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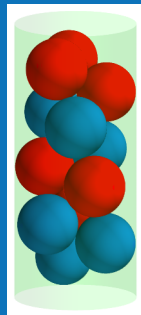


Coláiste na Tríonóide, Baile Átha Cliath  
Trinity College Dublin  
Ollscoil Átha Cliath | The University of Dublin

# Columnar packings of soft spheres

July 8, 2018 | Jens Winkelmann

*Co-authors:* A. Mughal, B. Haffner, D. Weaire and S. Hutzler

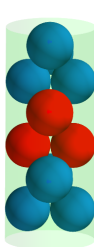


“Packing and stacking  
we lay waste our days!”<sup>1</sup>

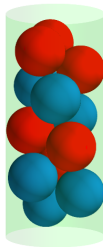
How many spheres fit in a cylinder?



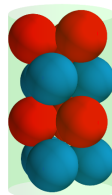
zig-zag



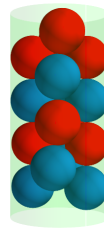
(2, 2, 0)  
uniform



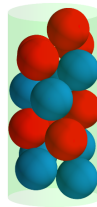
(3, 2, 1)  
uniform



(3, 3, 0)  
uniform



(4, 2, 2)  
uniform



(4, 3, 1)  
uniform

<sup>1</sup>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



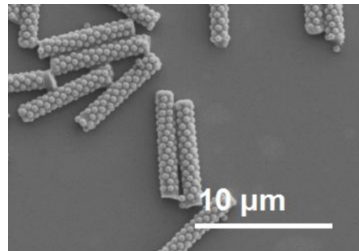
Bushy Park,  
Dublin



Dry foam



Wet foam



Si particles self-assembled to  
microrod inside PDMS pores<sup>1</sup>

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<sup>1</sup>Wu et al; *Confined Assemblies of Colloidal Particles with Soft Repulsive Interactions*; J Am Chem Soc 139, 5095–5101 (2017)



## Overview

Soft sphere model

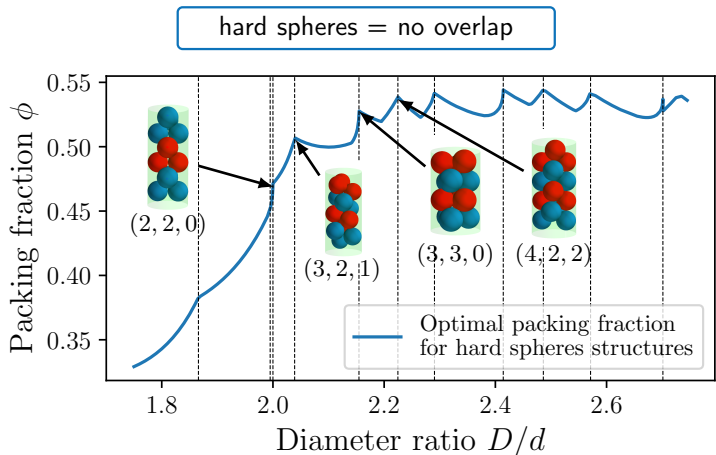
Phase diagram and the observation of a line-slip structure

Metastability and hysteresis

Conclusion

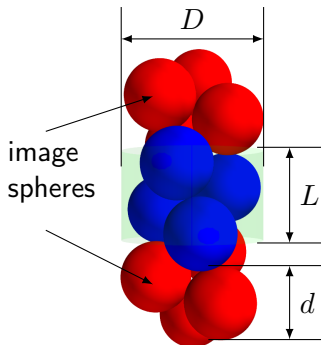


## Columnar hard sphere packings



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

## Simulation based on enthalpy minimisation



- Soft sphere model of **overlapping spheres** with overlap  $\delta_{ij}$
- Enthalpy  $H$ :

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

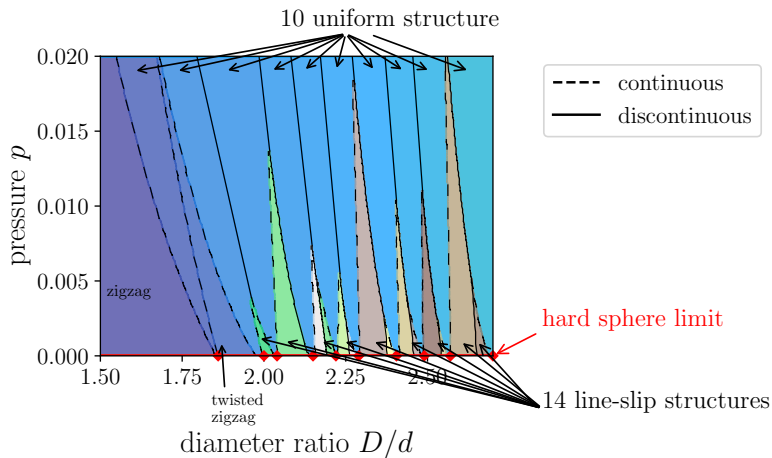
- Inner energy  $U \propto \delta_{ij}^2$
- Pressure term  $pV = p\pi \left(\frac{D}{2}\right)^2 L$
- image spheres are *twisted* by an angle  $\alpha$

### Enthalpy minimisation

Local minimum

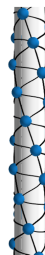
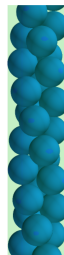
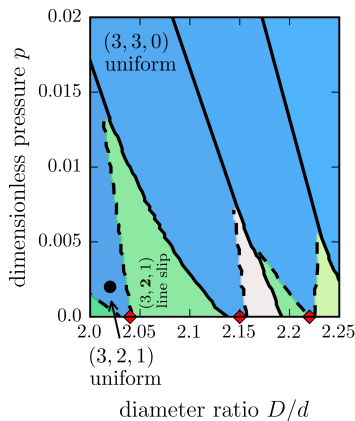
Global minimum

## The phase diagram



Phase diagram with all columnar structures *without inner spheres*

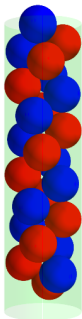
## Continuous and discontinuous transitions



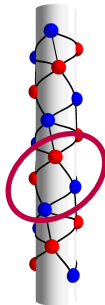
- Continuous (dashed): loss of contact
- Discontinuous (solid): complete change in structure

## What is a line-slip structure?

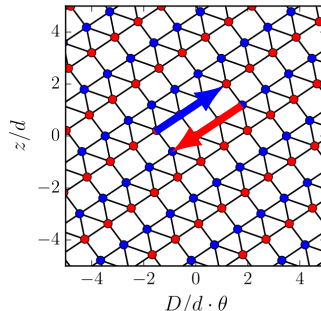
- Characterised by a **loss of contact** (gap)



(3,2,1) line slip



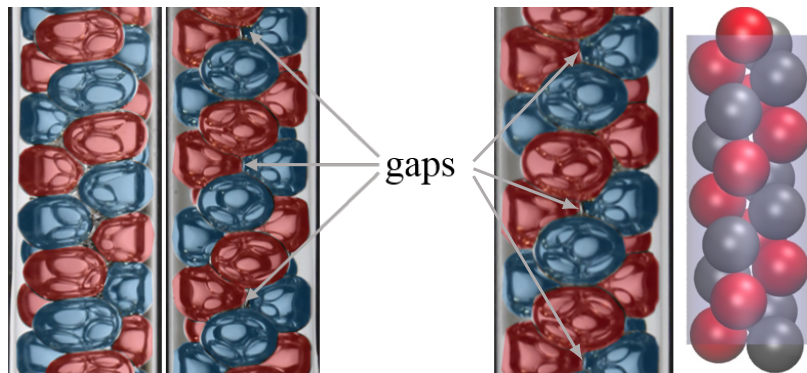
Contact network



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 $(3, 2, 1)$ line slip



$(3, 2, 1)$  uniform and  $(3, 2, 1)$  line-slip structure

$(3, 2, 1)$  line slip in experiment and simulation

<sup>0</sup>Winkermann 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

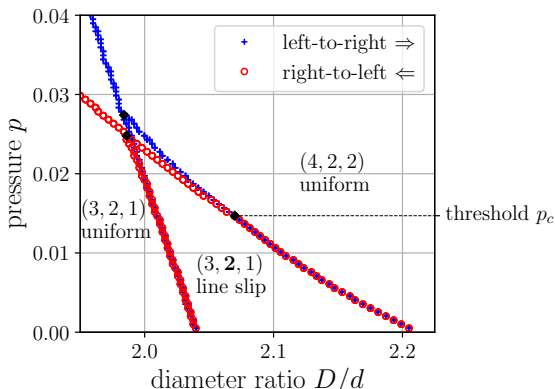
### Motivation:

- 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

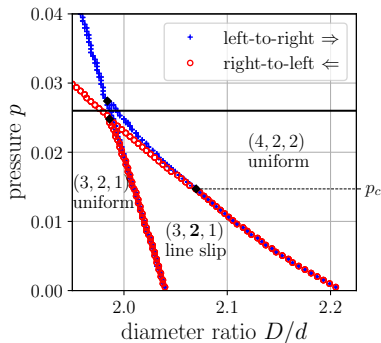
### Motivation:

- 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  $D/d$

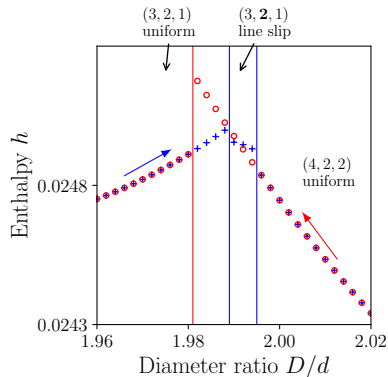




## Example for a hysteretic transition



Stability diagram



Enthalpy vs. diameter ratio

<sup>0</sup>Winkelmann et al; *Columnar structures of soft spheres: metastability and hysteresis*; Phys Rev E submitted (2018)

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

## Columnar bubble chains

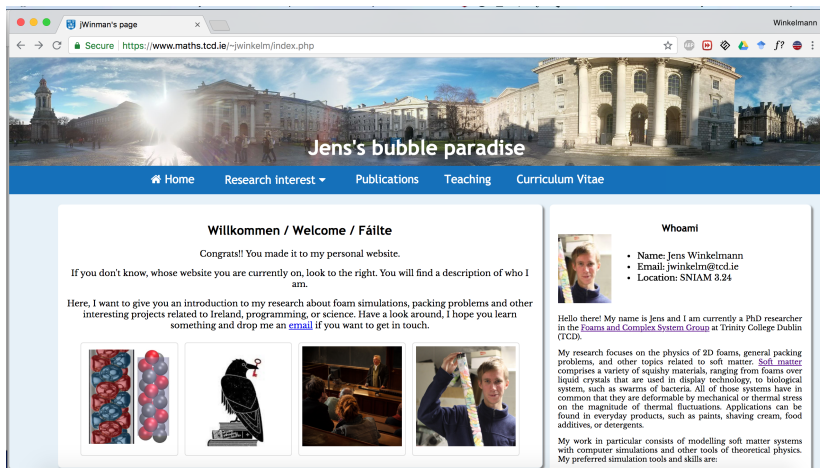
July 8, 2018

## Acknowledgement



this is Fritz  
Dunne

Website: <https://www.maths.tcd.ie/~jwinkelm>



Winman's page x

Secure <https://www.maths.tcd.ie/~jwinkelm/index.php>

Winkelmann

# Jens's bubble paradise

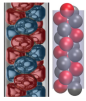



Home Research interest Publications Teaching Curriculum Vitae

## Willkommen / Welcome / Fáilte

Congrats!! You made it to my personal website.

If you don't know, whose website you are currently on, look to the right. You will find a description of who I am.

Here, I want to give you an introduction to my research about foam simulations, packing problems and other interesting projects related to Ireland, programming, or science. Have a look around, I hope you learn something and drop me an [email](#) if you want to get in touch.

### Whoami

- Name: Jens Winkelmann
- Email: [jwinkelm@tcd.ie](mailto:jwinkelm@tcd.ie)
- Location: SNIAM 3.24

Hello there! My name is Jens and I am currently a PhD researcher in the [Foams and Complex System Group](#) at Trinity College Dublin (TCD).

My research focuses on the physics of 2D foams, general packing problems, and other topics related to soft matter. [Soft matter](#) comprises a variety of squishy materials, ranging from foams over liquid crystals that are used in display technology, to biological systems, such as swarms of bacteria. All of those systems have in common that they are deformable by mechanical or thermal stress on the magnitude of thermal fluctuations. Applications can be found in everyday products, such as paints, shaving cream, food additives, or detergents.

My work in particular consists of modelling soft matter systems with computer simulations and other tools of theoretical physics. My preferred simulation tools and skills are: