



Multiscale Simulation of laser-textured surface wettability: toward understanding the role of surface oxidation and molecular adsorption

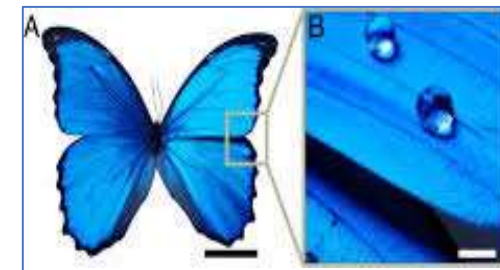
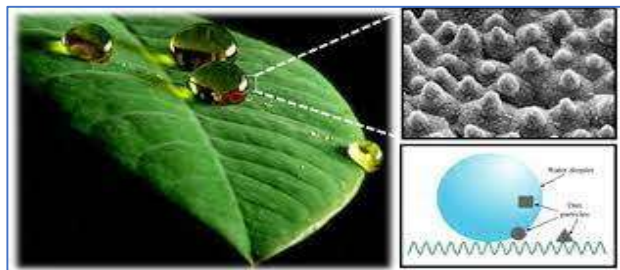
Ilemona S. Omeje¹, Patrick Ganster² and Tatiana Itina¹

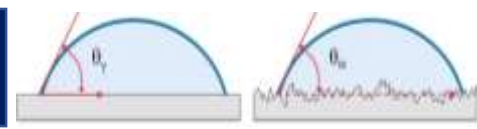
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10th International Conference on Multiscale Materials Modeling, Baltimore, USA

October 6, 2022





1 Motivation

2 Challenge

3 Objective

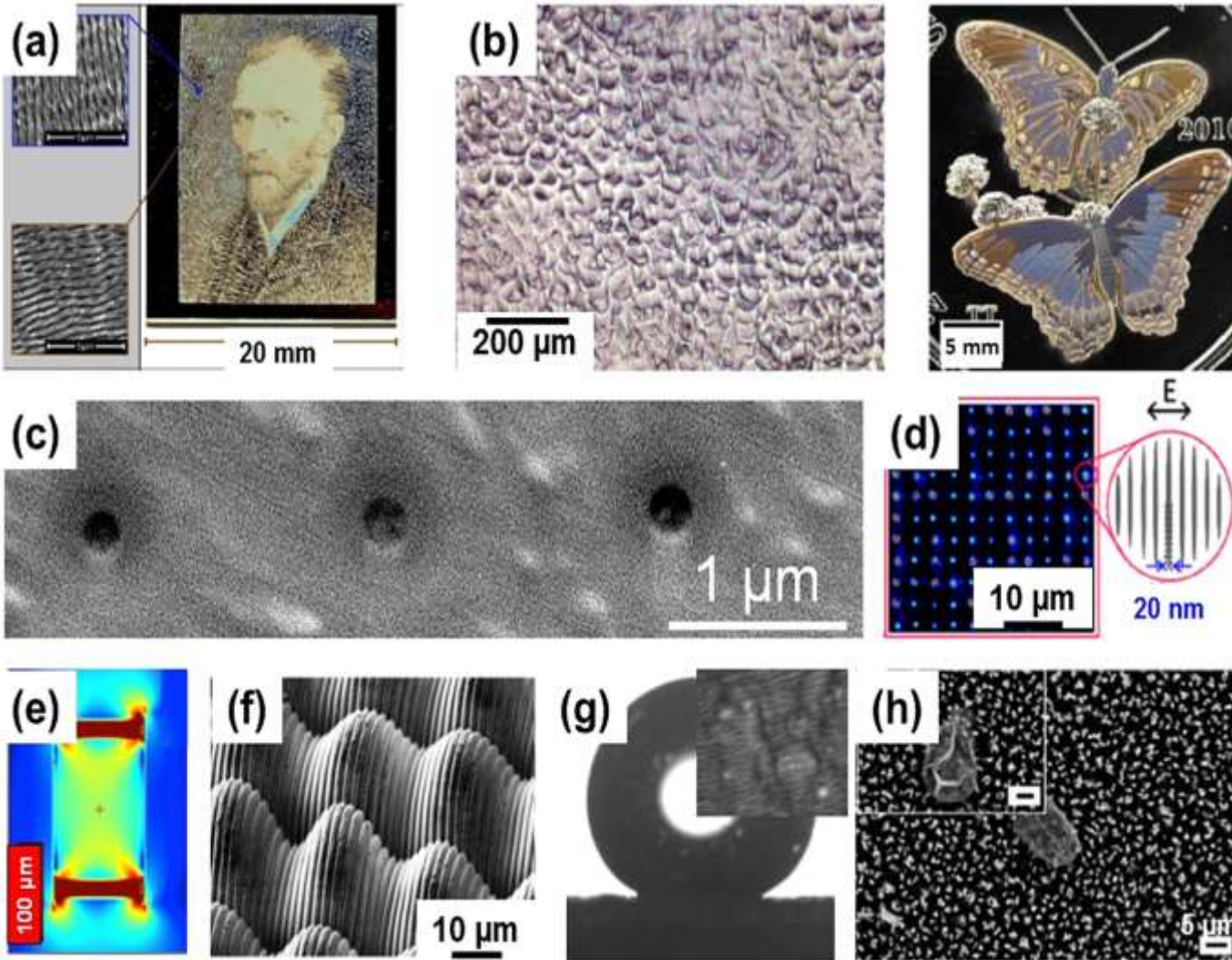
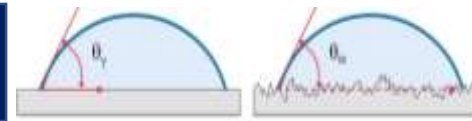
4 CFD Approach

5 Model Validation

6 CFD Results

7 Summary and Future Work

Motivation

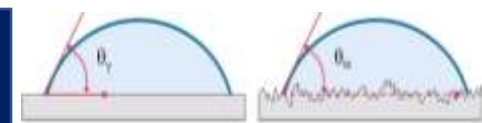


Functionalities of laser-induced nanostructures

- (a) Structural colors and optical marking
- (b) Plasmonic colors
- (c) Volume nanostructuring with Bessel beams for waveguide Bragg gratings
- (d) Encoding and data storage in nanogratings domains embedded in glass
- (e) Stress control using laser nanostructured domains
- (f) Biomimetic hierarchical structures
- (g) Superhydrophobic contact properties originating in hierarchical topographies
- (h) Bactericide properties of nanostructured surfaces

<https://doi.org/10.3390/nano10050864>

Challenge



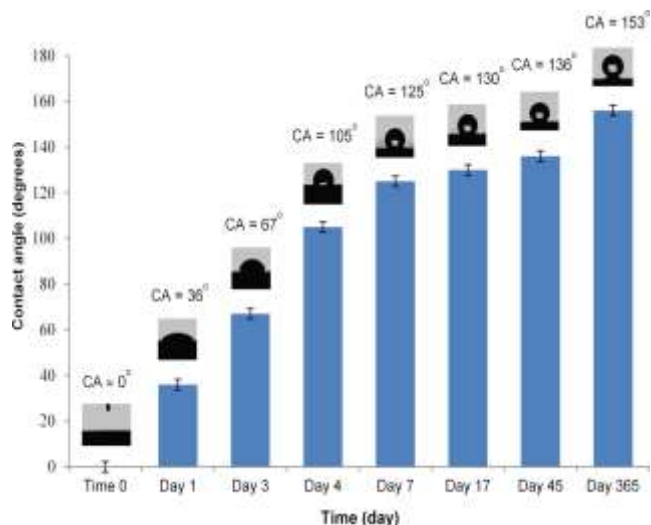
Challenge Wettability of laser textured surfaces

- Changes over time

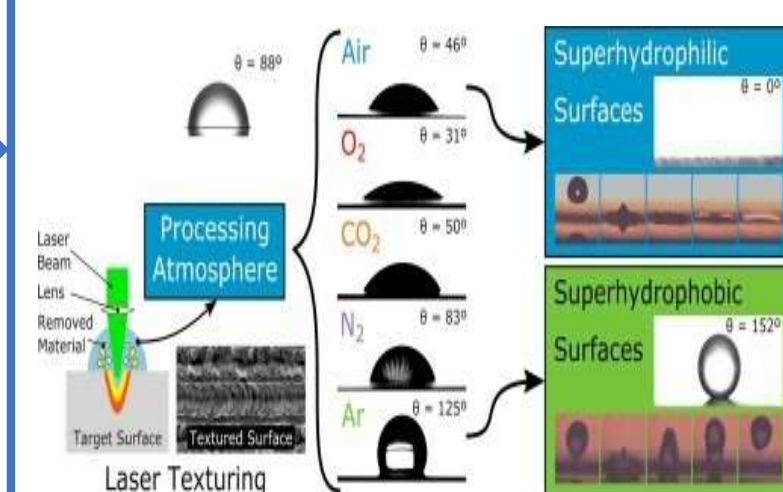
- Changes from superhydrophilic to superhydrophobic

- The existing wetting models is difficult to account for this wetting mechanism;
 - Wenzel and Cassie-Baxter

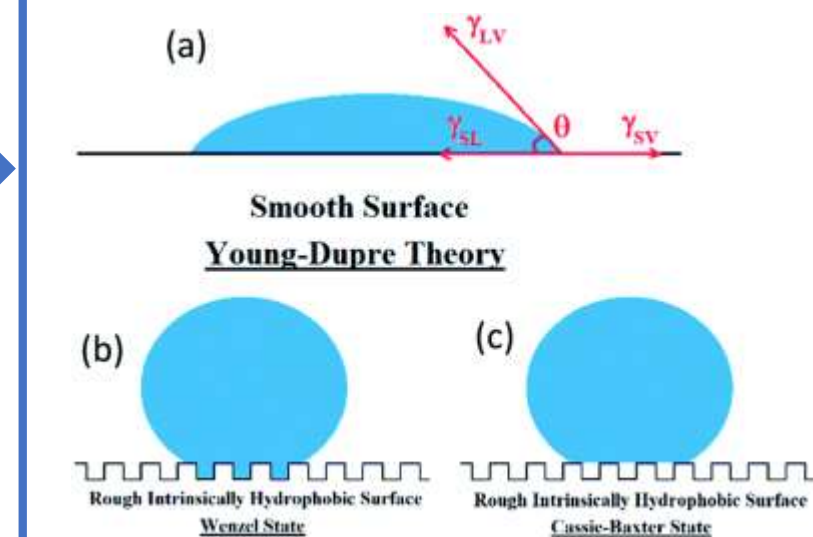
Wettability changes with time



Alternate hydrophobic and hydrophilic properties

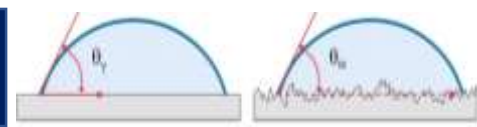


Existing wetting model



P. Bizi-bandoki et al. Time dependency of the hydrophilicity... Appl. Surf. Sci., 273 (2013), pp. 399-407

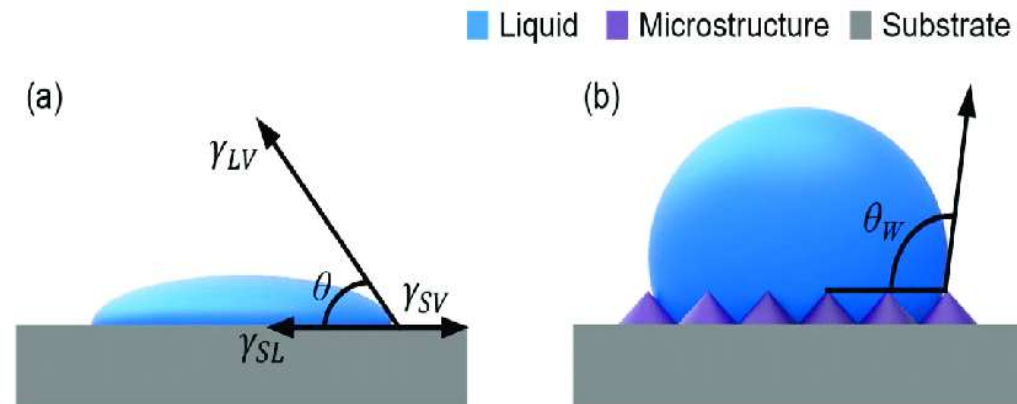
Objective



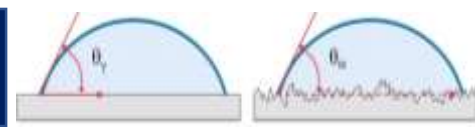
Develop a more realistic wettability model accounting for the changes in surface structure and wettability

First: We will start with simulation of water drop behavior on flat surface using CFD approach

Second: We introduce surface relief to understand the wetting dynamics.



Computation Fluid Dynamic (CFD) Approach



Navier Stokes Equation (Incompressible, time dependent)
(Solve Fluid Flow)

$$\nabla \cdot \vec{u} = 0$$

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right) = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{F}$$

Coupled with

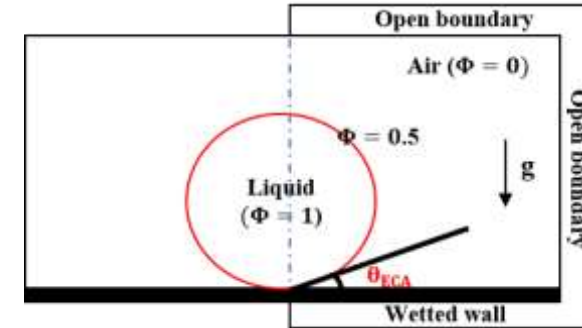
Level Set Method (Interface Tracking Method)

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

$$\begin{cases} \rho = \rho_1 + (\rho_2 - \rho_1)\phi \\ \mu = \mu_1 + (\mu_2 - \mu_1)\phi \end{cases}$$

Olsson, E.; Kreiss, G. A Comput. Phys. 2005, 210, 225–246.

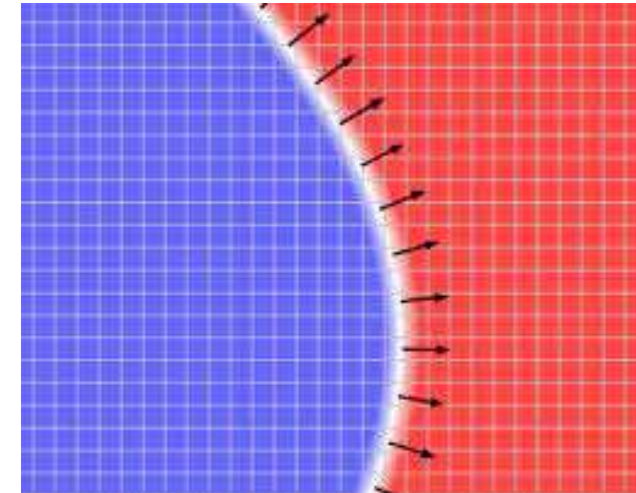
Simulation Set-up

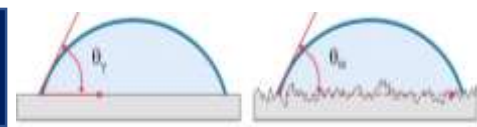


Schematic diagram of 2D axisymmetric setup

Computed by the finite-element solver discretized in
COMSOL Multiphysics 5.6 software

Comsol multiphysics CFD module user guide (version 5.6), COMSOL, 2020, 208–265.





Water Droplet on Glass

Properties

Diameter of droplet = 2 mm

Impact velocity = 0.52 m/s

Equili. Contact Angle = 106°

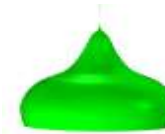
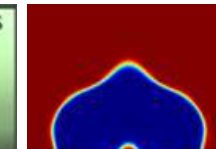
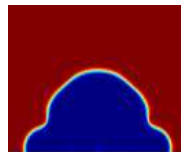
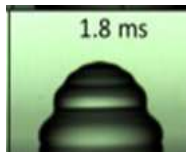
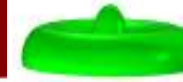
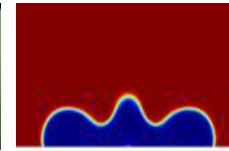
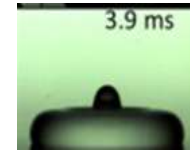
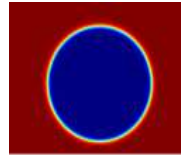
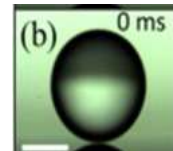


Experiment

Simulation 2D & 3D

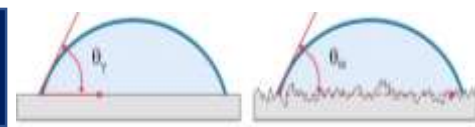
Experiment

Simulation 2D & 3D



Omeje, Ilemona S., et. al. Applied Surface Science Advances 9 (2022).

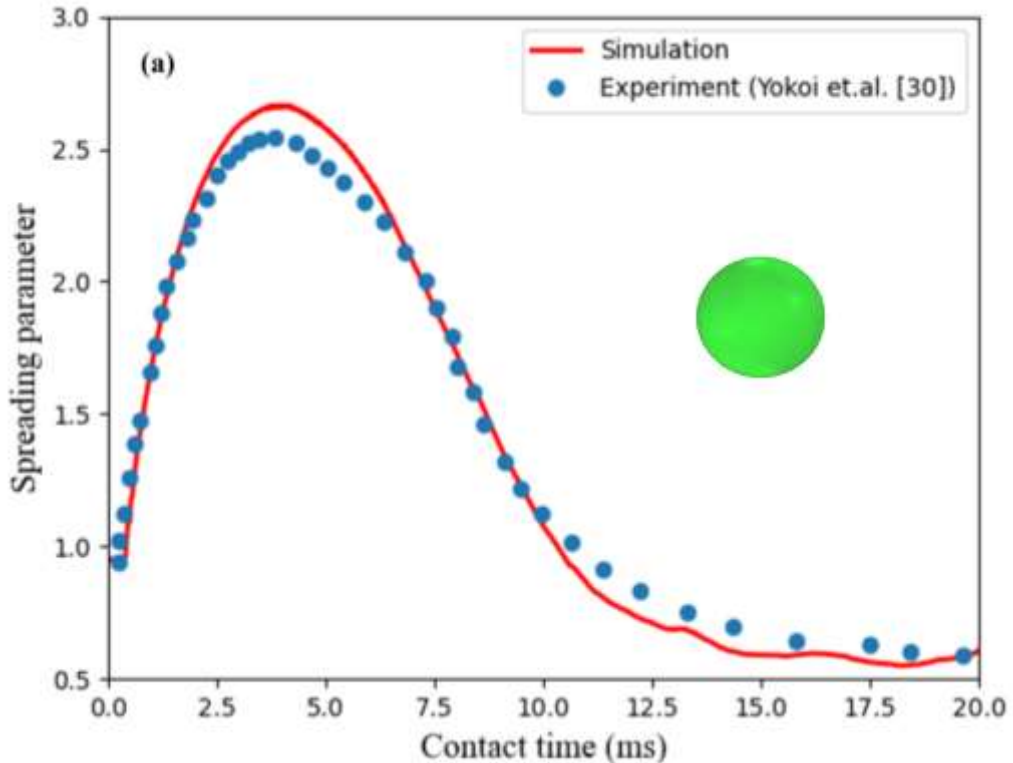
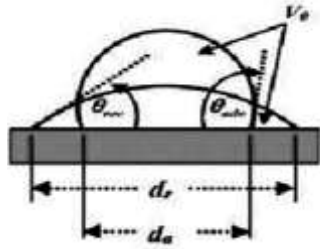
Model Validation: Spreading Parameter



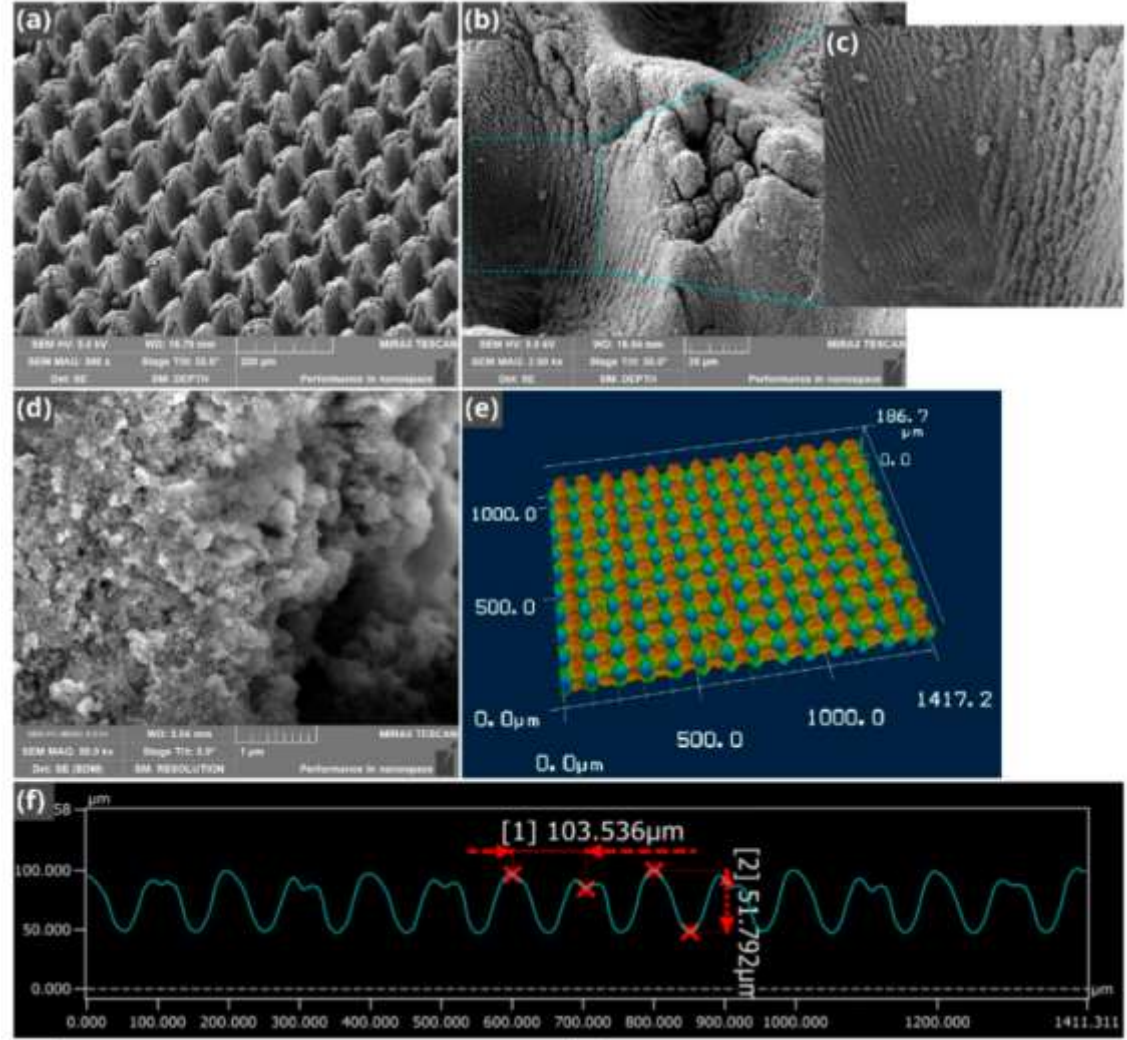
Spreading Parameter

Spreading Parameter $\beta^* = \frac{d_a}{D}$

Here d_a = diameter of droplet
 D = Initial diameter of droplet

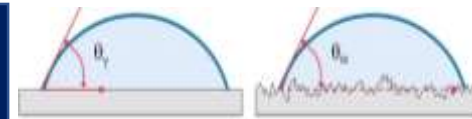


Surface of Superwicking Ti-6Al-4V Alloy Material Fabricated by Femtosecond Laser



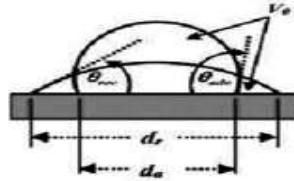
Omeje, Ilemona S., et al. Applied Surface Science Advances 9 (2022).

<https://doi.org/10.3390/nano11040899>

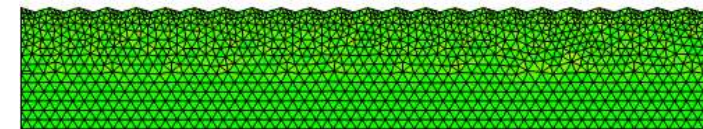
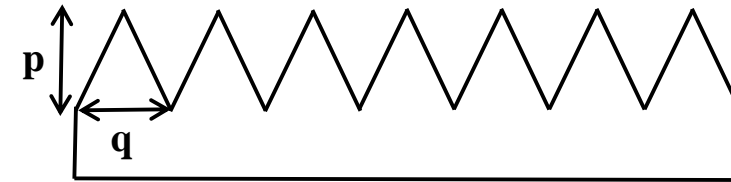


Performed wettings studies:

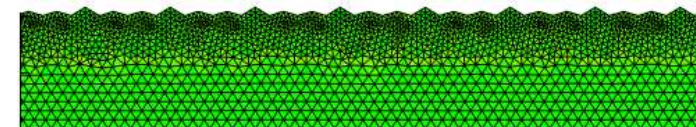
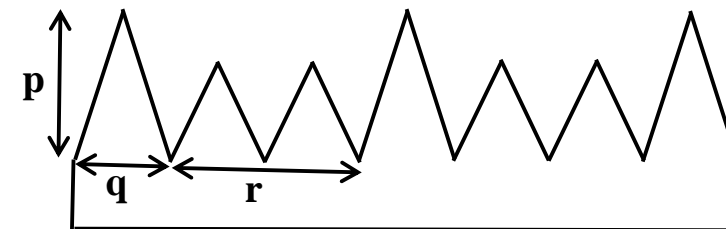
1. Plain **Ti-6Al-4V Surface**



2. Triangular relief **Ti-6Al-4V Surface**

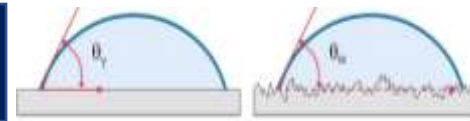


3. One with 2 periods and height



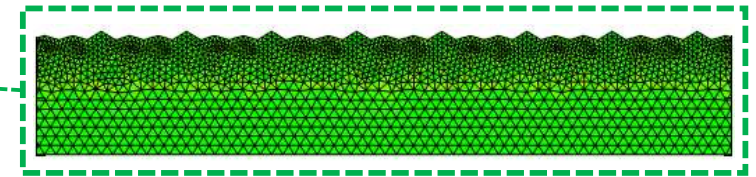
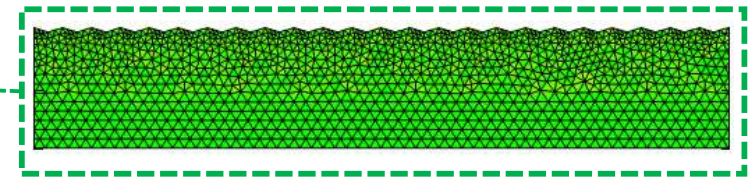
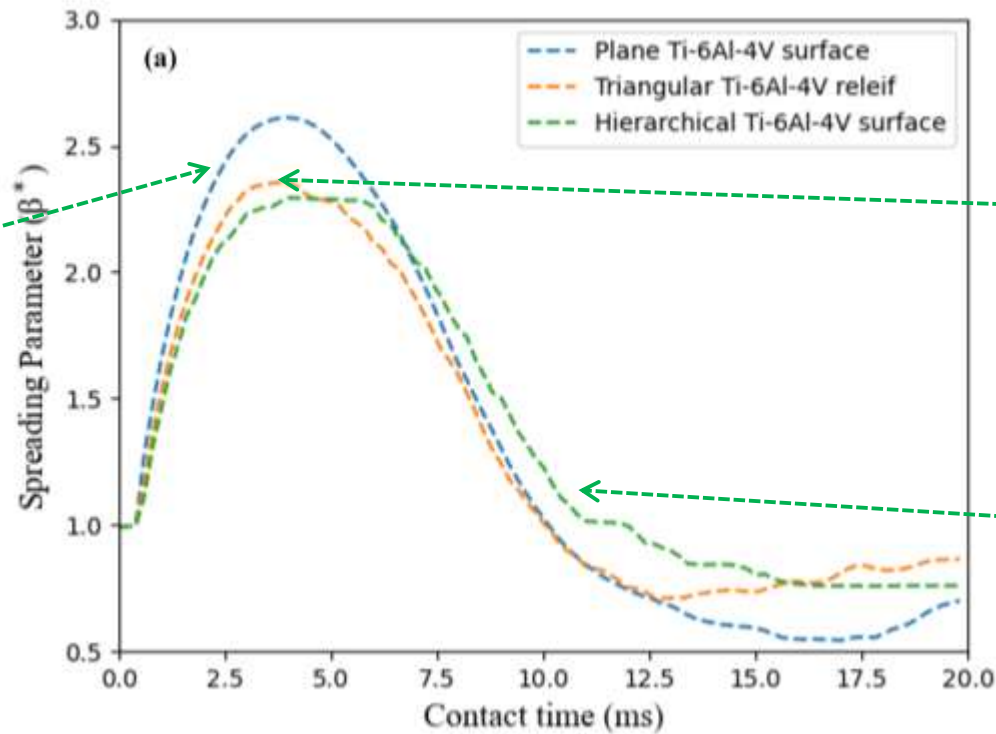
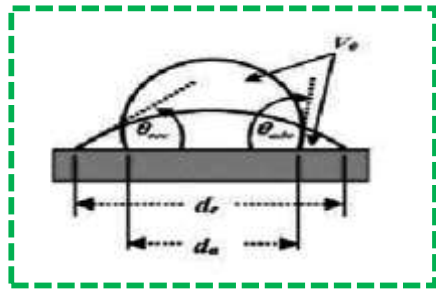
Explore the spreading parameter

CFD Results: Hierarchical Reliefs



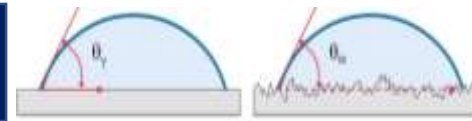
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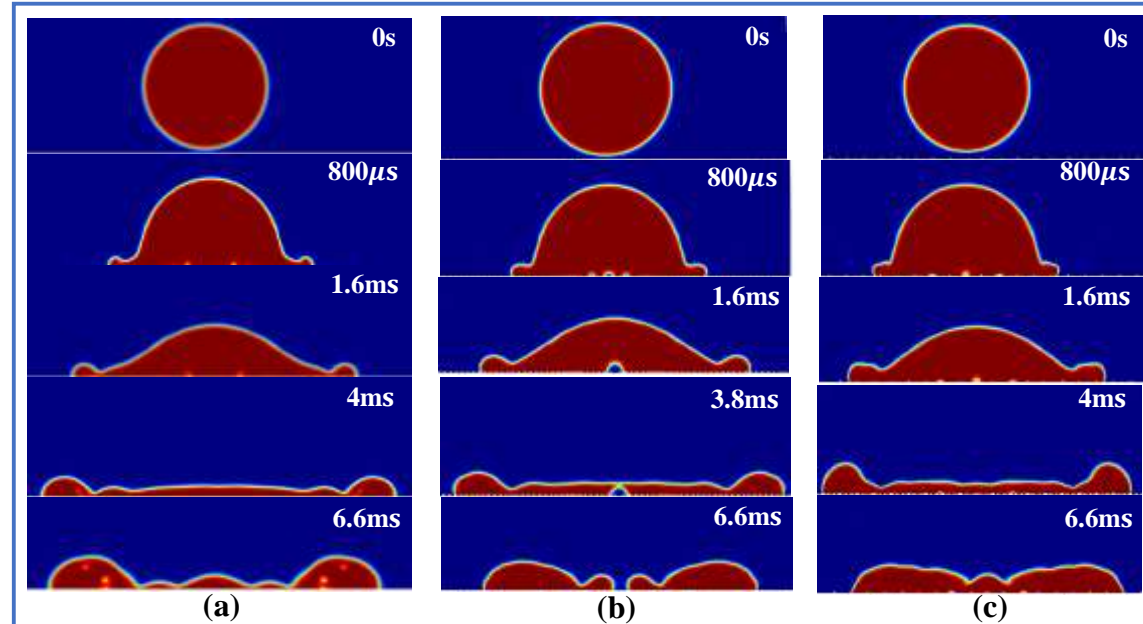
Omeje, Ilemona S., et. al. Applied Surface Science Advances 9 (2022).

CFD Results: Effect of Velocity and Viscosity



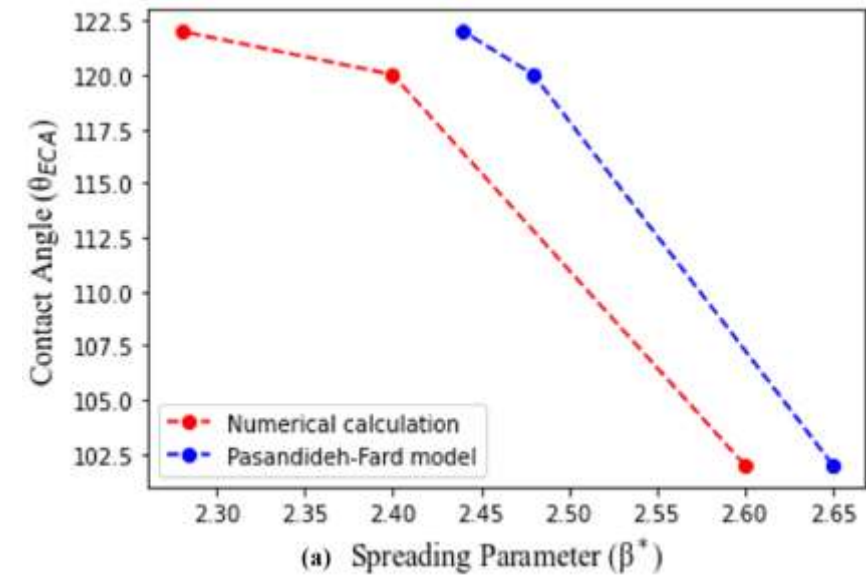
Snapshot of water impact on (a) **solid**, (b) **triangular**, and (c) **hierarchical Ti-6Al-4V alloy surface** at different time scale

Velocity of Impact = 1m/s
 $\theta_{ECA} = 96^\circ$



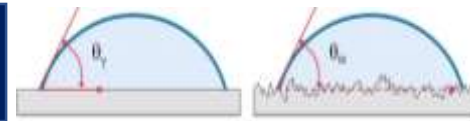
Maximum β^* of the current study and that of the analytical solution.

Surfaces	Max. β^* (current study)	Analytical solution [41]
Plain Ti-6Al-4V	2.60	2.65
Triangular Ti-6Al-4V	2.40	2.48
Two-period reliefs Ti-6Al-4V	2.28	2.44

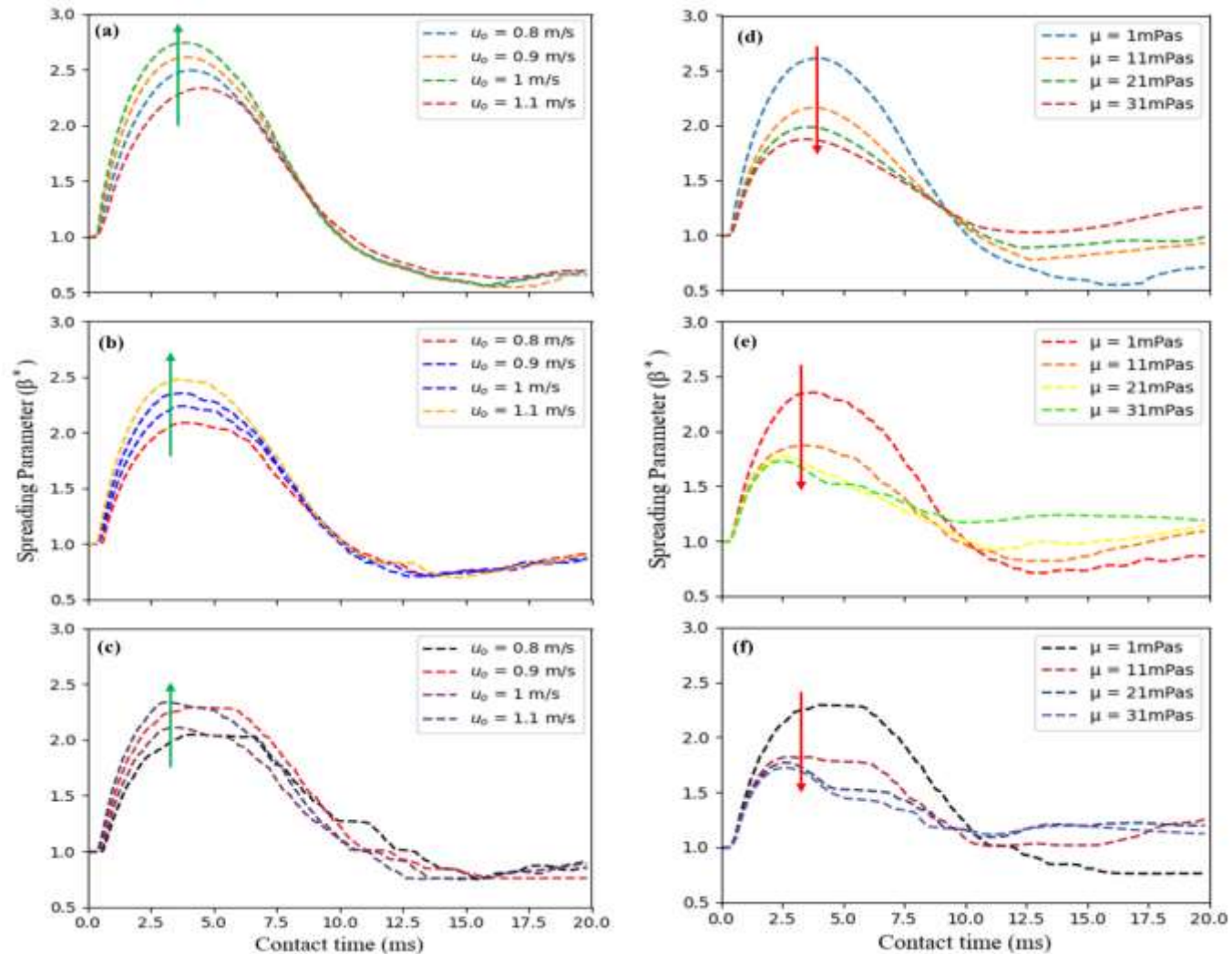


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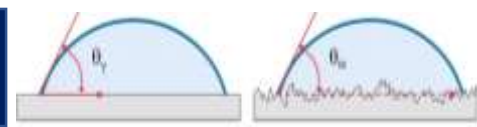
CFD Results: Effect of Velocity and Viscosity



Effect of velocity and viscosity of droplet



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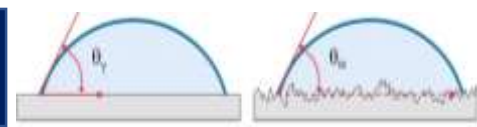


Summary

- Triangular surface reliefs alone are probably not well suitable for the increase in wettability properties, but rather two-period provide additional droplet capturing effects and are more promising for the wettability control.

Work in Progress

- **Multi-scale numerical approach such as the reactive MD (molecular dynamics) method to model** physico-chemical changes induced by laser.



**THANK YOU
FOR YOUR
ATTENTION**