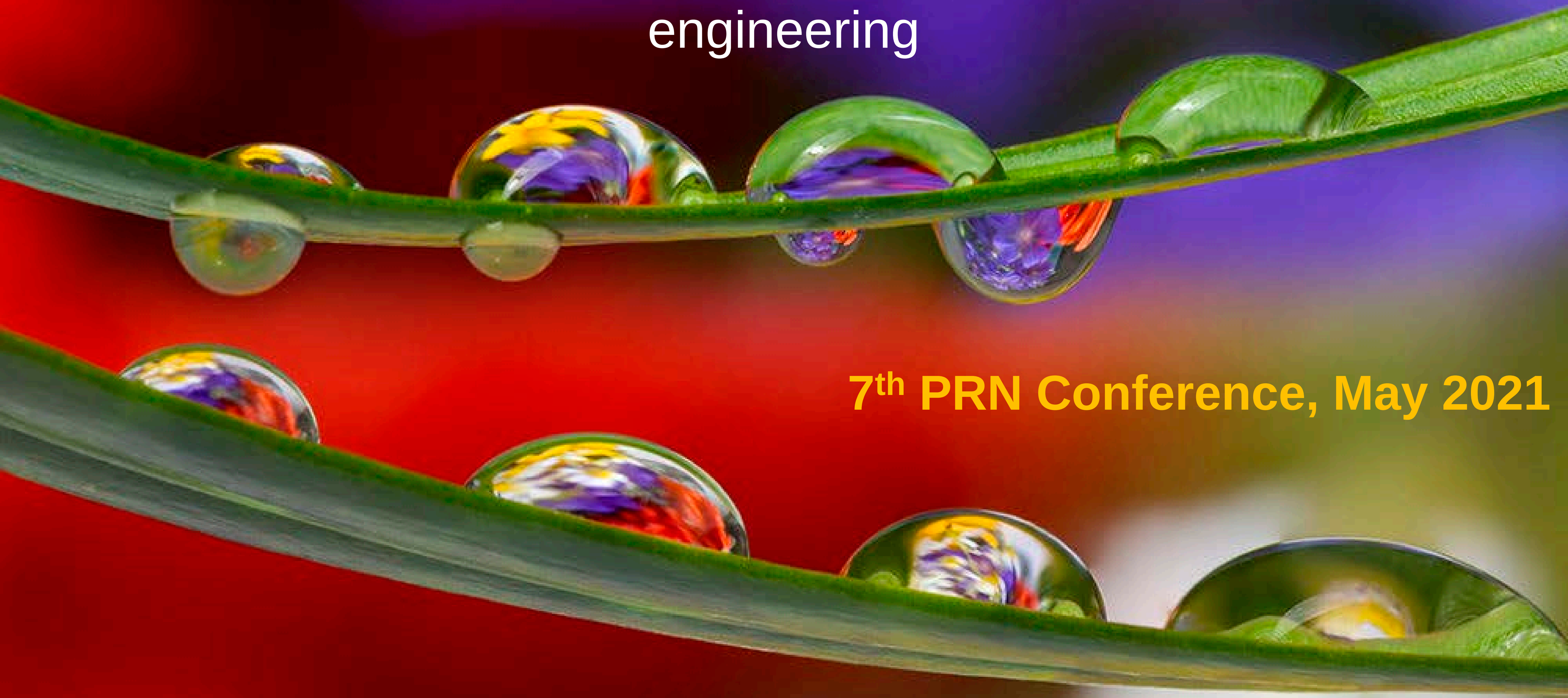
Controlling wettability through modeling-based surface topography engineering



7th PRN Conference, May 2021

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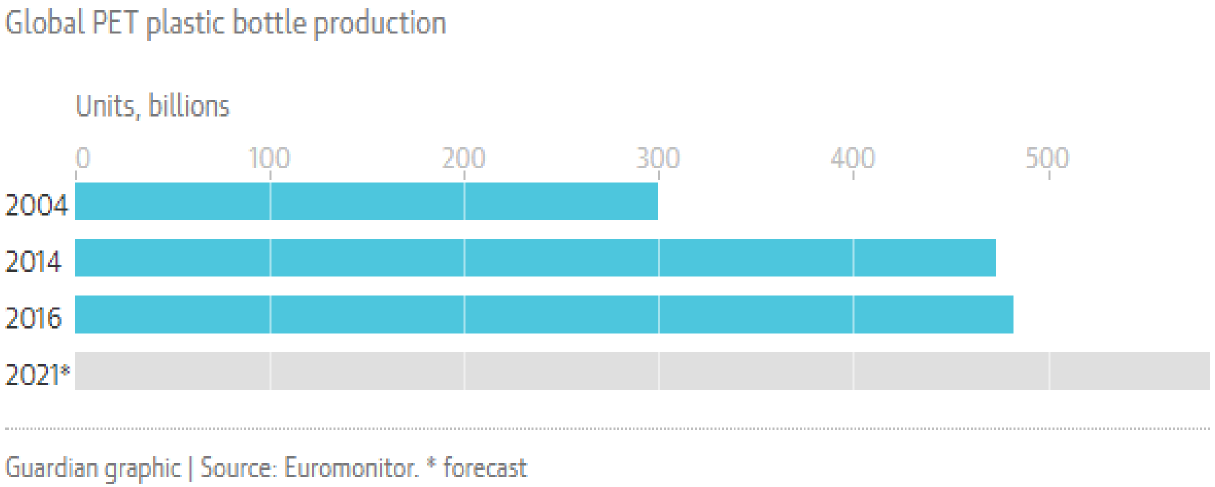
Presentation Outline

1. Problematic & Motivation
2. Proposed solution
3. Solution implementation
4. Solution validation
5. Conclusions & remarks

Problematic & Motivation

❑ **Surface wetting was identified as the prevalent mechanism related to adhesion of a liquid onto a solid surface**



More than **480bn** plastic bottles were made in 2016

By 2021 demand will climb up to **~580bn**

Equivalent to 1M/min or 17k/s

If placed end-to-end, they extend **more than halfway to the sun!**

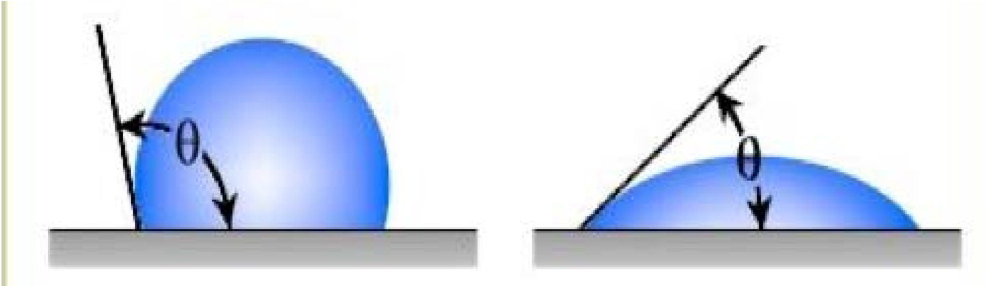
Approximately **6-8%** of packaged material sticks

About **0.03 km³** water loss/year

lake de l’ Hongrin

Solution: Superomniphobic surfaces

- The way to reduce product loss is through the design of superomniphobic surfaces
  - ***Omniphobic*** *(θ > 90º) and* ***superomniphobic*** *(θ > 150º) are surfaces that repel all kinds of liquids*

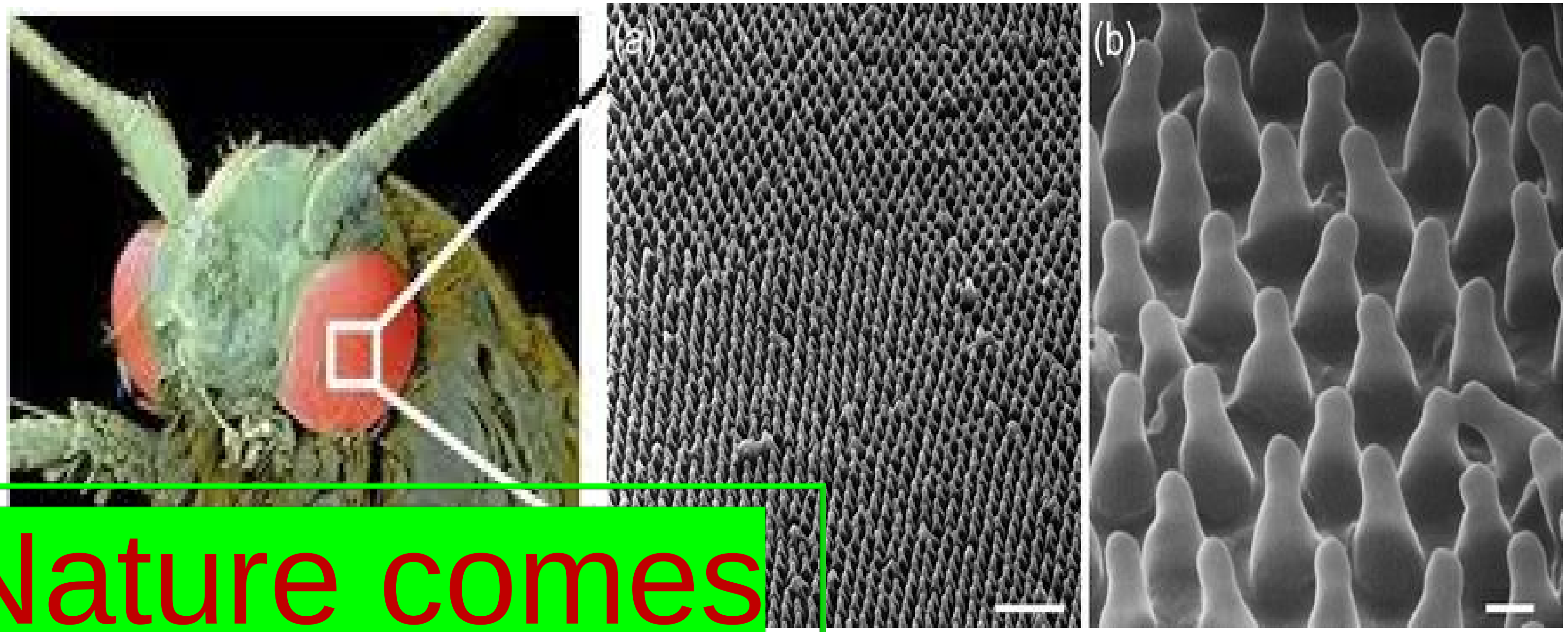


phobic (large θ)   **philic (small θ)**

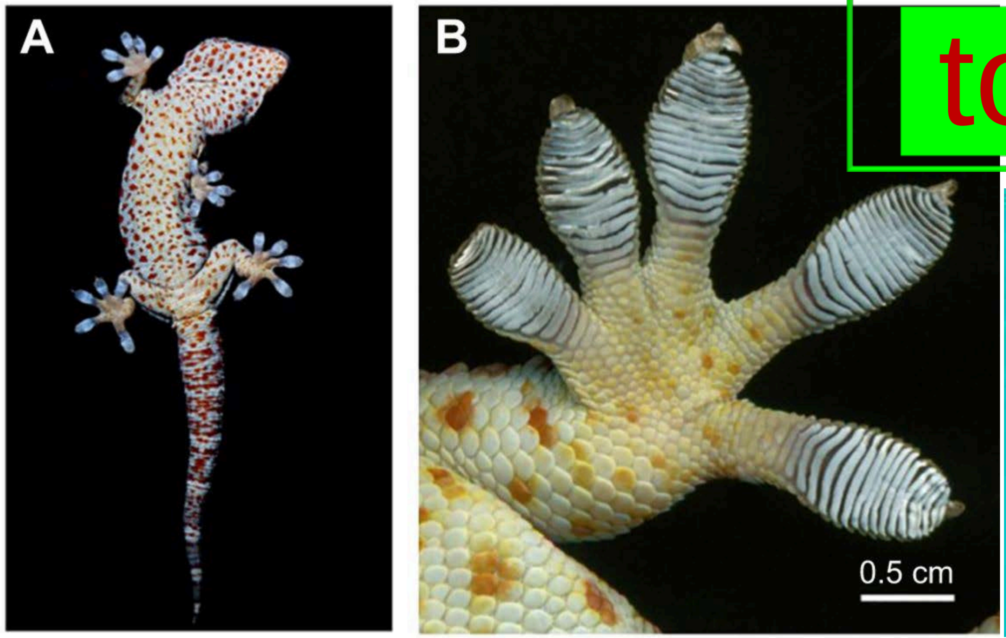
- *Possibilities to induce omniphobicity include:*
  - ***Chemical treatment*** *of surface (minor impact on wettability)*[1]
  - *Treatment of the* ***surface topography*** *(more promising)*

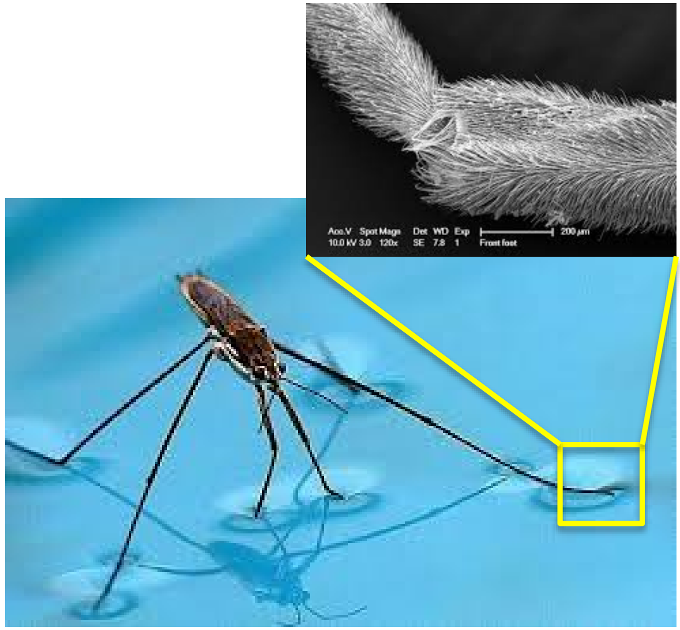
Task:
- *use* ***mathematical modelling*** *to quantify the relations between* ***surface topography and wetting***

1. Nishino, T et al. *Langmuir*, **1999**, *15*, 4321-4323



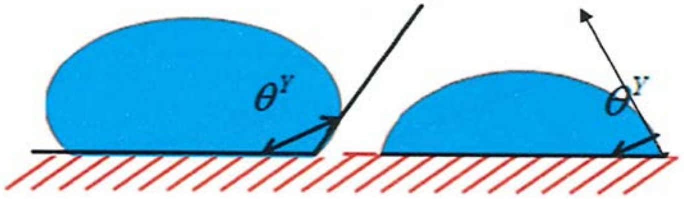
Nature comes to the rescue!





Solution: Bio-inspired surface topography manipulation

1. Young's Model[1] (1805)

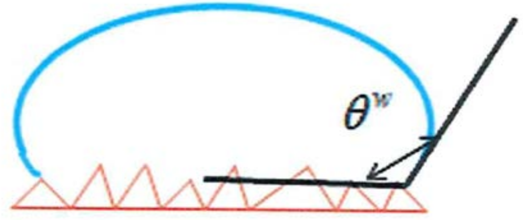


$$\cos\theta^Y = \frac{\gamma_s - \gamma_{sl}}{\gamma_l}$$

- Smooth surfaces 👎
- Full wetting 👎
- Unrealistic surface 👎

1. Young, T. *Phil. Trans. R. Soc. Lond.* **1805**, *95*, 65-87

2. Wenzel Model[2] (1936)

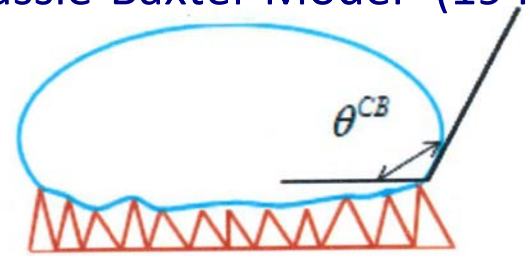


$$\cos\theta^W = roughness \cdot cos\theta^Y$$

- Rough surfaces 👍
- Full wetting 👎
- Unrealistic surface 👎

2. Wenzel, R. N. *Industrial and engineering chemistry*. **1936**, *28*(8)

3. Cassie-Baxter Model[3] (1944)



$$\cos\theta^{CB} = f_{sl}\cos\theta^Y - f_{la}$$

- Rough surfaces 👍
- Partial wetting 👍
- Realistic surface 👍
- Unrealistic interface 👎

3. Cassie, A. B. D.; Baxter, S. *Wettability of porous surfaces*. **1944**

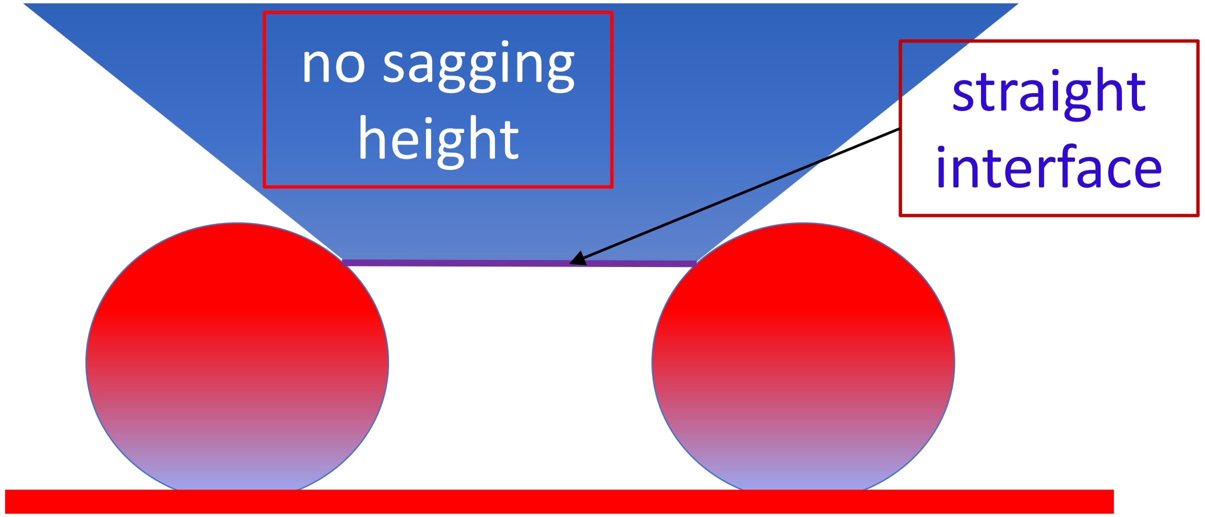
❑ It is evident that:

- ➢ *the **Cassie-Baxter** model is the most realistic one accounting for **rough surfaces** and **partial wetting***
- ➢ *However, **unrealistic interface**…*

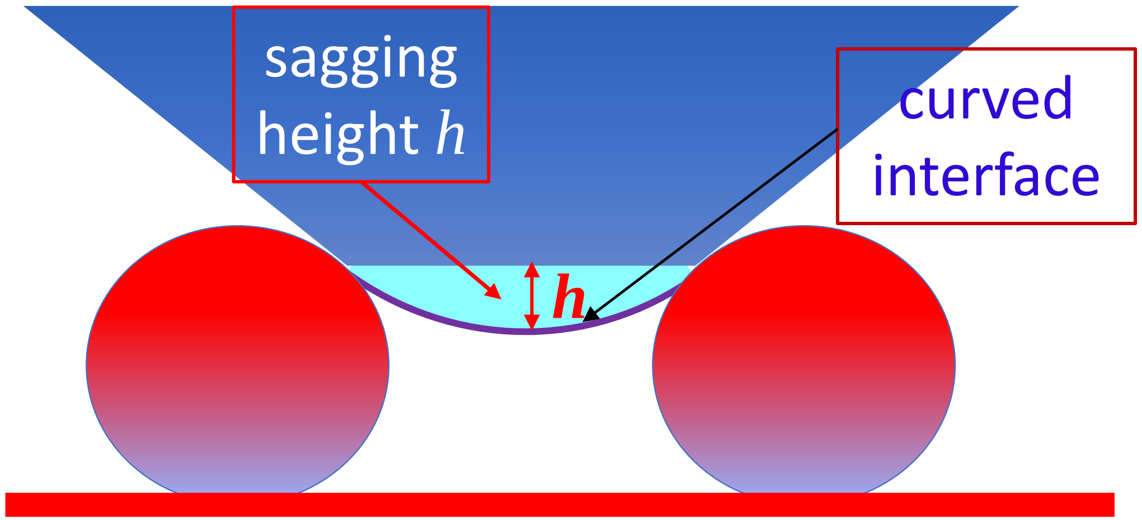
Solution: Model details & innovation

- The liquid properties are expressed in terms of the **sagging height *h*[1]**

Original Cassie-Baxter Model



Extended Cassie-Baxter Model (this work)



Sagging height

$$h = \frac{l^2}{l_{cap}}$$

l : characteristic length (topography dependent)

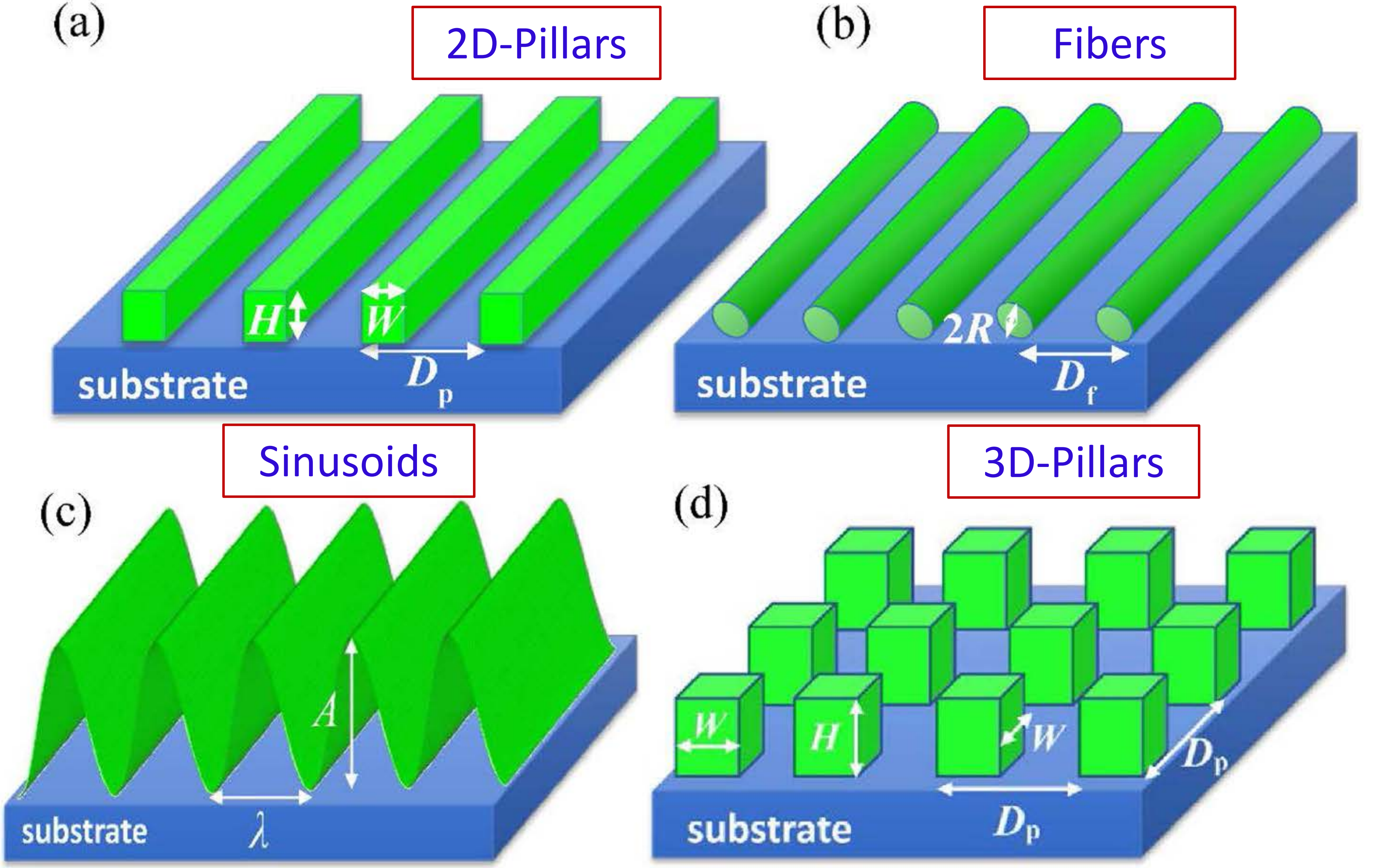
Capillary length

$$l_{cap} = \sqrt{\frac{\gamma_l}{\rho g}}$$

Liquid dependence

1. Tuteja, A. et al, *PNAS*, **2008**, *105*(47), 18200

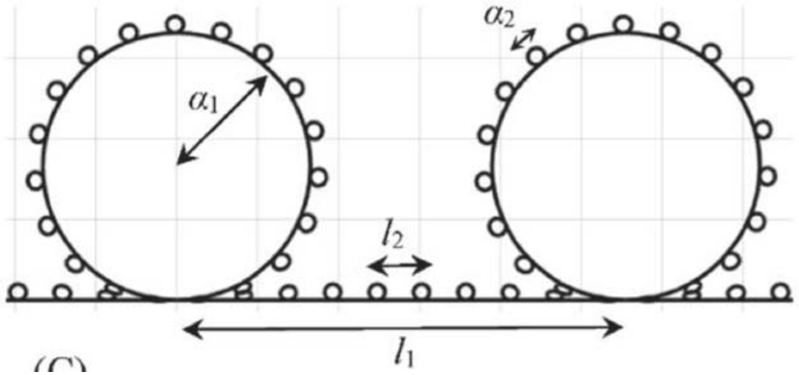
Single-level surface topographies



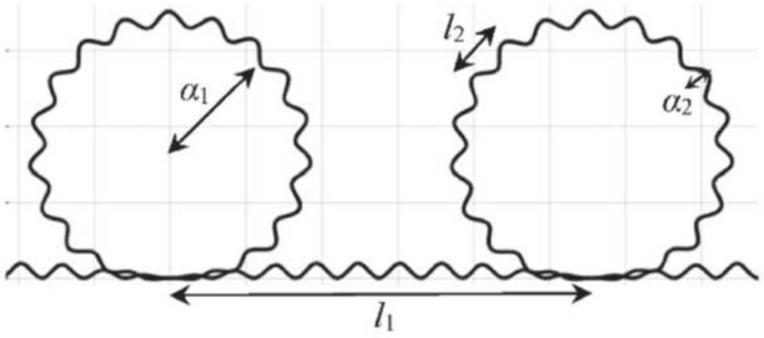
Topography	l
2D-Pillars	D_p
Fibers	D_f
Sinusoids	λ
3D-Pillars	D_p

Multi-level surface topographies

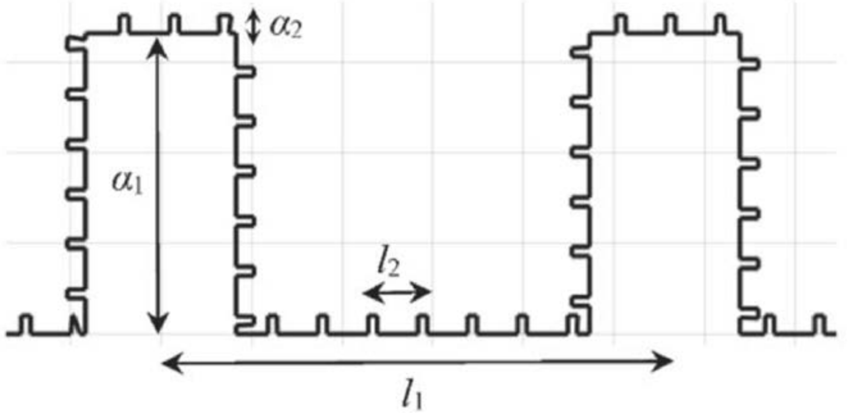
Fibers on Fibers



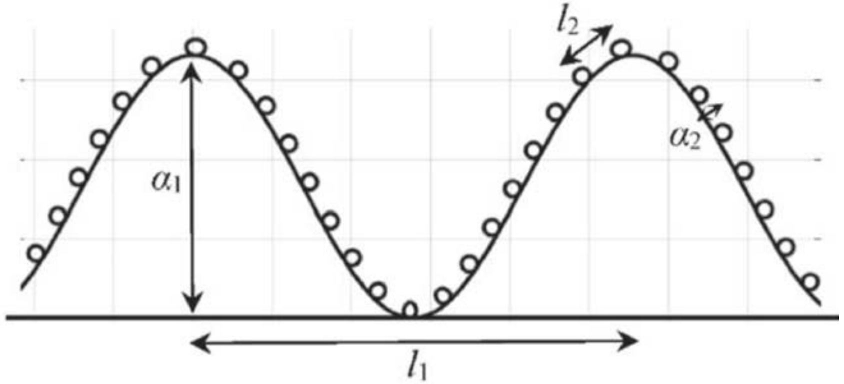
Sinusoids on Fibers



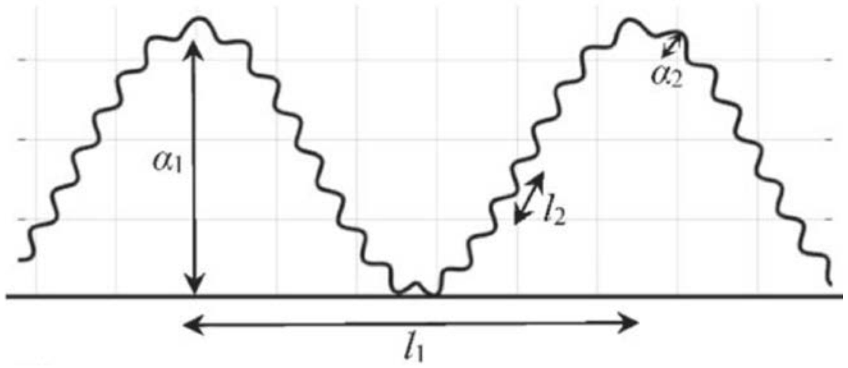
Pillars on Pillars



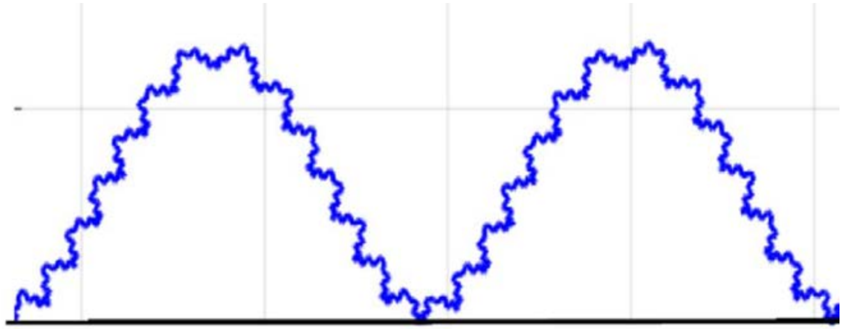
Fibers on Sinusoids



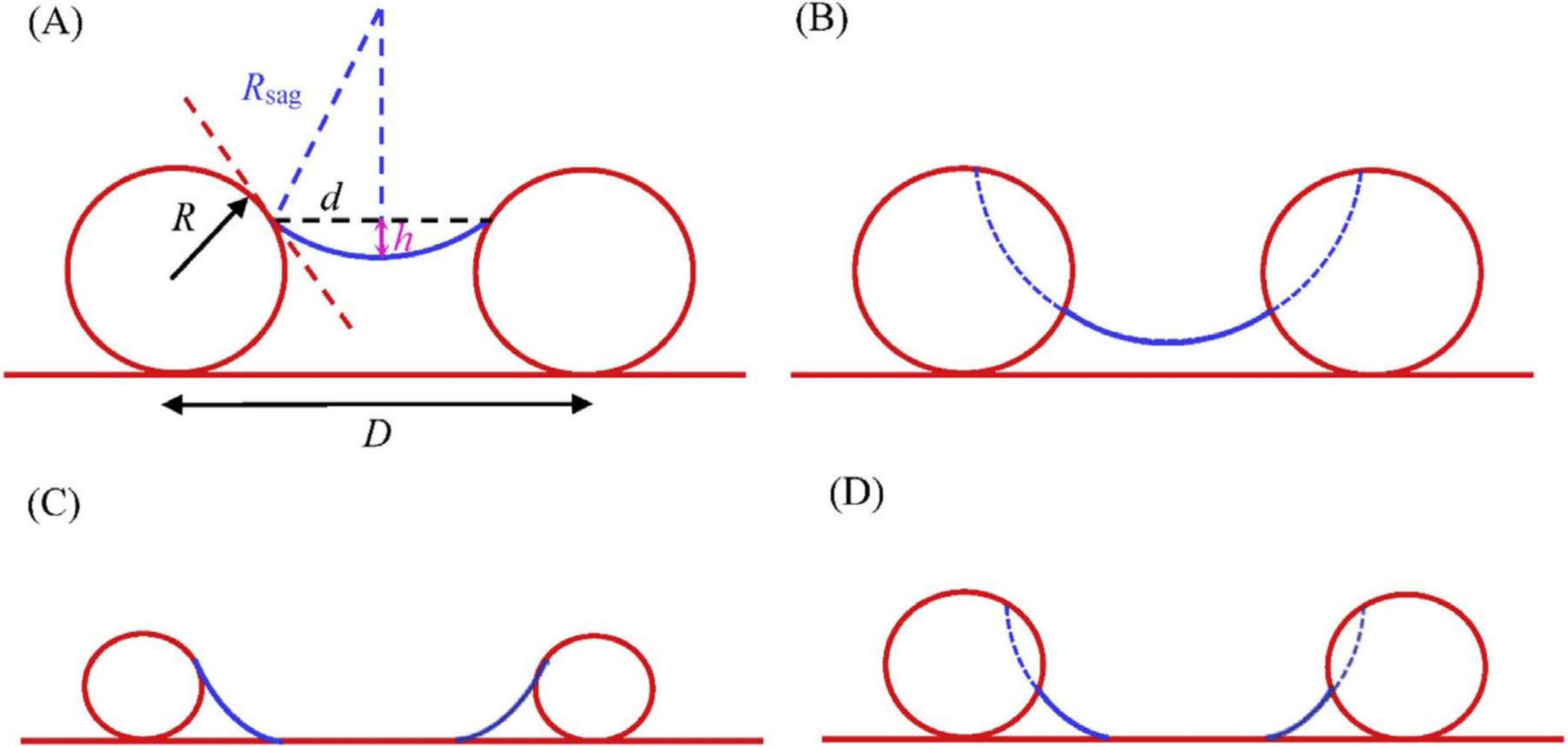
Sinusoids on Sinusoids



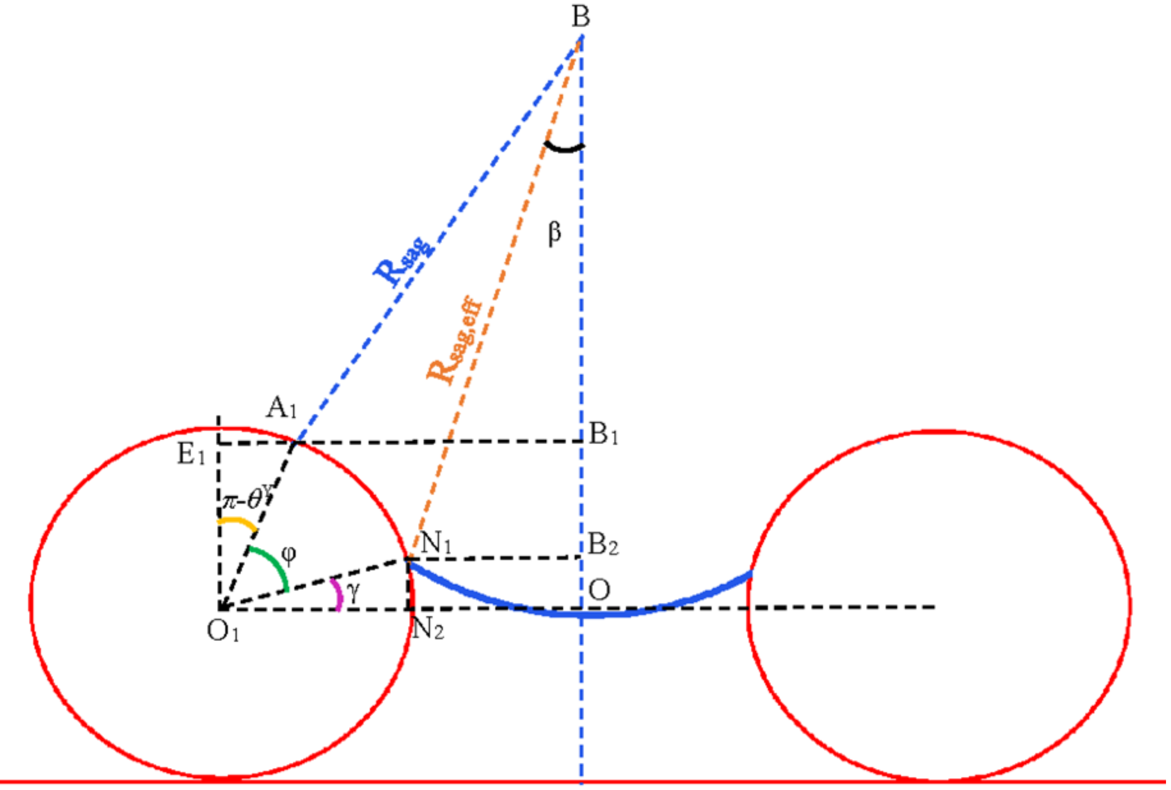
3x Sinusoids

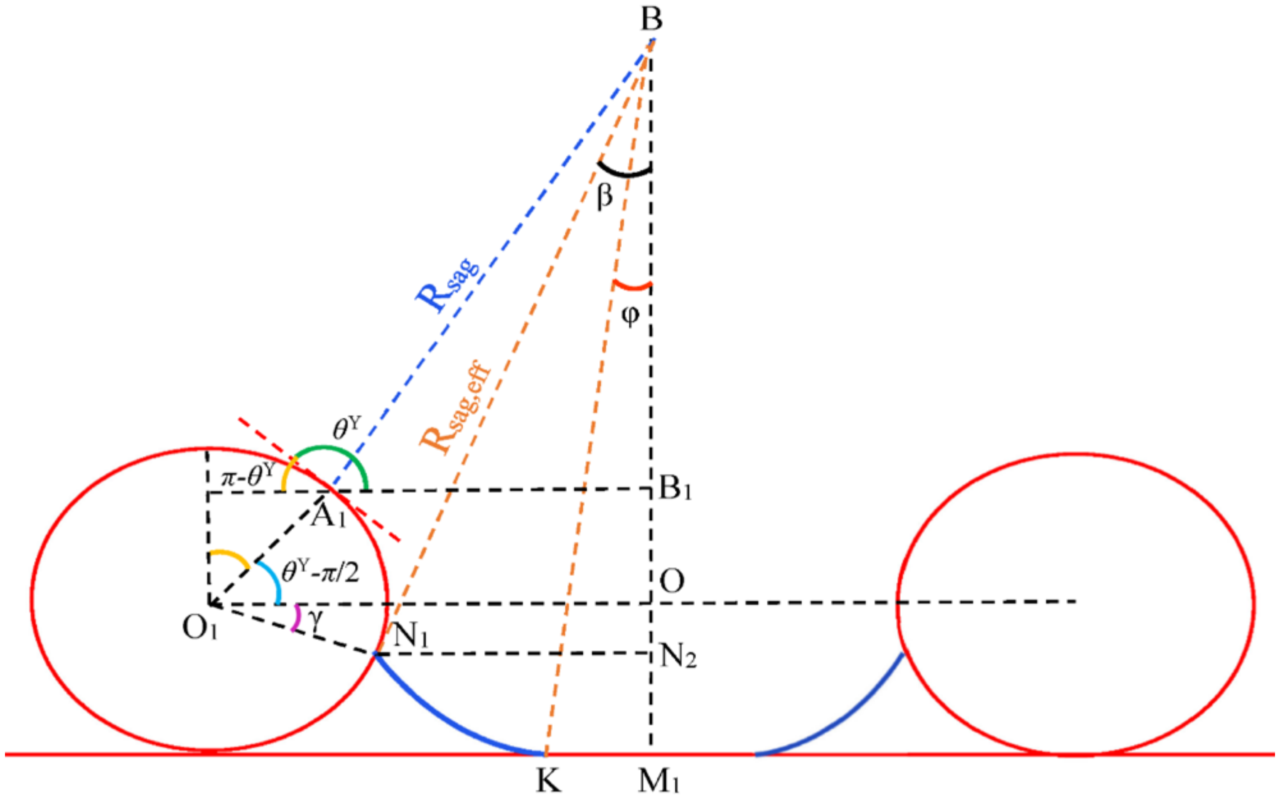


Fibers: Wetting scenarios



Fibers: Mathematical derivations





$$f_{sl} = \frac{\text{actual wetted area}}{\text{total projected area}} = \frac{2R(\pi - \theta^Y)}{D} + \frac{2R\left(\theta^Y - \frac{\pi}{2} - \gamma\right)}{D}$$

$$f_{la} = \frac{2\beta R_{sag,eff}}{D} = \frac{2R_{sag,eff}}{D}\arccos \times \left[\frac{\left(\sqrt{R_{sag,0}^2 - d^2} - R\cos\theta^Y - R\sin\gamma\right)}{R_{sag,eff}}\right]$$

$$f_{sl} = \frac{\text{actual wetted area}}{\text{total projected area}} = \frac{2R(\pi - \theta^Y)}{D} + \frac{2R_{sag}}{D}\sqrt{1 - \cos^2\varphi}$$

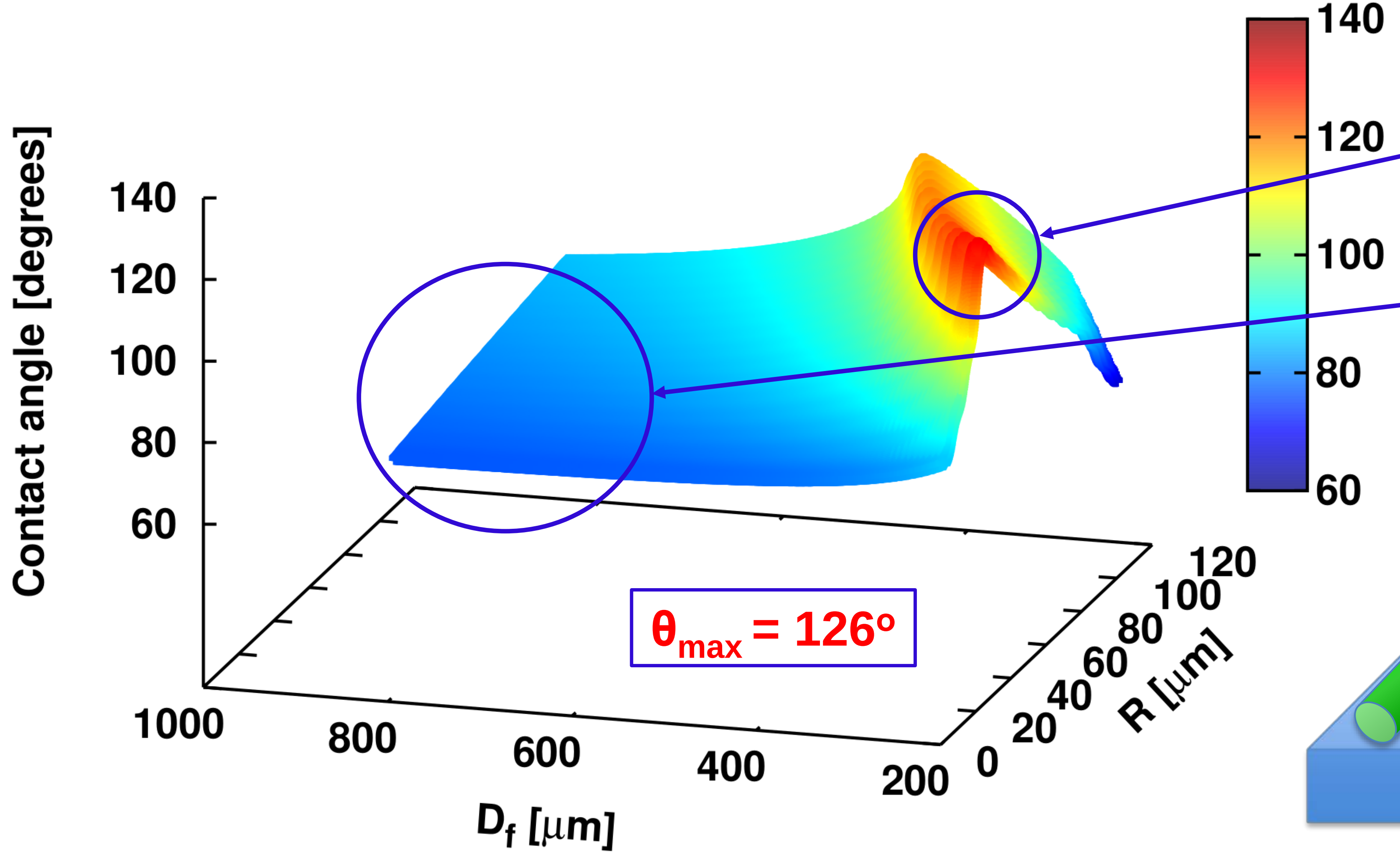
Lempesis et al., 2020

Model input

Parameter	Value
liquid	Water
surface	LDPE
Young's angle θ^{Y}	73^{o}
liquid density ρ	997 kg/m^3
liquid surface tension γ_l	72.8 mN/m

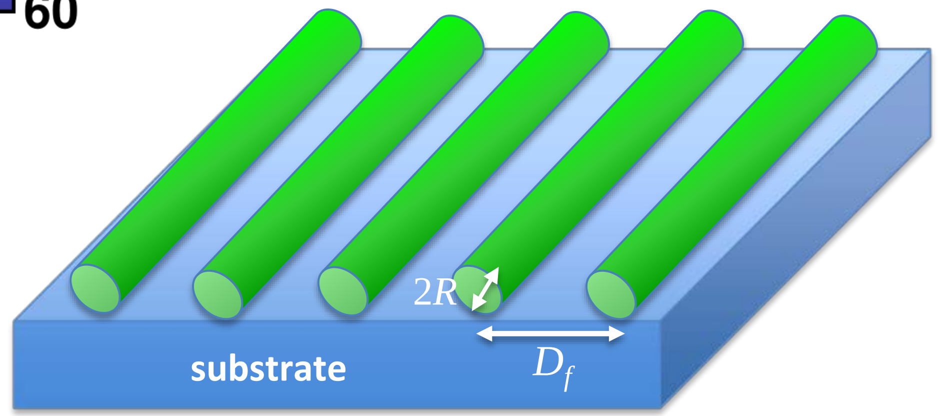
Lempesis et al., 2020

Fibers: Model output



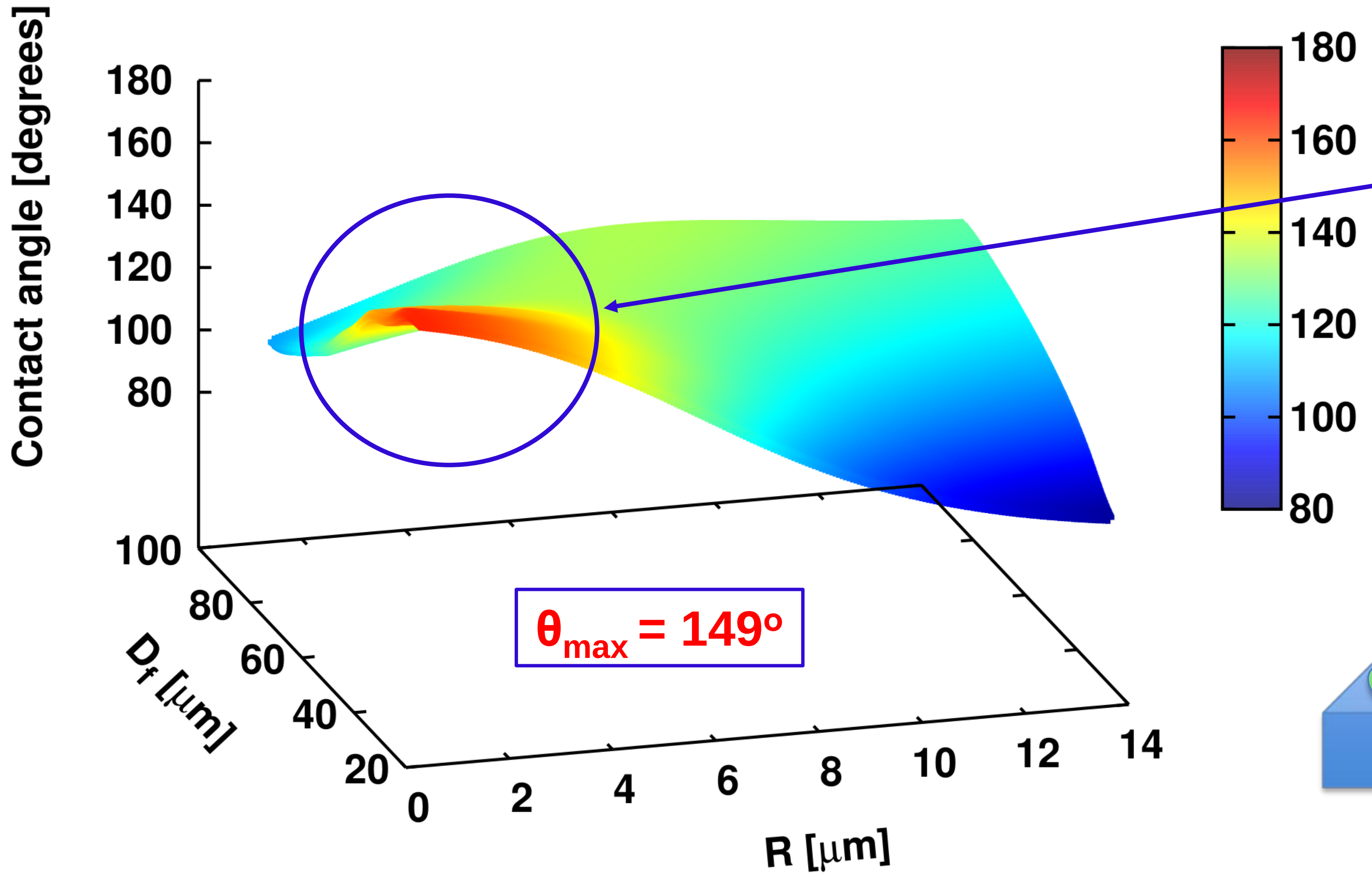
Comments

- Increase of contact angle as scale becomes smaller
- Our model captures the transition to the Young state ($\theta^Y = 73^o$)



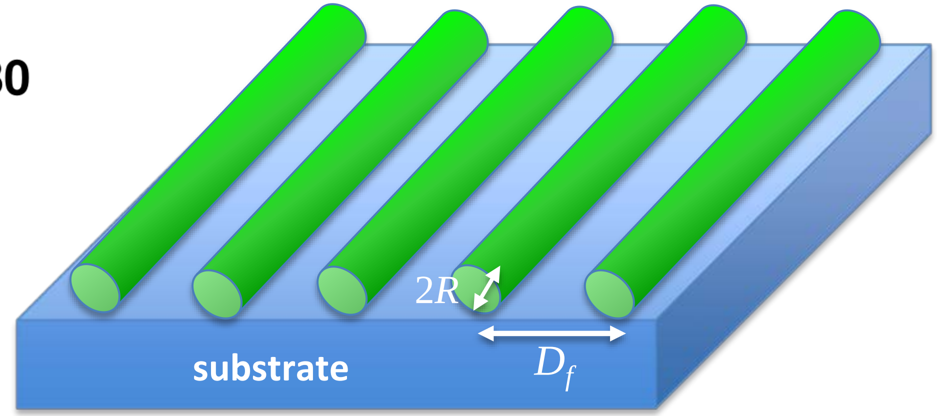
Lempesis et al., 2020

Fibers: Scale effect

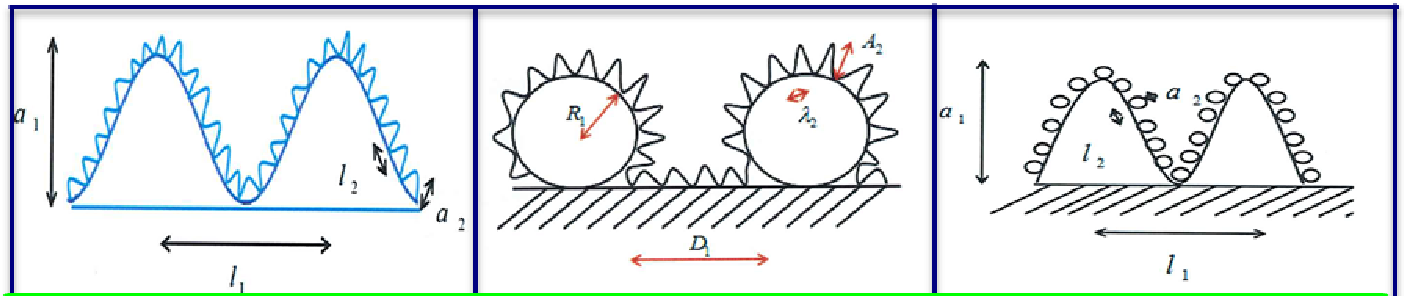


Comments

- As fiber scale drops, phobicity increases considerably
- Fabrication of **nanoscale** patterns is a formidable technological challenge

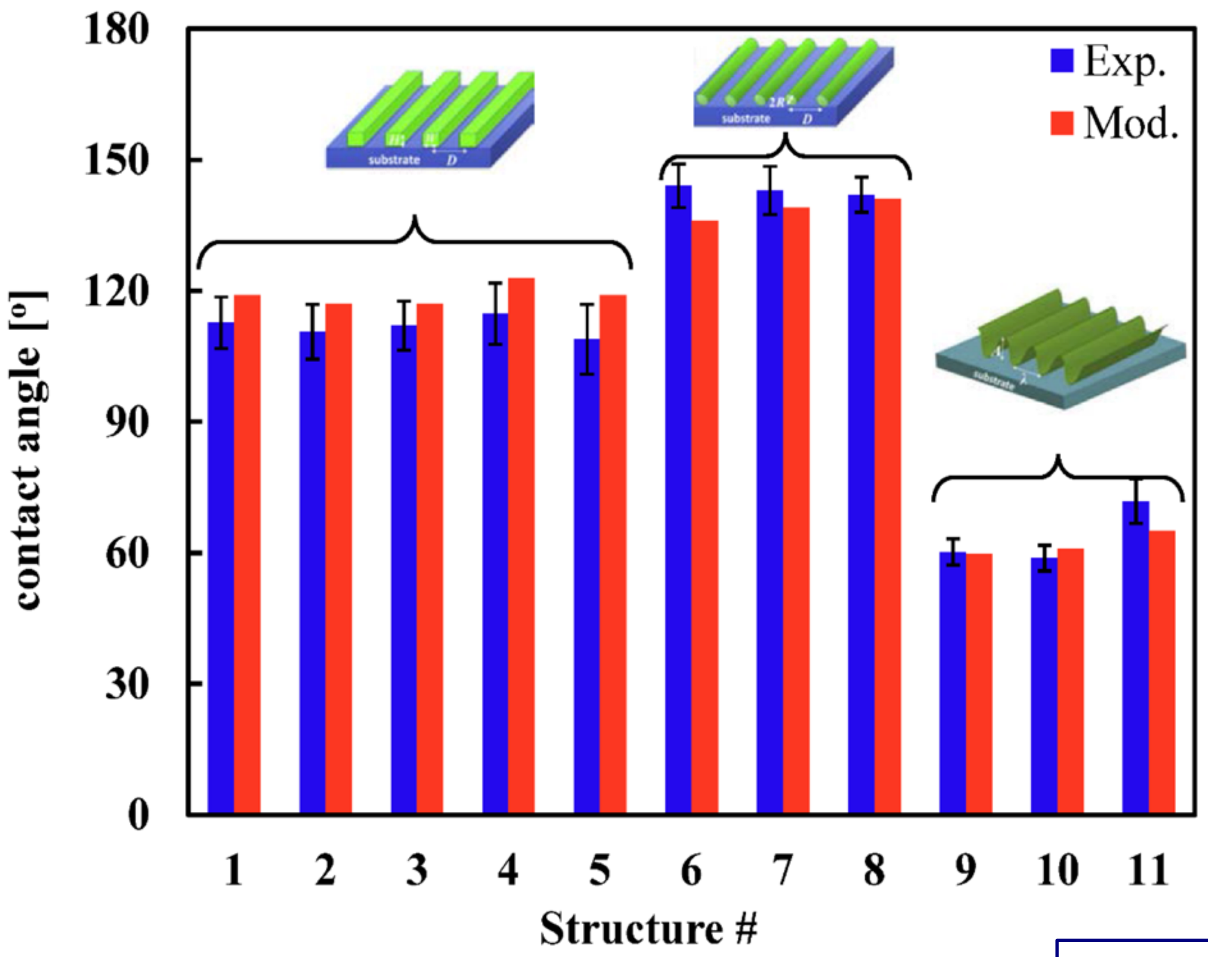


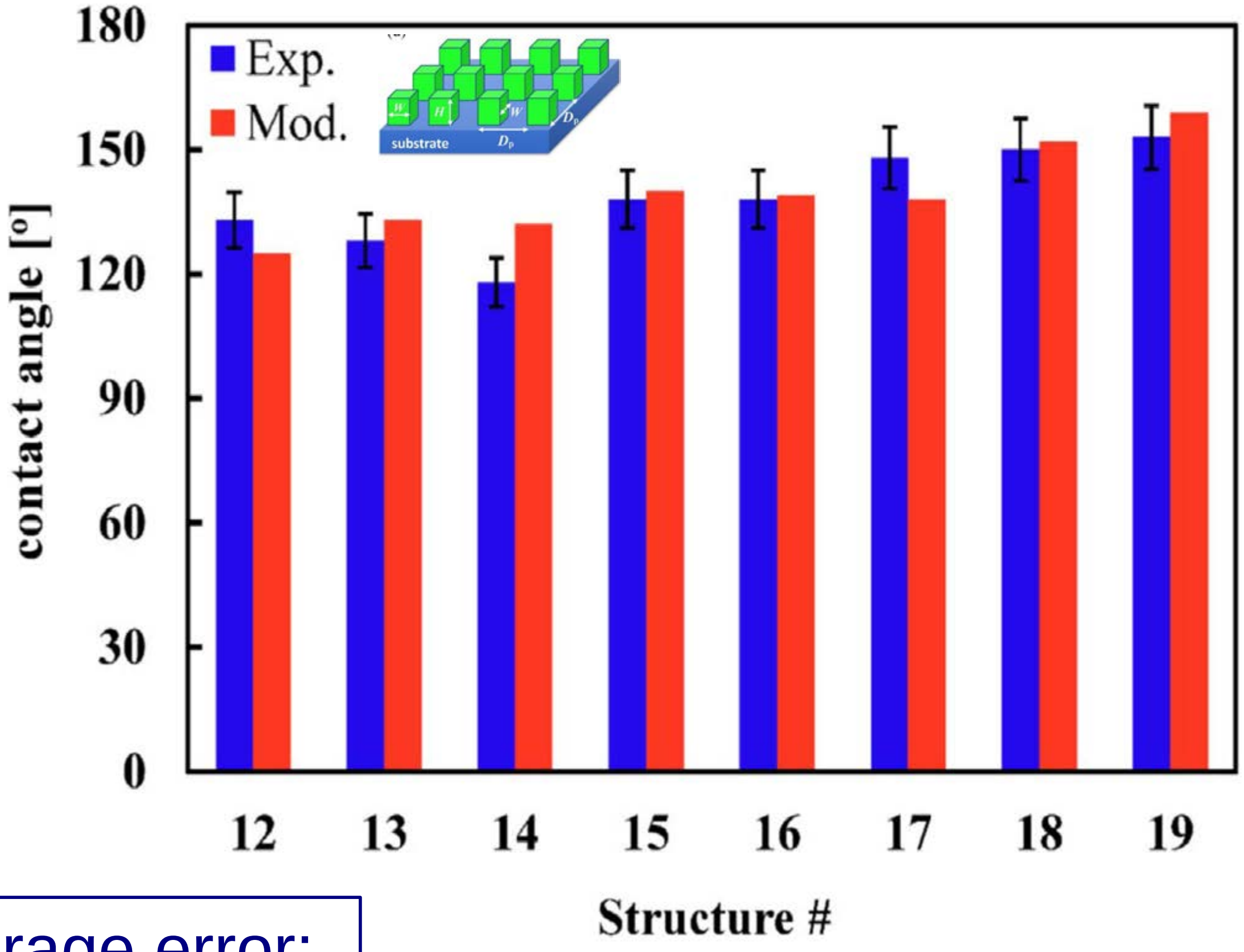
Lempesis et al., 2020



	Two-level topography			Single-level topography
Ext. Cassie/Baxter	Sine on Sine	Sine on Fibers	Fibers on Sine	Sine
Max. Contact Angle [º]	140	149	**162**	100
Scale1 [µm] (coarse scale)	A_1 = 161	R = 28	A = 161	A = 81
	λ_1 = 252	D_f = 217	λ = 252	λ = 126
Scale2 [µm] (fine scale)	A_2 = 16	A = 32	R = 7	n/a
	λ_2 = 25	λ = 50	D_f = 28	n/a

Model validation: single-level topographies

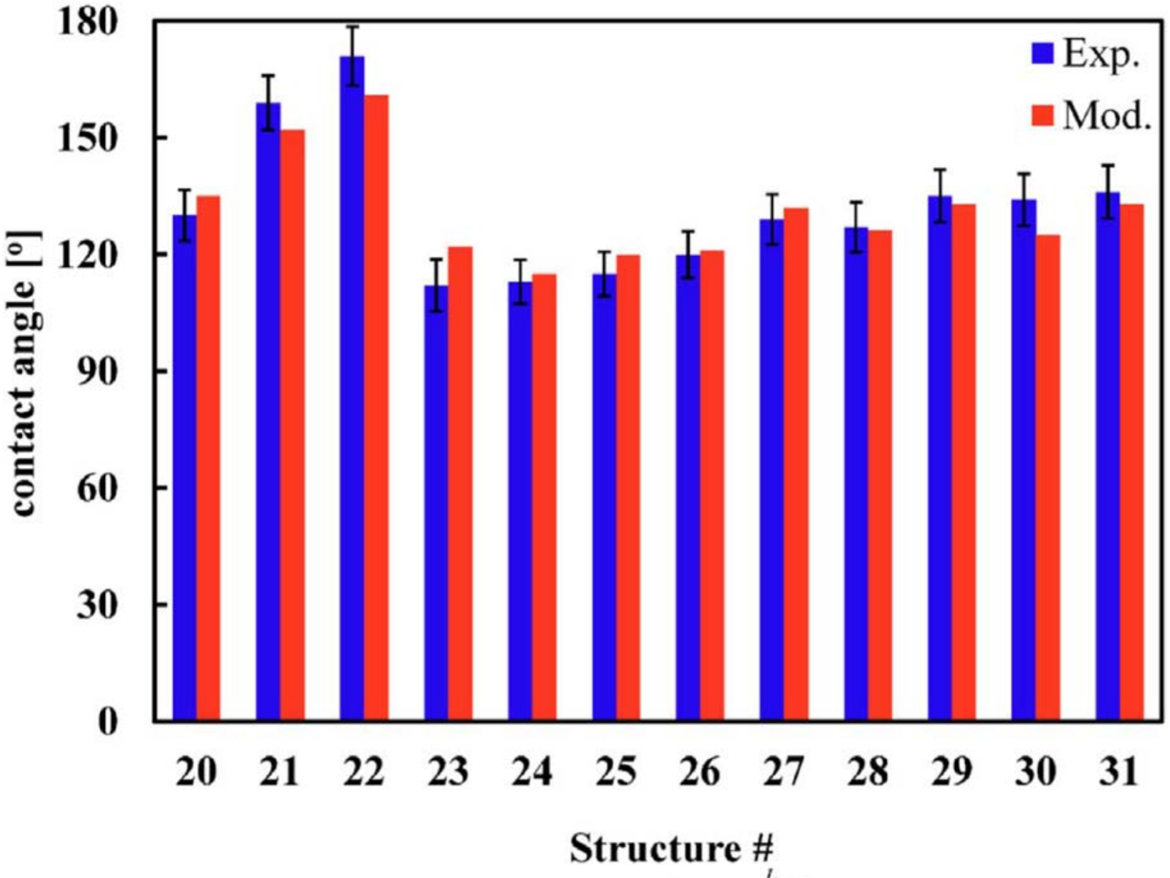


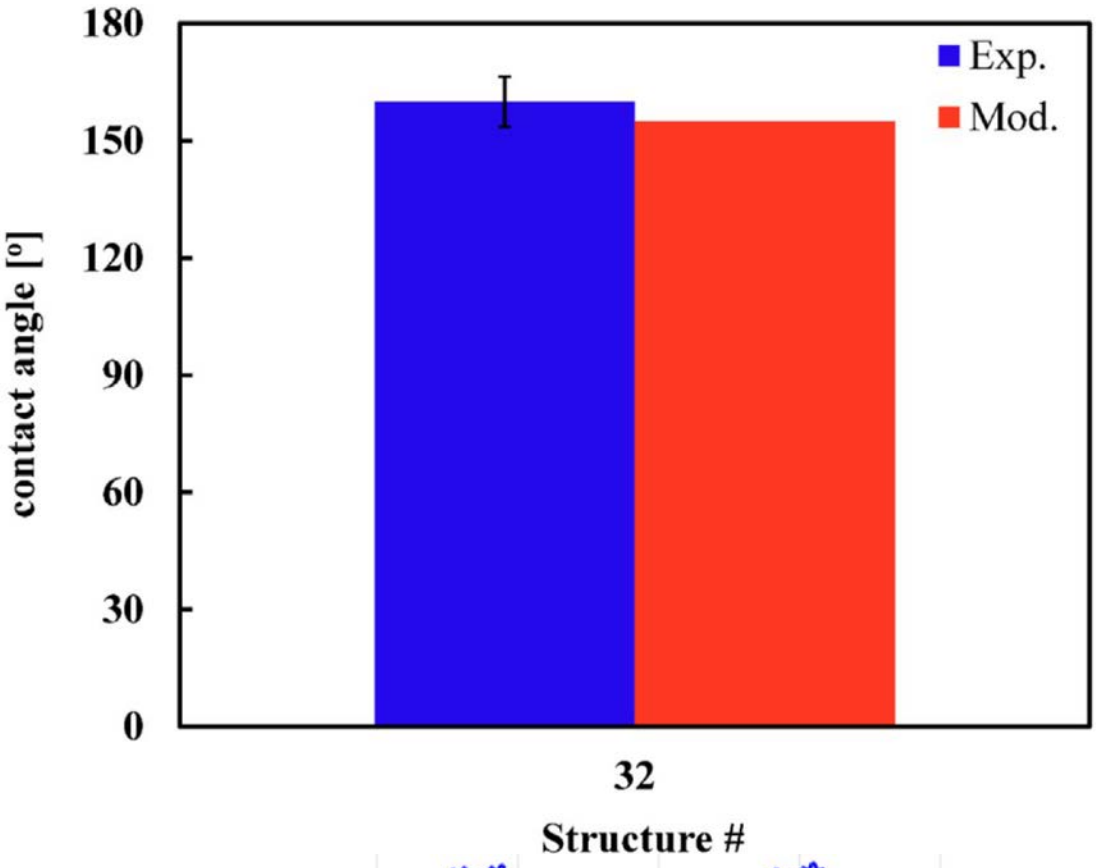


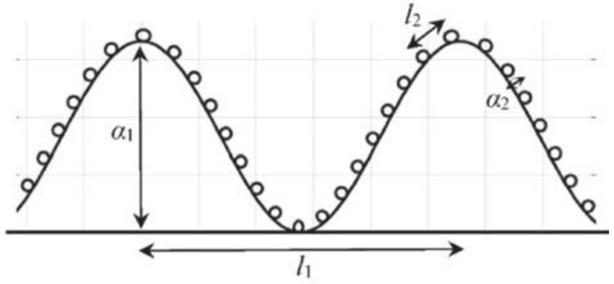
Average error:
4.6 %

Lempesis et al., 2021

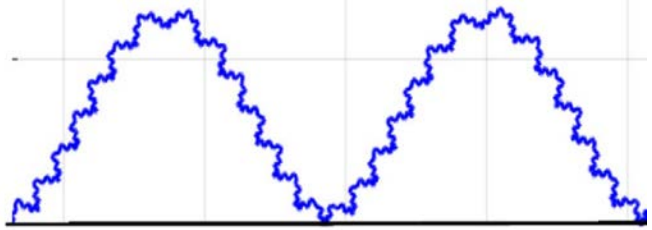
Model validation: multi-level topographies







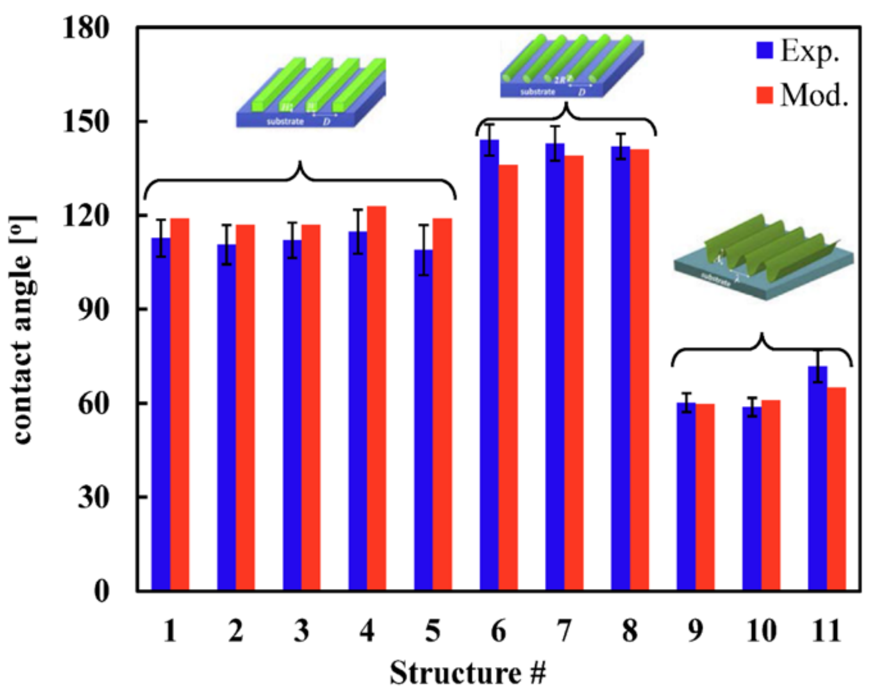
Average error:
3.5 %



Lempesis et al., 2021

Summary and next steps

- An extended Cassie-Baxter model with realistic interfaces was developed for single- and multi-level topographies
- Our model captures the transitions to the Wenzel and Young states and length scale effect
- Model results deviated on average from exp. data by (~4%)
- Addition of a 2^{nd} level almost doubled the contact angle, while a 3^{rd} level brought about an additional 12.5% increase



- Creation of a user-friendly Graphical User Interface (GUI)
- Extension of formalism to more surface topography types
- Modeling the wetting behavior of moving droplets (self-cleaning)

Acknowledgements

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