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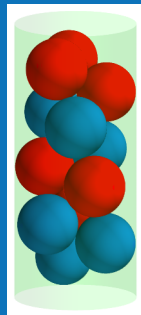www.research.ie

Coláiste na Tríonóide, Baile Átha Cliath
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Columnar packings of soft spheres

July 8, 2018 | Jens Winkelmann

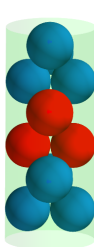*Co-authors*: A. Mughal, B. Haffner, D. Weaire and S. Hutzler
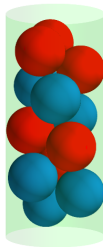
"Packing and stacking
we lay waste our days!"[1]

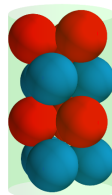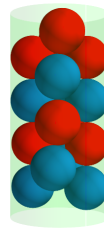## How many spheres fit in a cylinder?
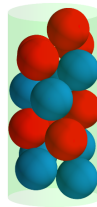

| zig-zag | $(2, 2, 0)$ uniform | $(3, 2, 1)$ uniform | $(3, 3, 0)$ uniform | $(4, 2, 2)$ uniform | $(4, 3, 1)$ uniform |

[1]Aste, Weaire; *Pursuit of perfect packing*; Boca Raton, USA: Taylor & Francis (2008)

Examples for columnar structures

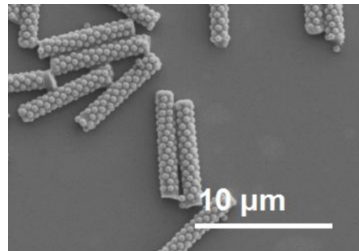- Appearance from botany, over foam to self-assembly on micro-scale

Bushy Park, Dublin

Dry foam

Wet foam

Si particles self-assembled to microrod inside PDMS pores[1]

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[1]Wu et al; *Confined Assemblies of Colloidal Particles with Soft Repulsive Interactions*; J Am Chem Soc 139, 5095–5101 (2017)
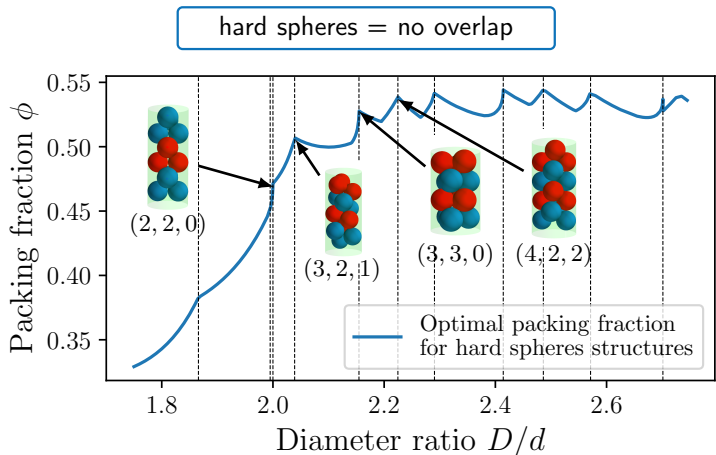
Overview

Soft sphere model

Phase diagram and the observation of a line-slip structure

Metastability and hysteresis

Conclusion

Columnar hard sphere packings

hard spheres = no overlap

$(2, 2, 0)$ $(3, 2, 1)$ $(3, 3, 0)$ $(4, 2, 2)$

Packing fraction ϕ

Diameter ratio D/d

Optimal packing fraction
for hard spheres structures

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[0]Mughal, Chan, Weaire, Hutzler; *Dense packings of spheres in cylinders: Simulations*; Phys Rev E 85, 051305 (2012)

Simulation based on enthalpy minimisation

D

image spheres

L

d
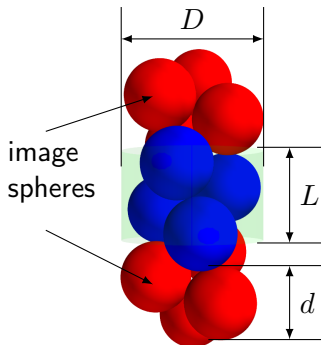
- Soft sphere model of overlapping spheres with overlap δ_{ij}

- Enthalpy H:

$$H(\{\vec{r}_i\}, L, \alpha) = \underbrace{U(\delta_{ij})}_{\text{inner energy}} + \underbrace{pV}_{\text{pressure term}}$$
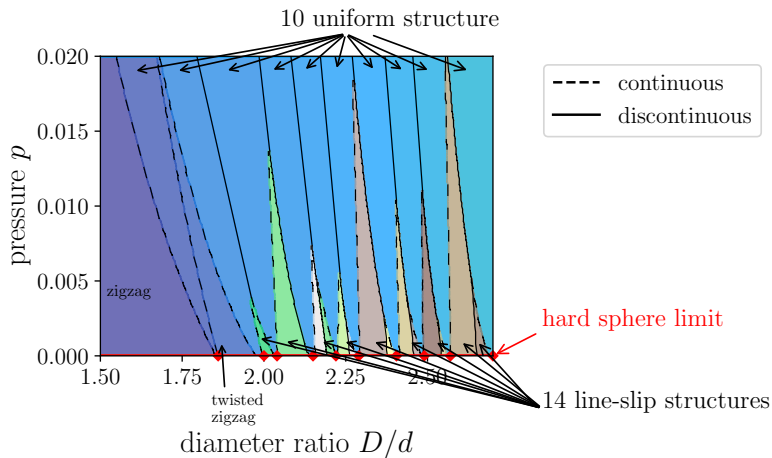
  - Inner energy $U \propto \delta_{ij}^2$

  - Pressure term $pV = p\pi \left(\frac{D}{2}\right)^2 L$

- image spheres are *twisted* by an angle α
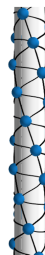
Enthalpy minimisation
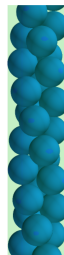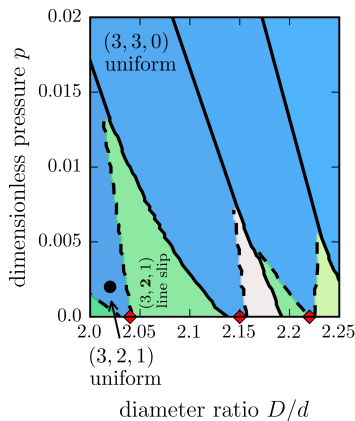
Local minimum   Global minimum

The phase diagram

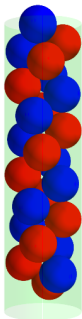Phase diagram with all columnar structures *without inner spheres*

Continuous and discontinuous transitions

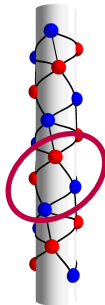- Continuous (dashed): loss of contact
- Discontinuous (solid): complete change in structure
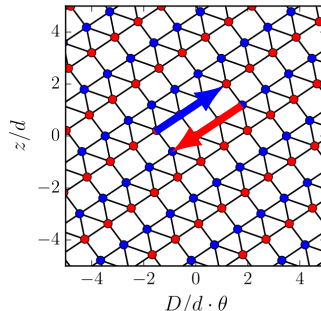
What is a line-slip structure?

- Characterised by a loss of contact (gap)

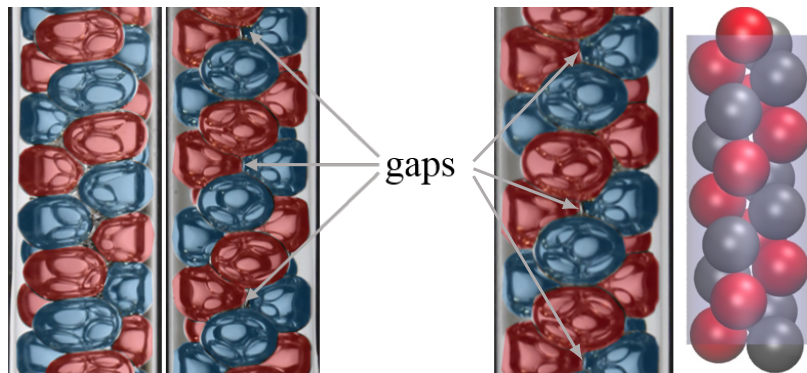$(3, \mathbf{2}, 1)$ line slip   Contact network   Rolled out contact network

- Line slip is adjustable with pressure/compression
- For *microrods*: Stiffness/conductivity are adjustable by compression

The simulation and observation of a $(3, \mathbf{2}, 1)$ line slip

$(3, 2, 1)$ uniform and $(3, \mathbf{2}, 1)$ line-slip structure

$(3, \mathbf{2}, 1)$ line slip in experiment and simulation

[0]Winkelmann et al; *Simulation and observation of line-slip structures in columnar structures of soft spheres*; Phys Rev E 97, 059902 (2017)
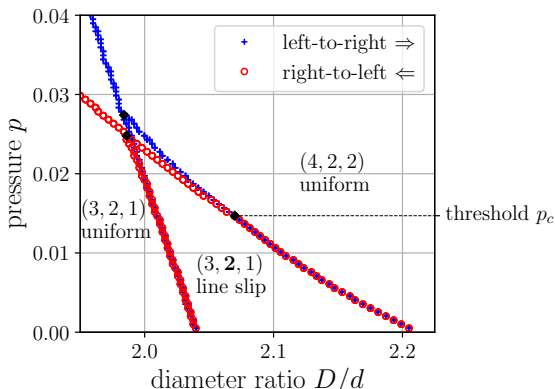
Stability diagram of metastable phases

Motivation:

- Phase diagram: structures of *global* minimal enthalpy

  - Experiment starts in certain structure
  - Structure changes with hysteresis
  - Not comparable with our experiments

- Stability diagram: change in structure by varying p or D/d
  - Displays region of metastable structures
  - Start in $(3, 2, 1)$, increase D/d, decrease D/d
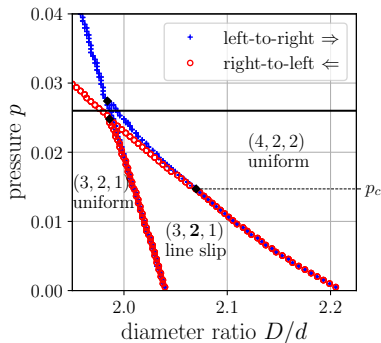
Stability diagram of metastable phases

Motivation:

- Phase diagram: structures of *global* minimal enthalpy
- Stability diagram: change in structure by varying p or D/d
  - Start in $(3, 2, 1)$, increase D/d, decrease D/d

Example for a hysteretic transition

Stability diagram
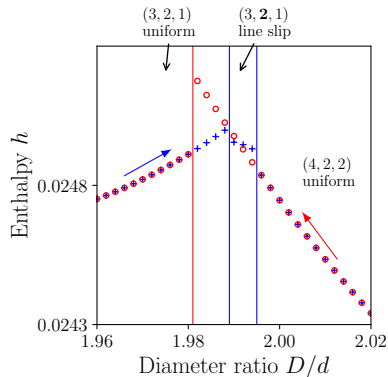
Enthalpy vs. diameter ratio

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[0]Winkelmann et al; *Columnar structures of soft spheres: metastability and hysteresis*; Phys Rev E *submitted* (2018)

Conclusion and Outlook

Conclusions

1. Phase diagram displays conditions to generate columnar structures
2. Experimental observation of a $(3, \mathbf{2}, 1)$ line slip
3. Stability diagram for $(3, 2, 1) \Leftrightarrow (4, 2, 2)$ transition
4. Hysteresis appears above threshold pressure

Columnar bubble chains
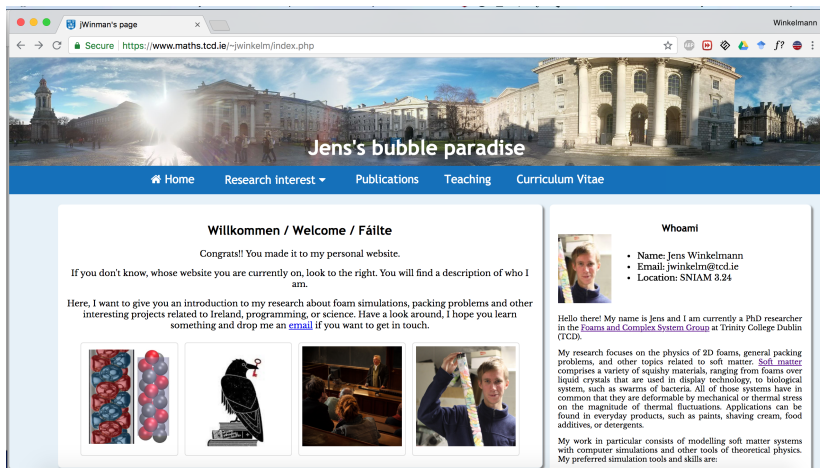
Acknowledgement

this is Fritz
Dunne

Website: `https://www.maths.tcd.ie/~jwinkelm`