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The University of Dublin

Columnar structures: Packing spheres into cylinders

J. Winkelmann, A. Mughal(*), D. Weaire and S. Hutzler
School of Physics, Trinity College Dublin, The University of Dublin, Ireland
(*) Department of Mathematics, Aberystwyth University, Aberystwyth, Wales

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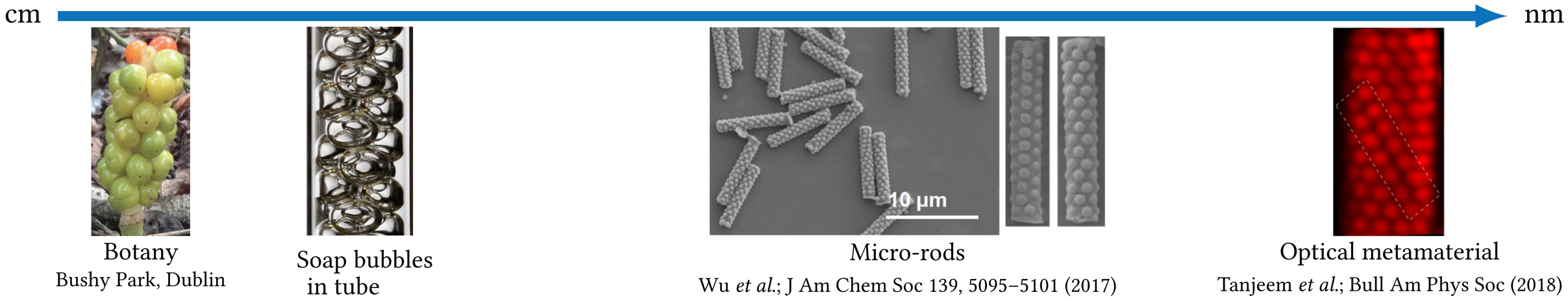
Appearance in nature and man-made objects



Botany
Bushy Park, Dublin

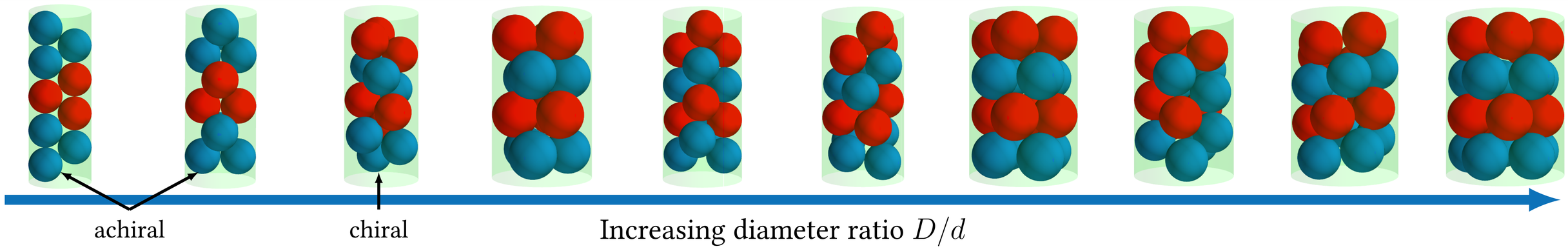
Soap bubbles in tube

Micro-rods
Wu *et al.*; J Am Chem Soc 139, 5095–5101 (2017)

Optical metamaterial
Tanjeem *et al.*; Bull Am Phys Soc (2018)

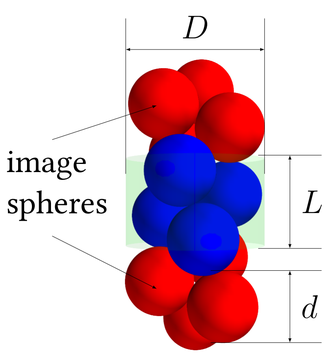
Columnar structures occur when spheres are *densely* packed inside cylinders. From simulation and theory we predict dense packings created with various assembly methods and compare them with experiments.

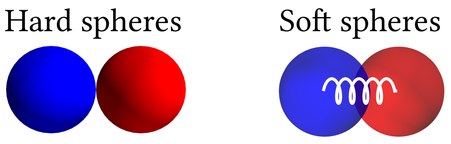
Simulated examples of columnar packings



We present simulation of *soft* (overlapping) spheres packed inside tubes. Special structures are so-called *line-slip* structures, which we also observed in experiments using soap bubbles.

Packing *soft* spheres into cylinders



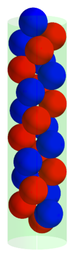


- *Soft spheres:* Energy $\propto$ overlap δ_{ij}^2
- Generate structure at const pressure p

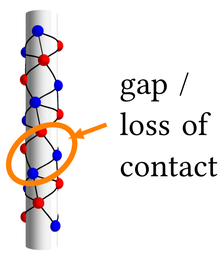
$$\text{Enthalpy } H = \underbrace{U(\delta_{ij})}_{\text{internal energy}} + \underbrace{pV}_{\substack{\text{pressure x}\\ \text{volume term}}}$$

Enthalpy minimisation

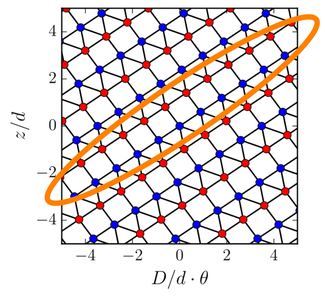
What is a *line-slip* structure?



line-slip packing



Contact network

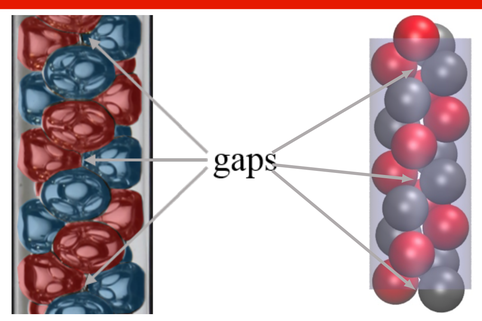


Rolled-out network

Experimental line slip in a foam

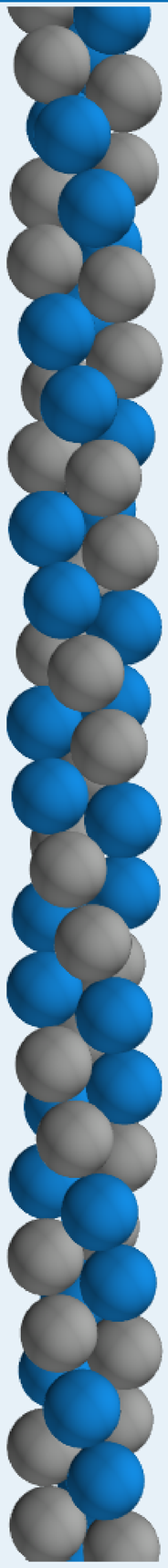
Experiment:
- add liquid to soap bubbles in glass tube

⇒ gaps occure



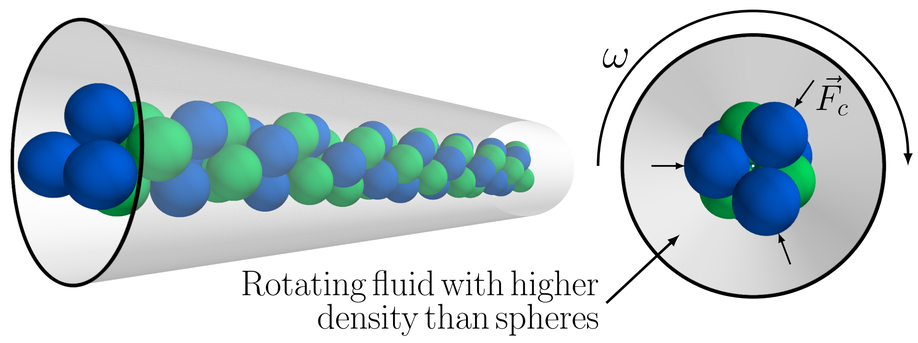
Comparison with **simulation**

Winkelmann *et al.* Phys Rev E 97, 059902 (2017)



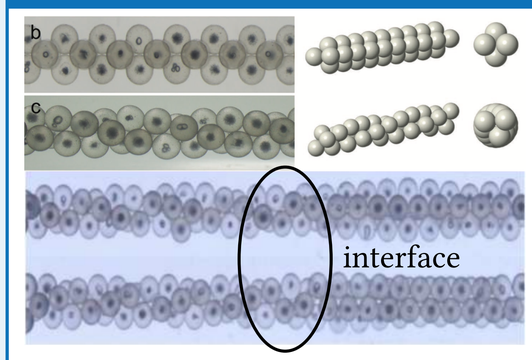
A novel assembly method [Lee *et al.*] involves rapid rotations of spheres surrounded by a liquid of higher density. We present a phase diagram for *soft* spheres derived from analytic energy calculations.

Columnar structures by rapid rotations



- The centripetal force $\vec{F}_c$ pushes the spheres towards the central axis

Experiments with hard spheres [Lee *et al.*]

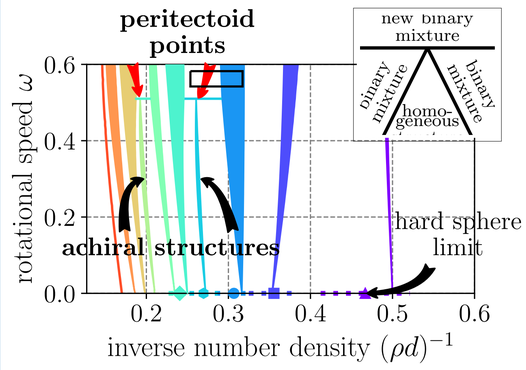


homogeneous structure:
→ fills up the whole tube

binary mixture:
→ two structures

Lee *et al.* Adv. Mater. 29, 1704274 (2017)

Theory for soft spheres



- coloured area: homogeneous structures
- white area: binary mixtures

Prediction:
Achiral structures vanish together with their adjacent binary mixtures in **peritectoid points**!

Winkelmann *et al.* Phys Rev E 99, 020602(R) (2019)

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Science Foundation Ireland

Further readings

[1] L. Fu et al. *Hard sphere packings within cylinders.* In: *Soft Matter* 12.9 (2016), pp. 2505–2514. [2] L. Fu et al. *Assembly of hard spheres in a cylinder: a computational and experimental study.* In: *Soft Matter* 13.18 (2017), pp. 3296–3306. [3] A. Meagher et al. *An experimental study of columnar crystals using monodisperse microbubbles.* In: *Colloids Surf. A* 473 (2015), pp. 55–59. [4] A. Mughal and D. Weaire. *Theory of cylindrical dense packings of disks.* In: *Phys Rev E* 89.4 (2014), p. 042307. [5] A. Mughal et al. *Dense packings of spheres in cylinders: Simulations.* In: *Phys Rev E* 85.5 (2012), p. 051305. [6] A. Mughal et al. *Columnar structures of soft spheres: metastability and hysteresis.* In: *Phys Rev E, accepted* (2018). [7] D. Wood, C. Santangelo, and A. Dinsmore. *Self-assembly on a cylinder: a model system for understanding the constraint of commensurability.* In: *Soft Matter* 9.42 (2013), pp. 10016–10024. [8] G. Wu et al. *Confined assemblies of colloidal particles with soft repulsive interactions.* In: *J. Am. Chem. Soc.* 139.14 (2017), pp. 5095–5101.