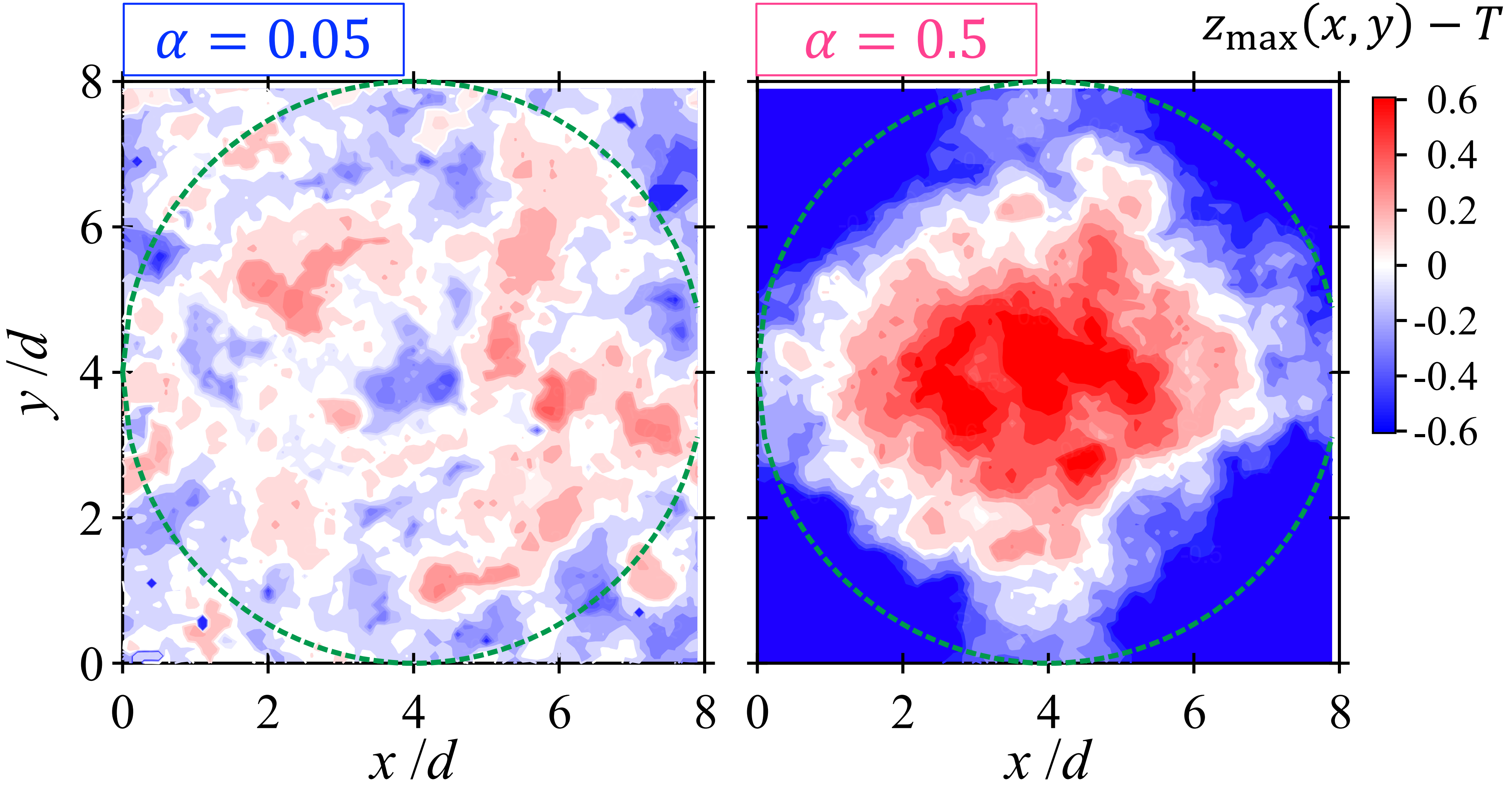
$$Ra = \frac{1}{A}\int_A \mathrm{d}x\mathrm{d}y\,|z_{\mathrm{max}}(x, y) - T|$$

Surface roughness (sc)



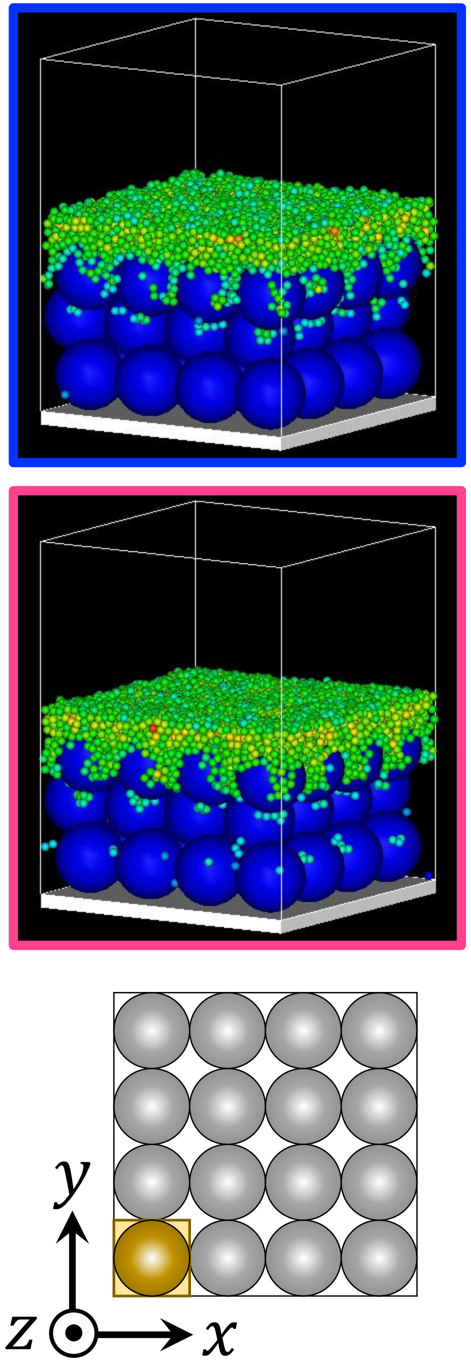


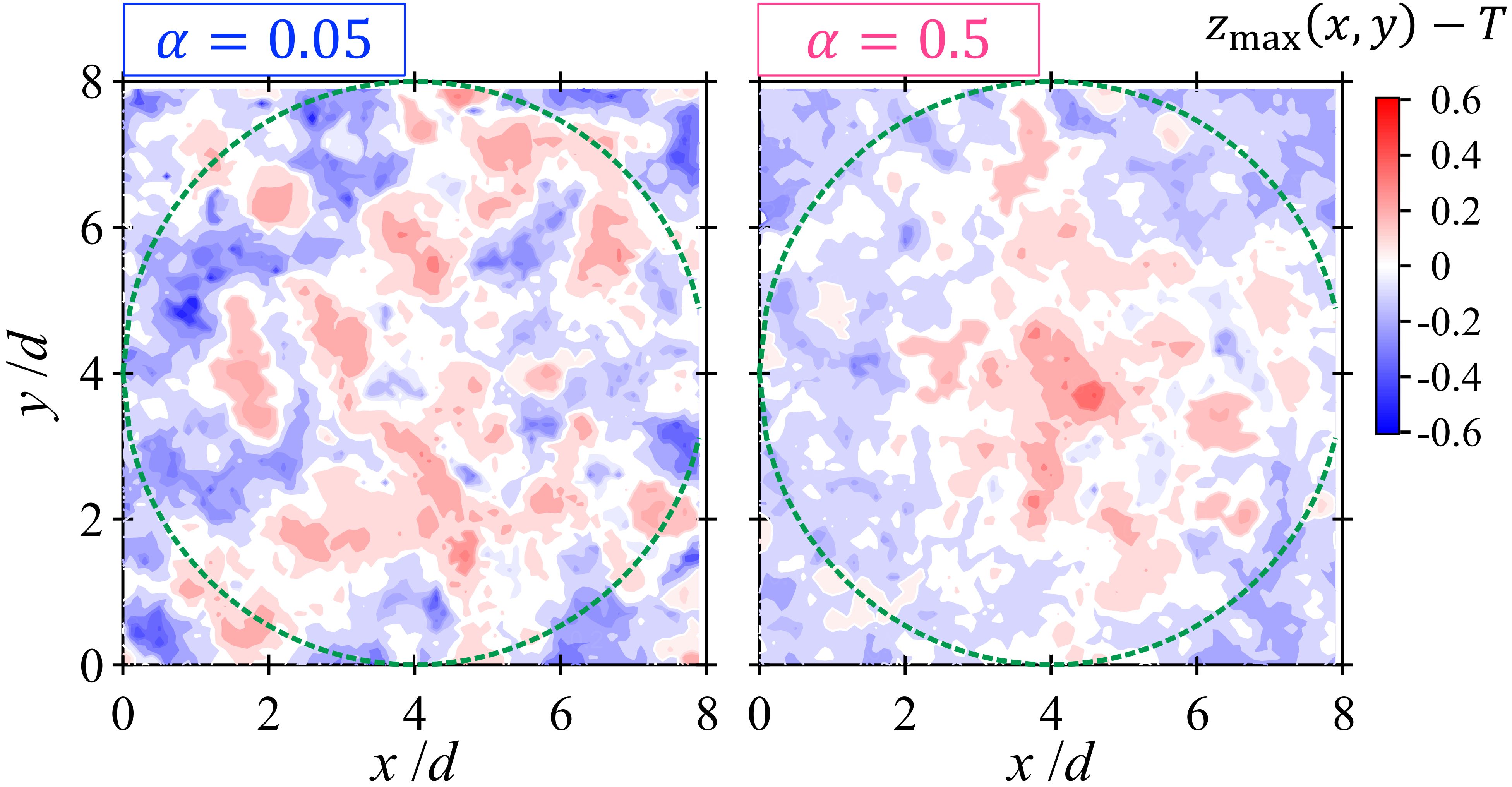




Thickness, T/d	2.9	0.72
Roughness, Ra/d	0.12	0.30

Surface roughness (fcc)



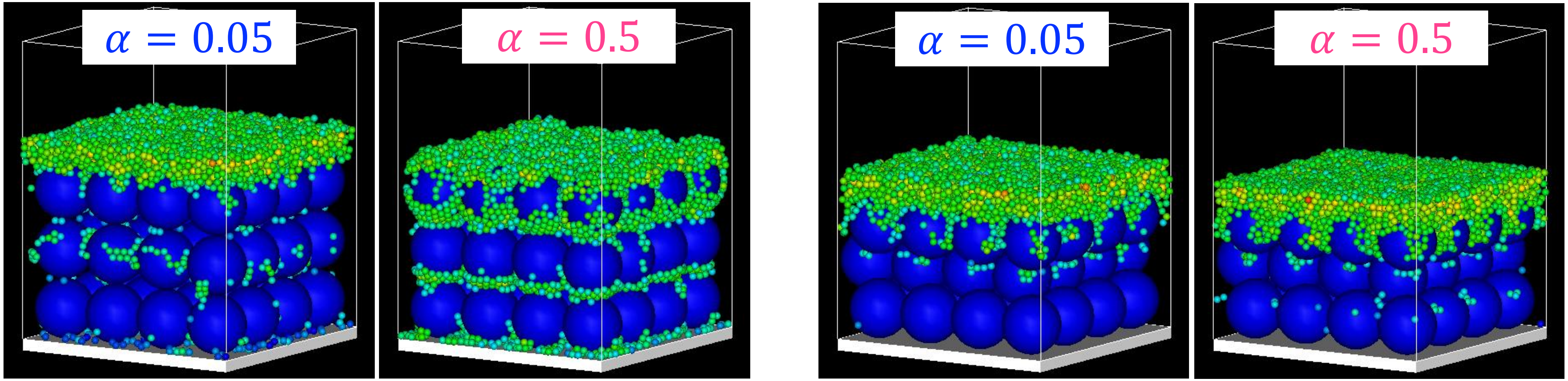


	$\alpha = 0.05$	$\alpha = 0.5$
Thickness, T/d	3.1	1.9
Roughness, Ra/d	0.11	0.08

Summary

- Effects of larger porosity of particulate layer (sc > fcc):
  - Invasion of particles
  - Surface roughness reflecting particulate layer structure

- These effects are remarkable for larger surface tension of solvent (relative to inter-particle adhesion)



sc

fcc