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Numerical Simulation of Nanoparticle Network Formation in Transparent Conductive Coating

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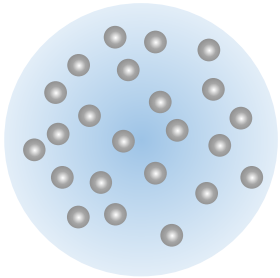
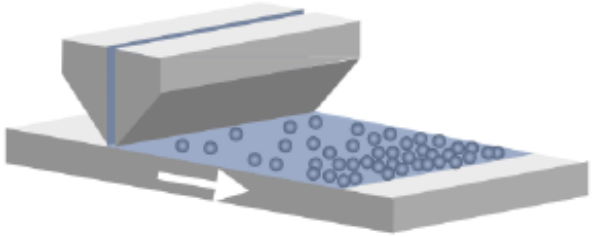
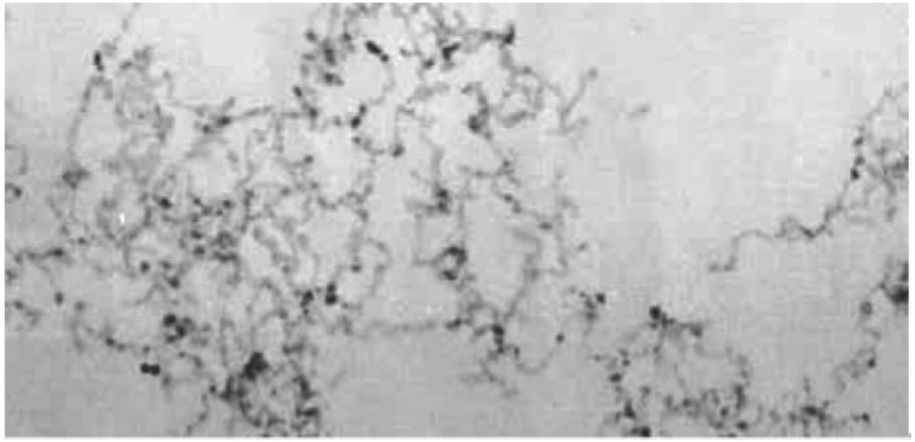
Network formation of particles





Coating
Drying

Aqueous suspensions
of nanoparticles



Transparent conductive films

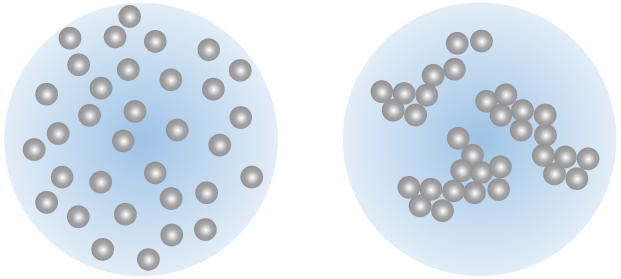
Example of network structure:
Wakabayashi *et al*., Langmuir (2007).

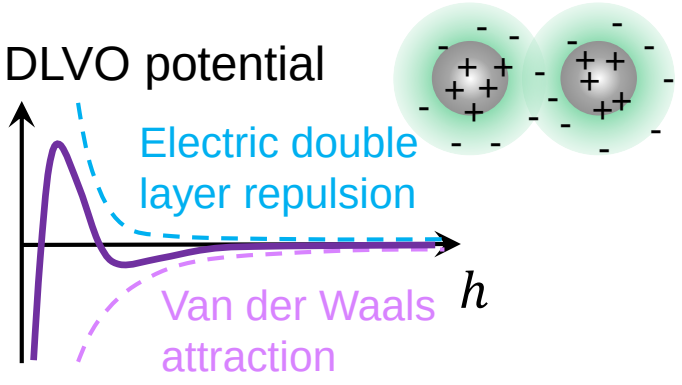
How do network structures form?

← Consideration by numerical simulations

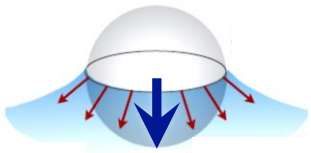
Structure formation during drying

Particle dispersion/aggregation

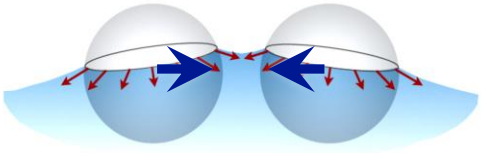




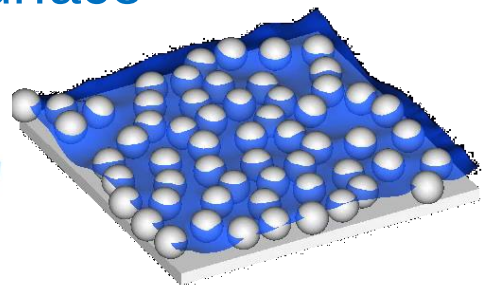
Drying: capillary force induced by free surface



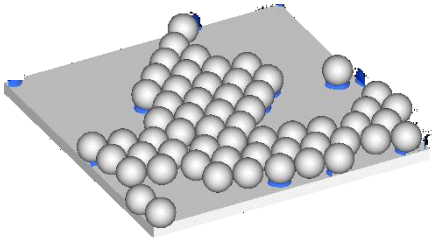
Vertical push into liquid

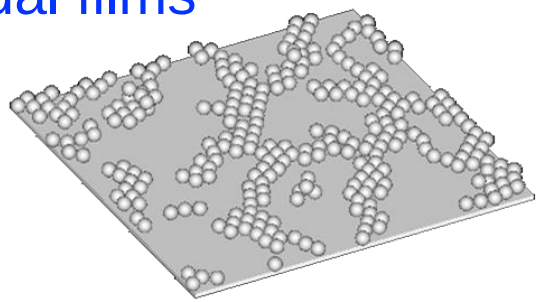


Lateral attraction

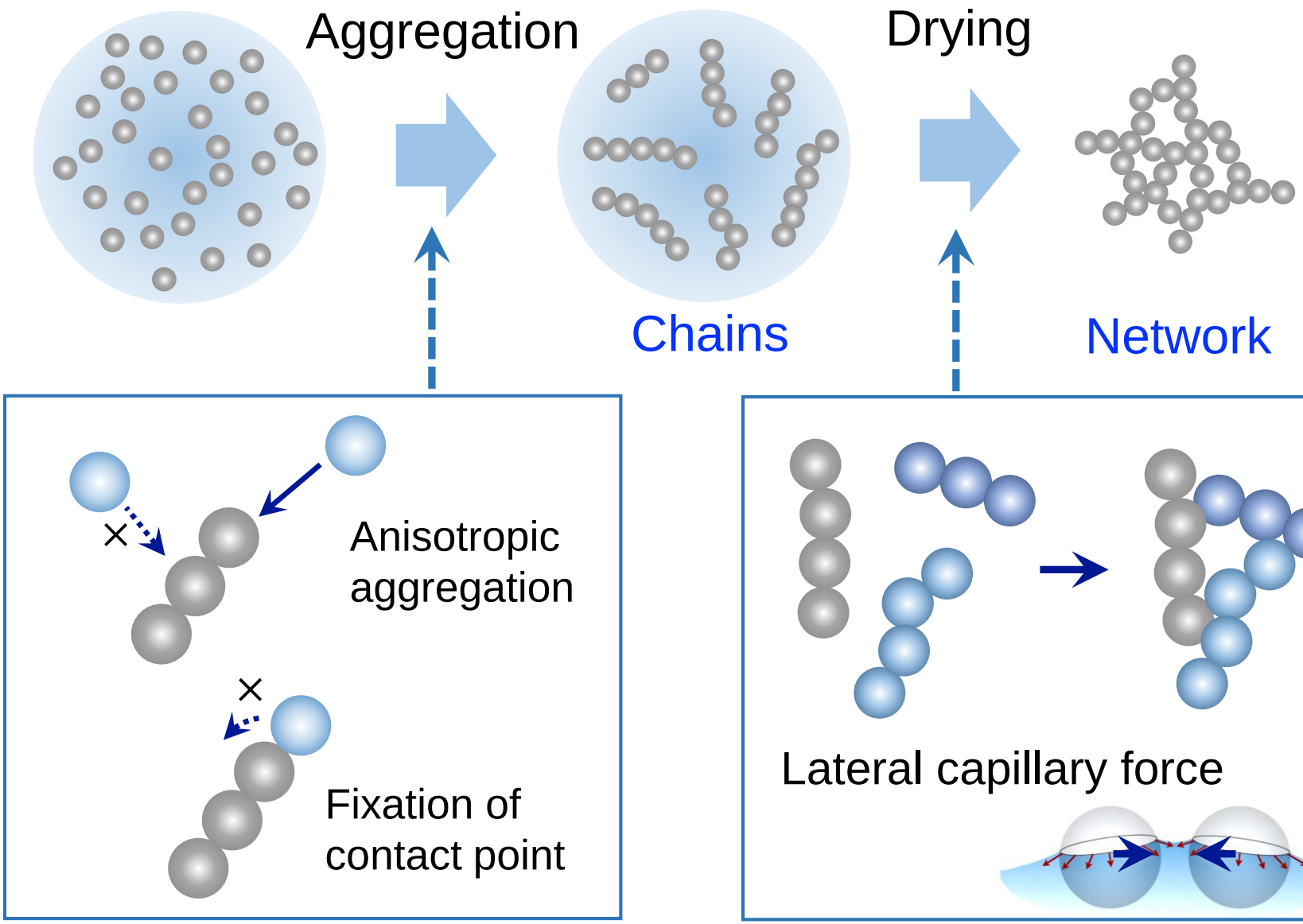


Structure of colloidal films



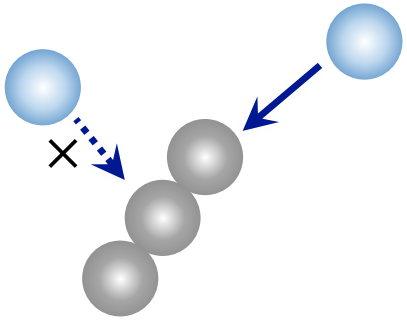


A possible mechanism

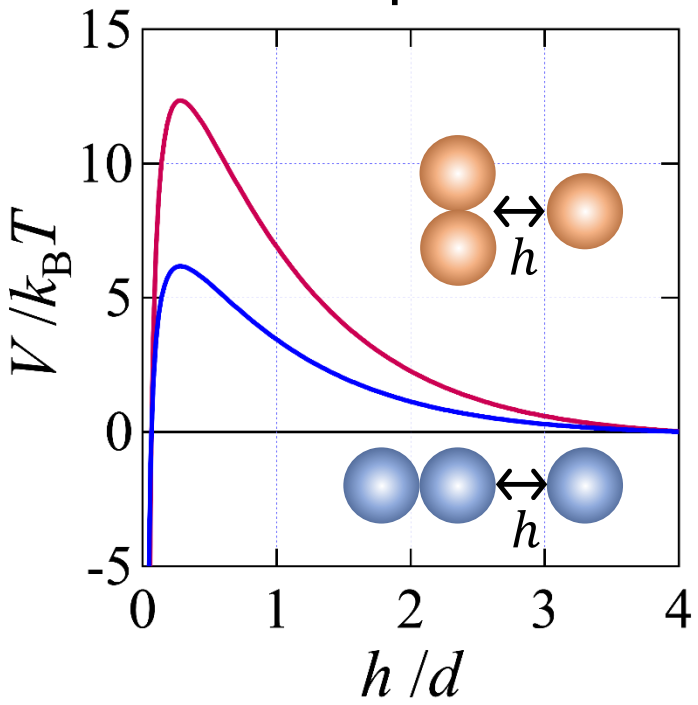


Chain formation

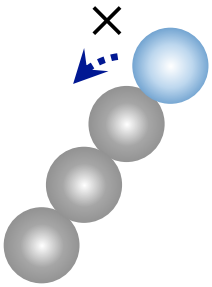
Anisotropic aggregation

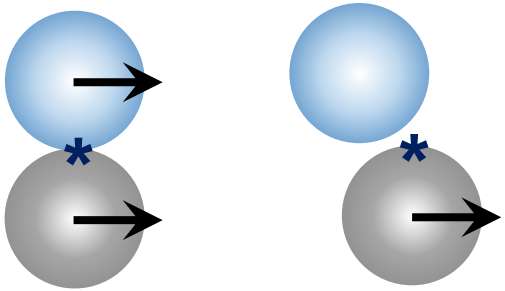


DLVO potential



Fixation of contact point



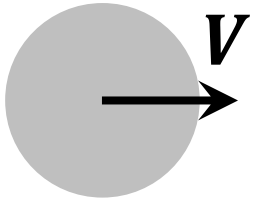


Stick Slip

Particles' Motion

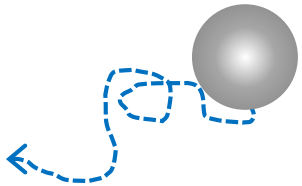
$$M\dot{\boldsymbol{V}} = -\xi \boldsymbol{V} + \boldsymbol{F}^{\mathrm{R}} + \boldsymbol{F}^{\mathrm{cpl}} + \boldsymbol{F}^{\mathrm{cnt}} + \boldsymbol{F}^{\mathrm{DLVO}}$$

Liquid Free surface Interparticle

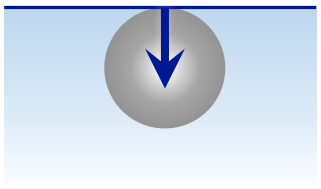


- **Drag force**: $-\xi \boldsymbol{V}$ (Stokes' law: $\xi = 3\pi\eta d$)
- **Random force**: $F_{\alpha}^{\mathrm{R}}(t) \sim N(0, 2\xi k_{\mathrm{B}} T \Delta t)$ (Gaussian dist.)

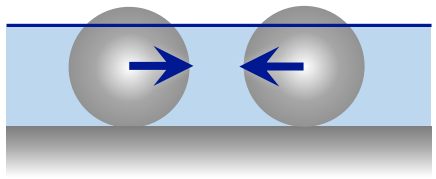
  → **Brownian motion**



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



Vertical

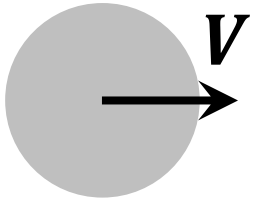


Lateral

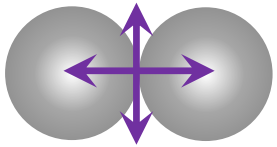
Particles' Motion

$$M\dot{\boldsymbol{V}} = -\xi \boldsymbol{V} + \boldsymbol{F}^{\mathrm{R}} + \boldsymbol{F}^{\mathrm{cpl}} + \boldsymbol{F}^{\mathrm{cnt}} + \boldsymbol{F}^{\mathrm{DLVO}}$$

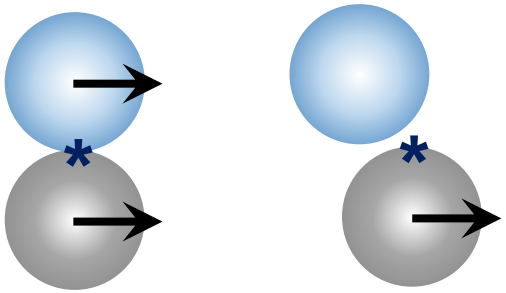
Liquid　Free surface　Interparticle



- **Contact force/torque**: $\boldsymbol{F}^{\mathrm{cnt}}, \boldsymbol{T}^{\mathrm{cnt}}$

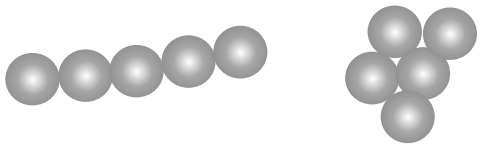


Contact point



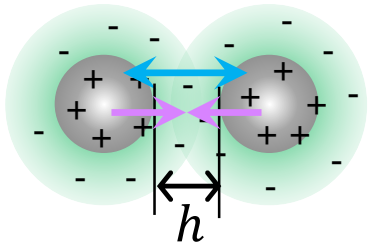
Stick　Slip

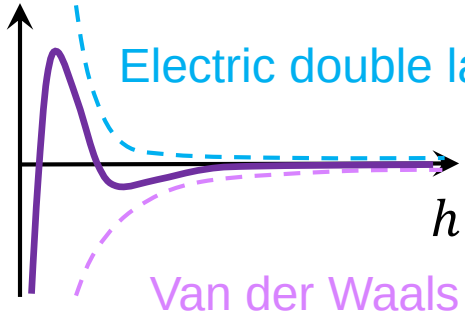
→ Aggregation shapes: Chain / Block



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

DLVO potential





→ Dispersion / Aggregation

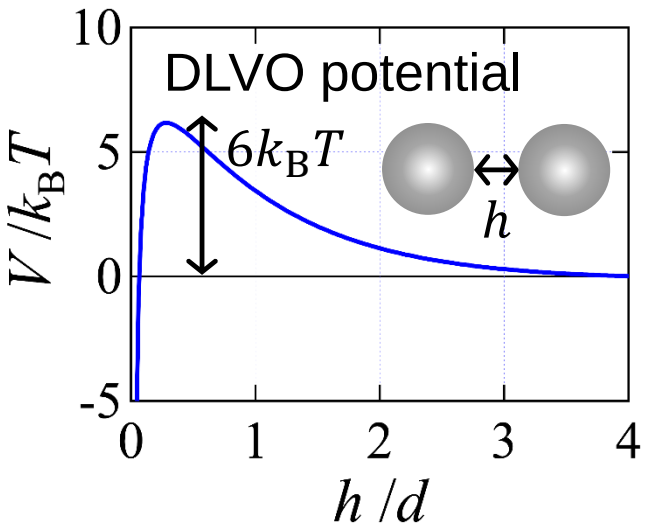
Simulation Conditions

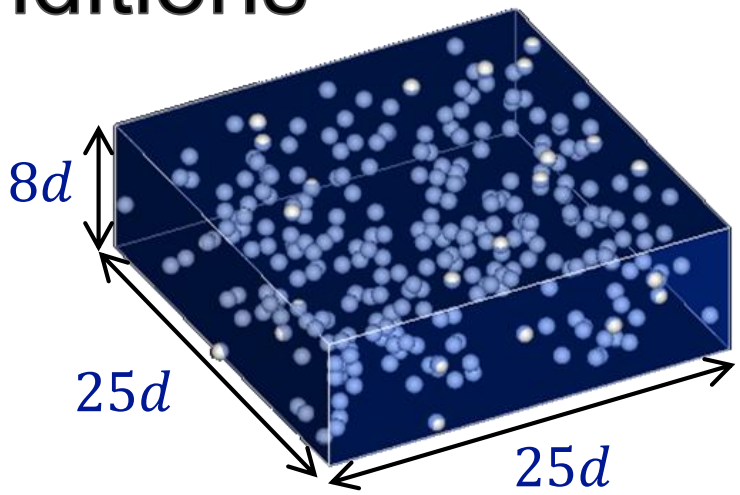
Particles

- Diameter $d = 10\ \mathrm{nm}$
- Zeta potential $-50\ \mathrm{mV}$
- Coverage on substrate $\mathbf{30, 40, 50\%}$
  (Initial volume fraction $2.3,\ 3.0,\ 3.8\ \mathrm{vol\%}$)
- Particle contact point **stick**, **slip**

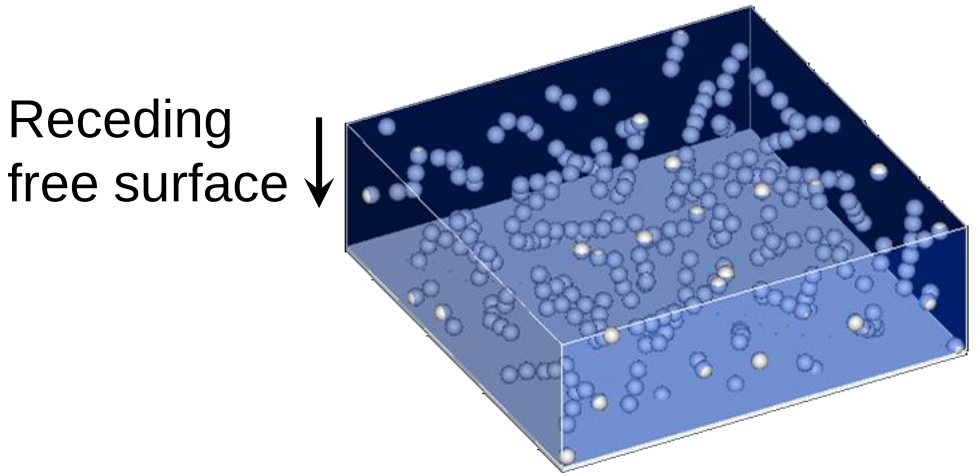
Liquid (water)

- Ion concentration $10^{-3}\ \mathrm{M}$
- Drying rate $2.2 \times 10^{-3}\ \mathrm{m/s}$



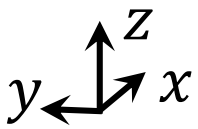


(1) Aggregation in liquid



(2) Drying on substrate

Periodic boundaries x, y

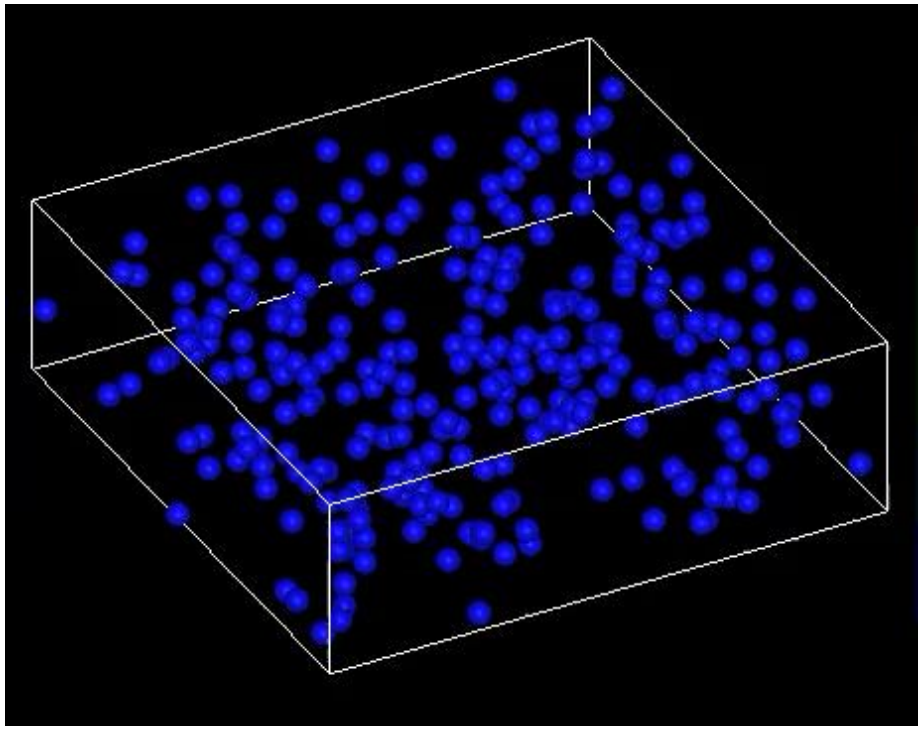


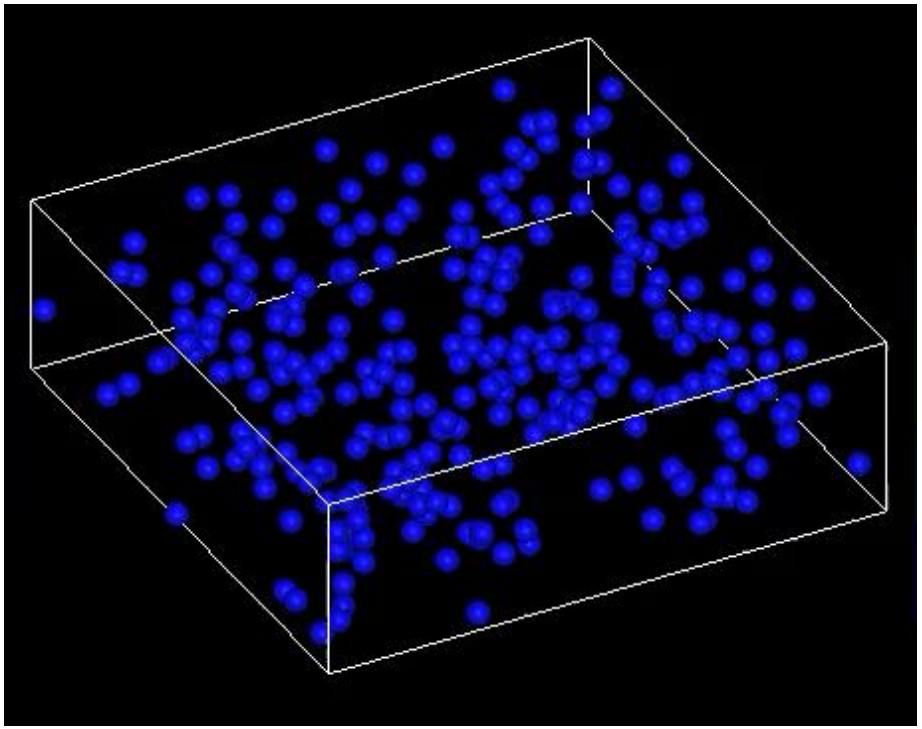
Aggregation

Coverage 40%

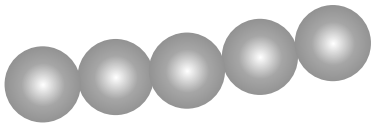
Contact number

0  4



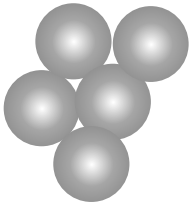


Stick



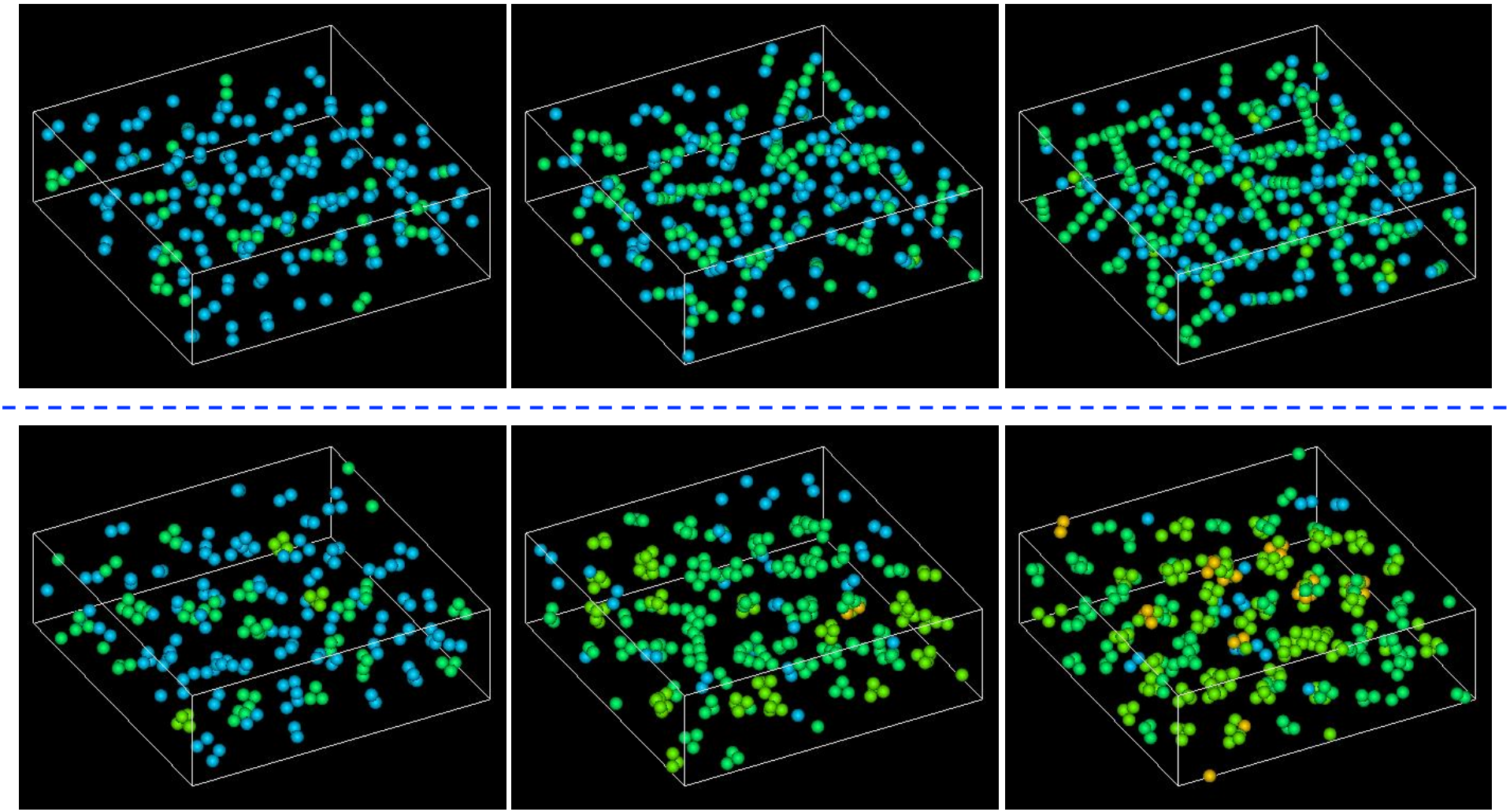
Chain

Slip



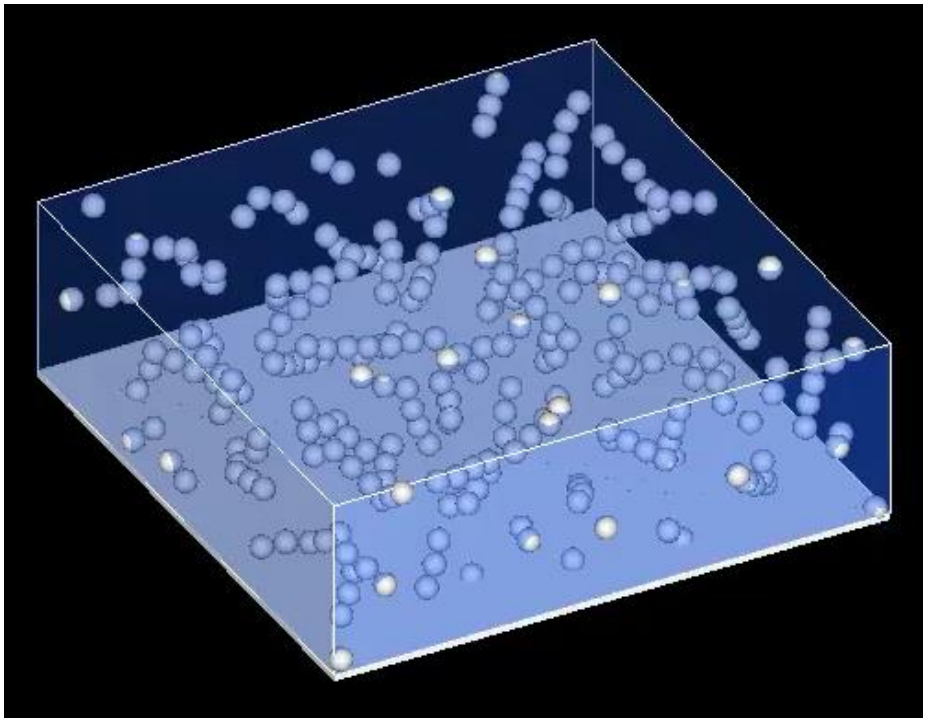
Block

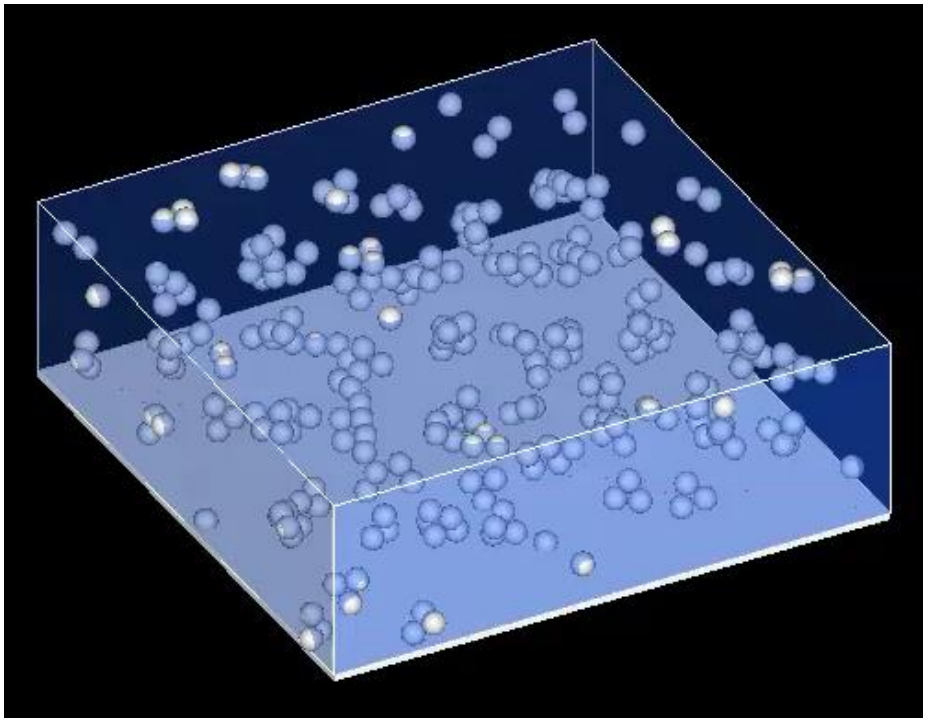
Aggregation



Drying

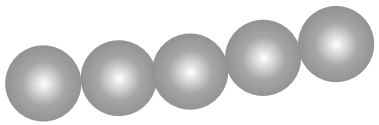
Coverage 40%



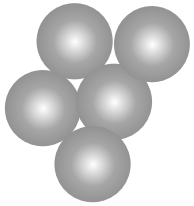


Stick

Slip

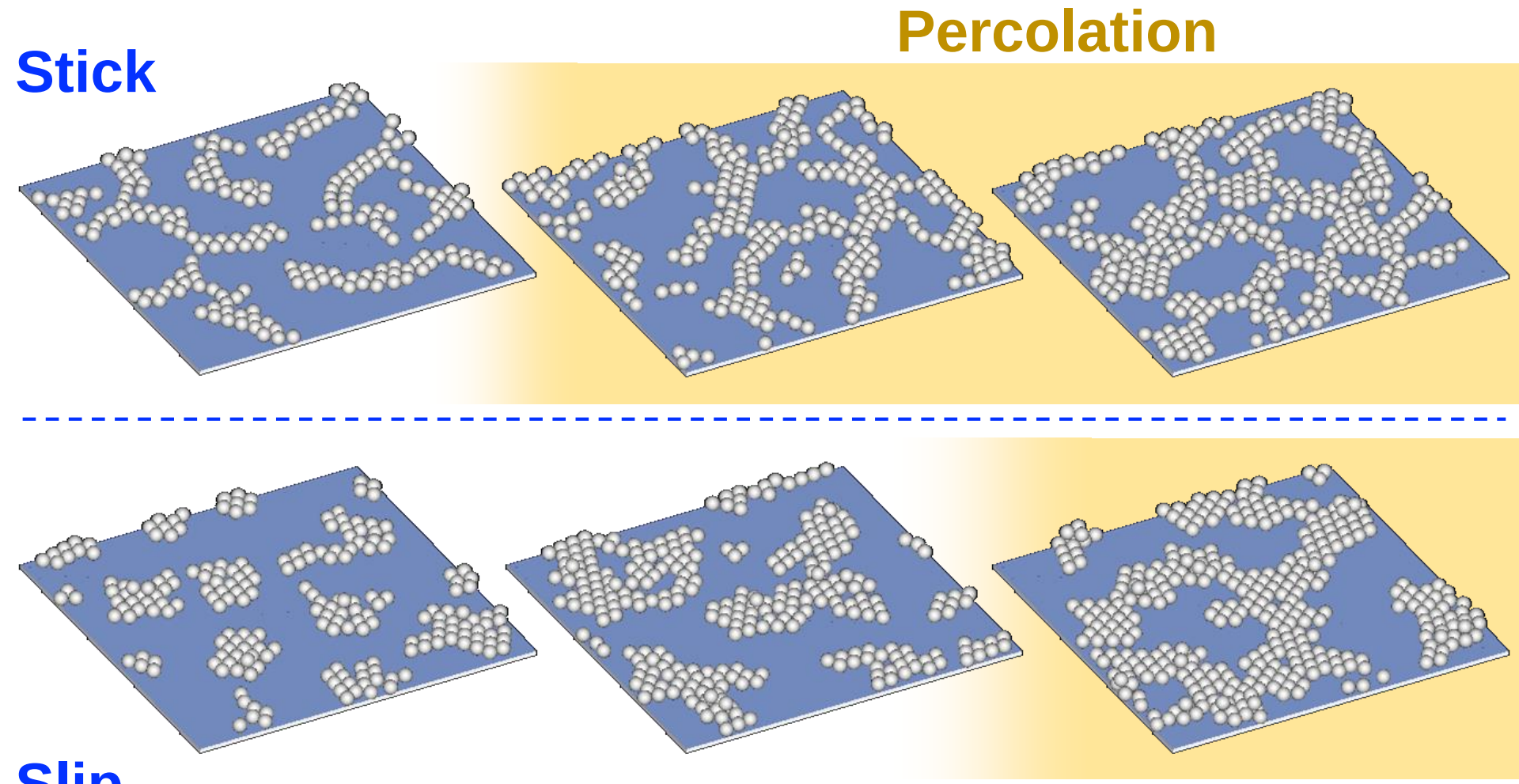


Chain



Block

Drying



Summary

- Consideration of the mechanism of particle network formation during drying by numerical simulations

- A possible mechanism of network formation
  - Chain formation in liquid:
    Anisotropic aggregation by DLVO potential
    + Fixation of contact point between particles
  - Connection of chains by capillary force during drying

- Effects of stick/slip particle contact on network formation

  Stick → lower percolation coverage ($\sim 40\%$)