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

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

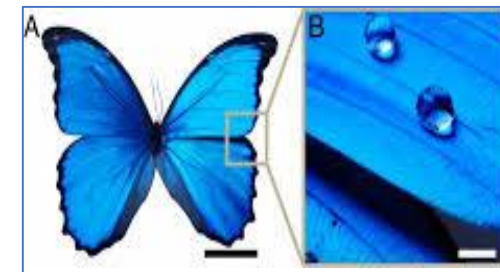
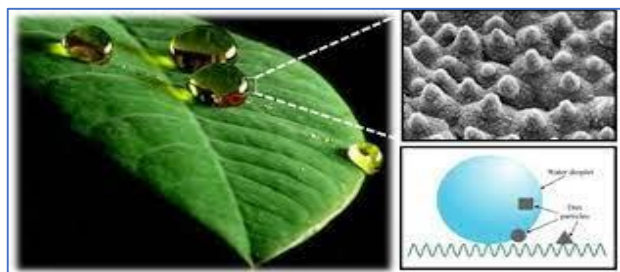
Ilemona S. Omeje<sup>1</sup>, Patrick Ganster<sup>2</sup> and Tatiana Itina<sup>1</sup>

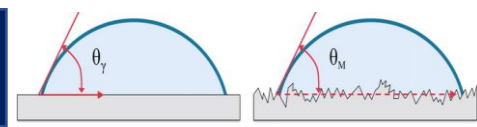
<sup>1</sup>*Laboratoire Hubert Curien, UMR 5516, Université de Lyon/Université Jean Monnet, Saint-Etienne, France*

<sup>2</sup>*Laboratoire Georges Friedel, Ecole des Mines, Saint-Etienne, France*

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

October 6, 2022





**1** Motivation

**2** Challenge

**3** Objective

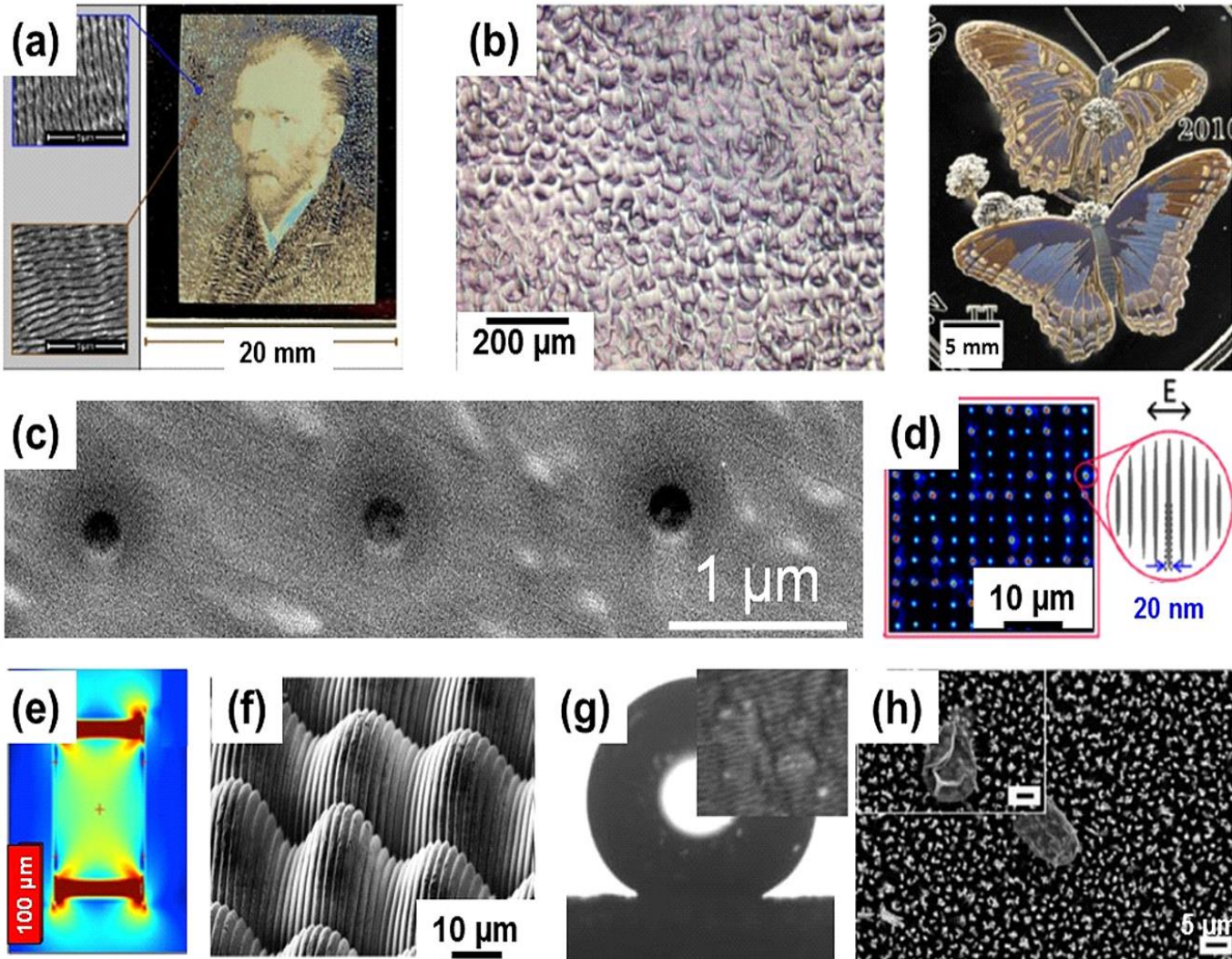
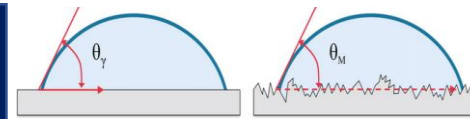
**4** CFD Approach

**5** Model Validation

**6** CFD Results

**7** Summary and Future Work

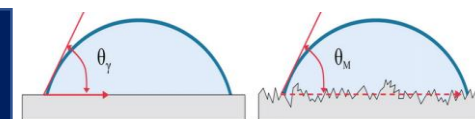
# Motivation



## 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>



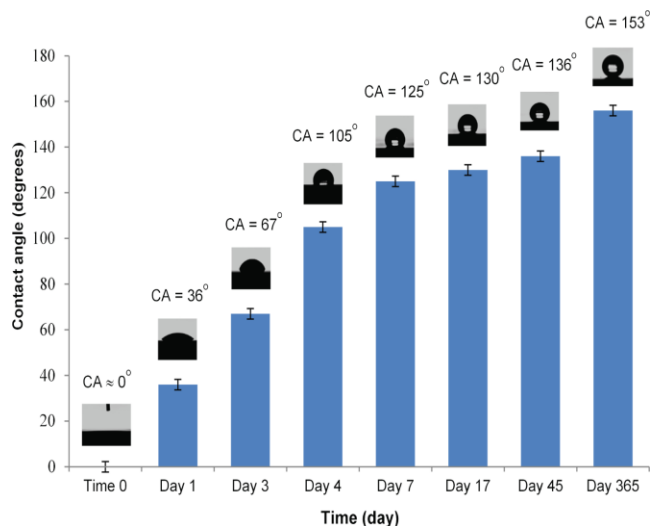
## Challenge Wettability of laser textured surfaces

- Changes over time

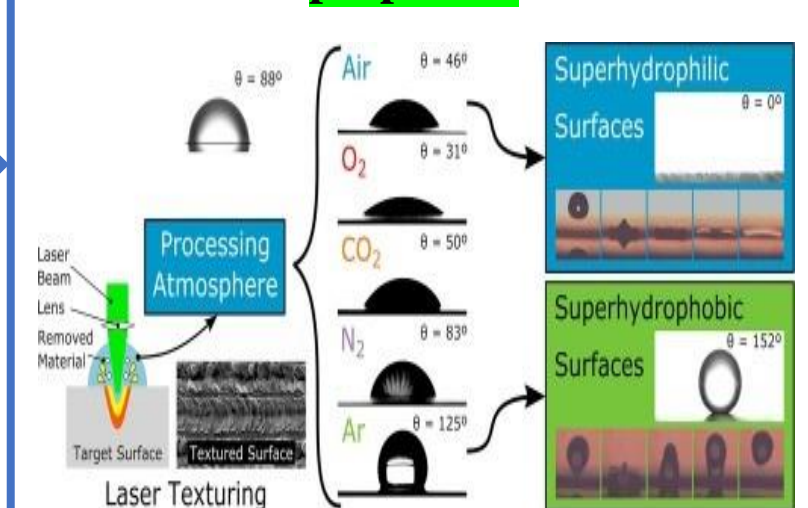
- Changes from superhydrophilic to superhydrophobic

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

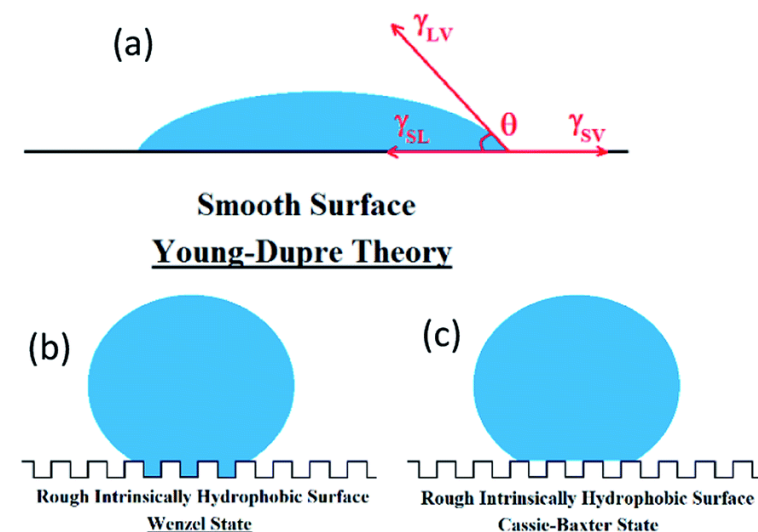
### Wettability changes with time

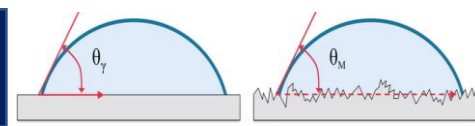


### Alternate hydrophobic and hydrophilic properties



### Existing wetting model

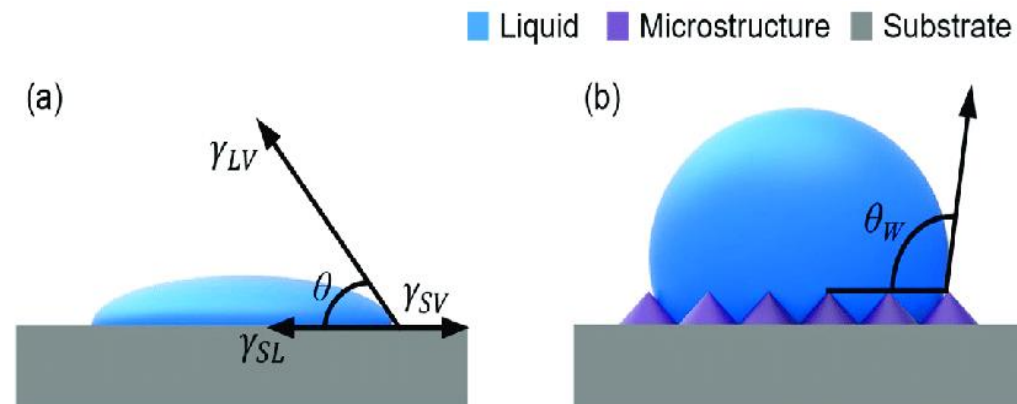




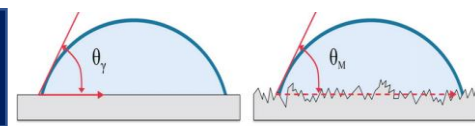
Develop a more realistic wettability model accounting for the changes in surface structure and wettability

**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**

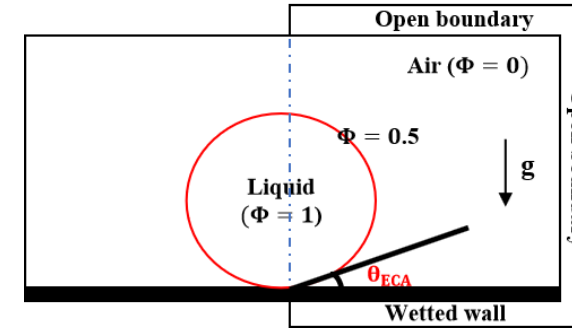
**Level Set Method (Interface Tracking Method)**

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

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

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

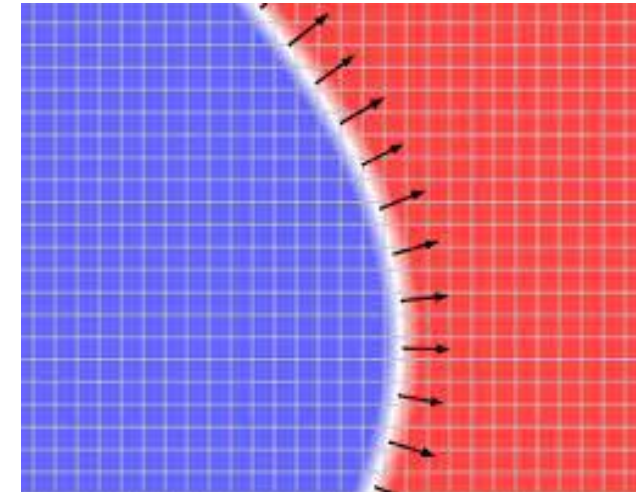
## Simulation Set-up

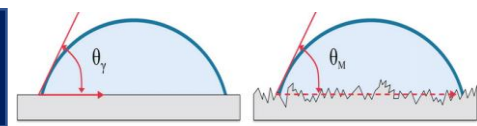


Schematic diagram of 2D axisymmetric setup

**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.*





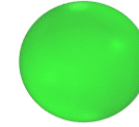
## Water Droplet on Glass

### Properties

Diameter of droplet = 2 mm

Impact velocity = 0.52 m/s

Equili. Contact Angle =  $106^\circ$

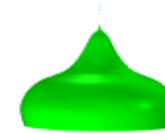
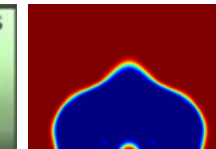
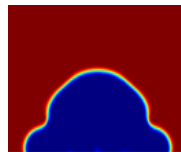
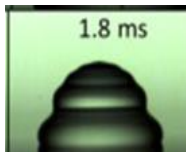
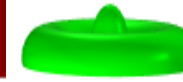
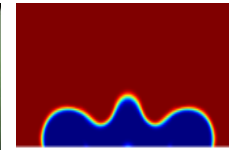
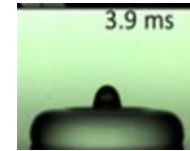
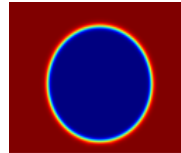
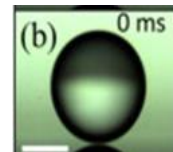


Experiment

Simulation 2D & 3D

Experiment

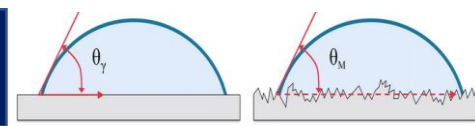
Simulation 2D & 3D



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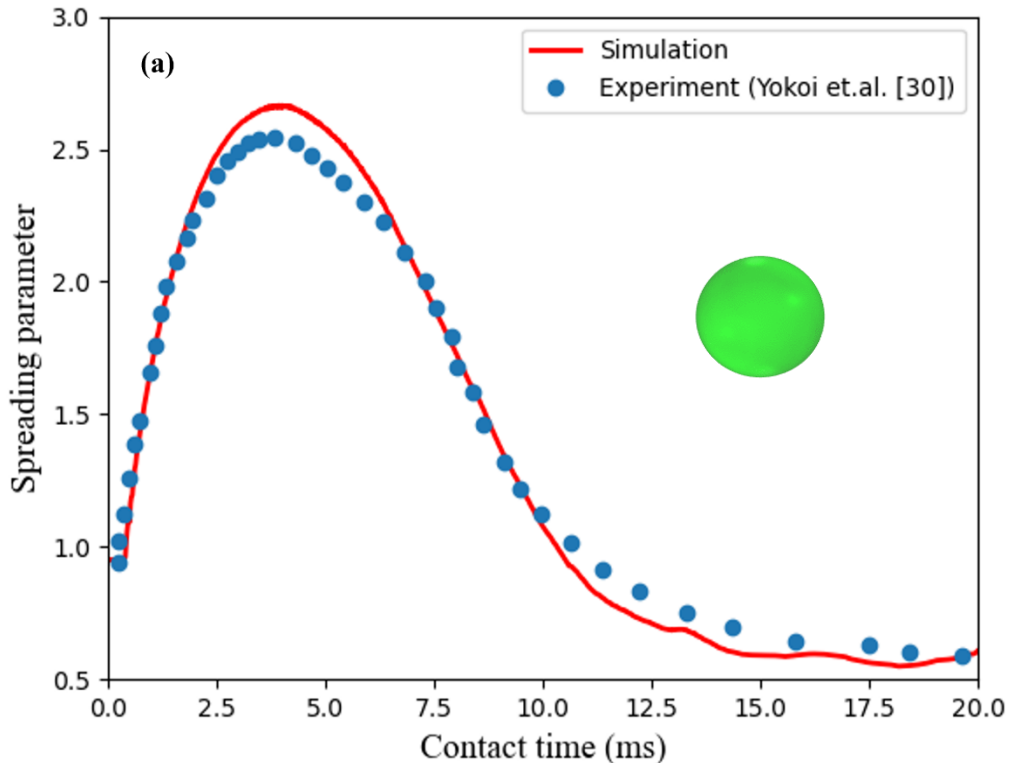
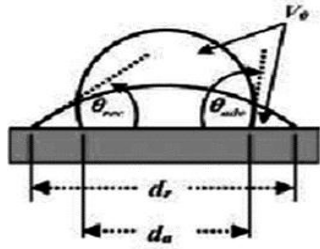
# Model Validation: Spreading Parameter



## Spreading Parameter

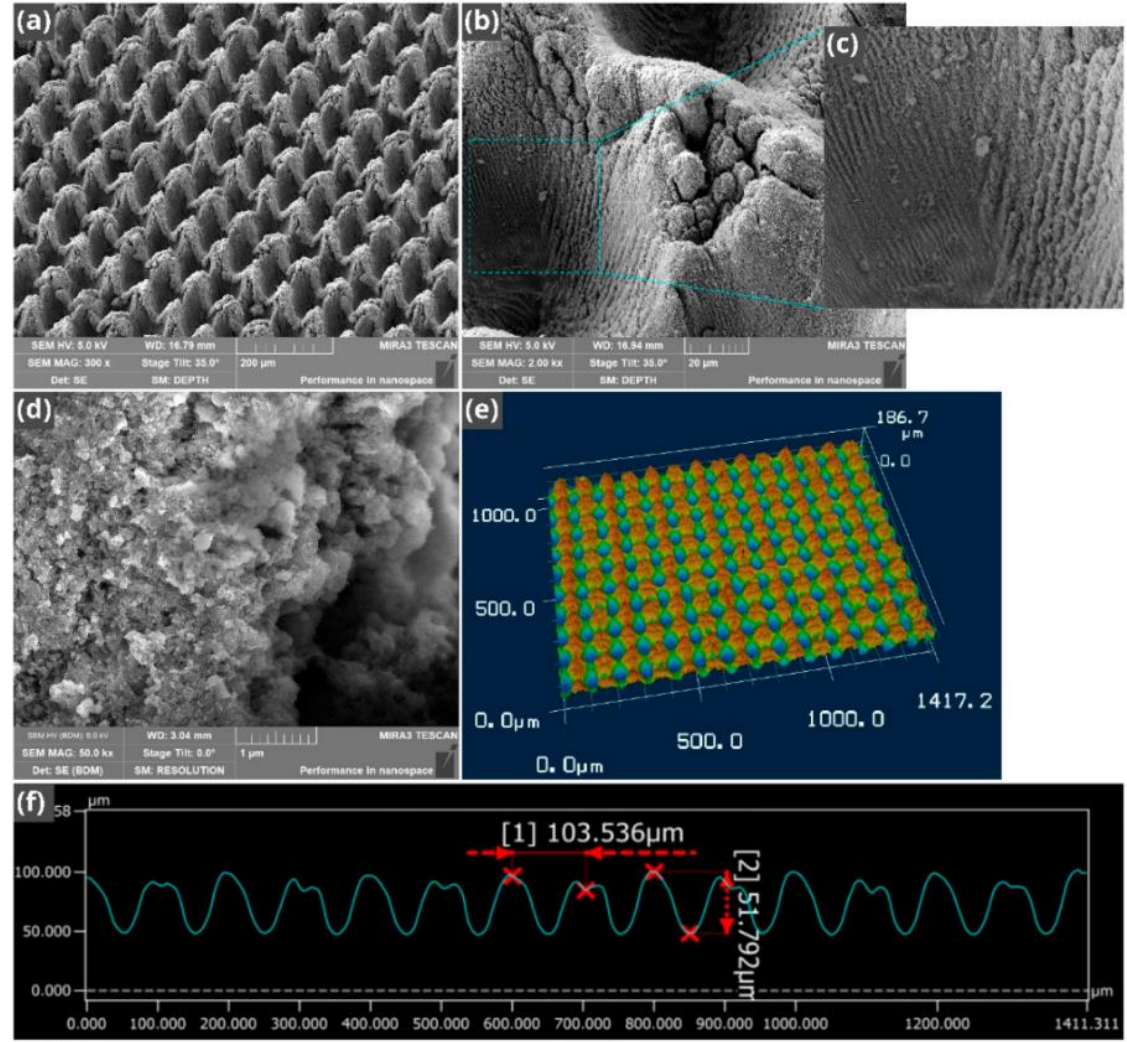
**Spreading Parameter  $\beta^* = \frac{d_a}{D}$**

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

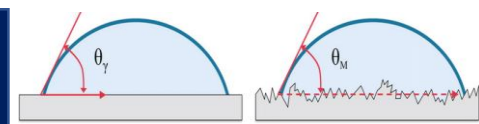


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## Surface of Superwicking Ti-6Al-4V Alloy Material Fabricated by Femtosecond Laser

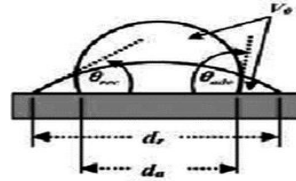


<https://doi.org/10.3390/nano11040899>

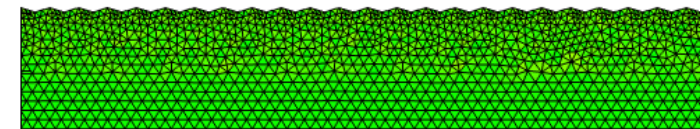
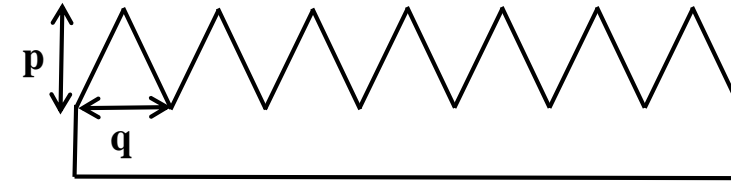


## Performed wettings studies:

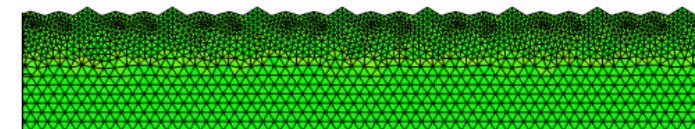
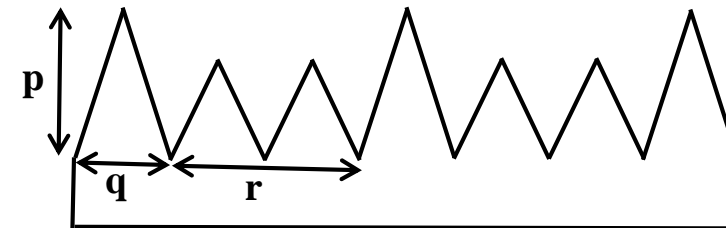
1. Plain **Ti-6Al-4V Surface**



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

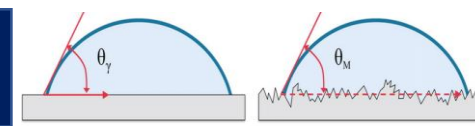


3. One with 2 periods and height



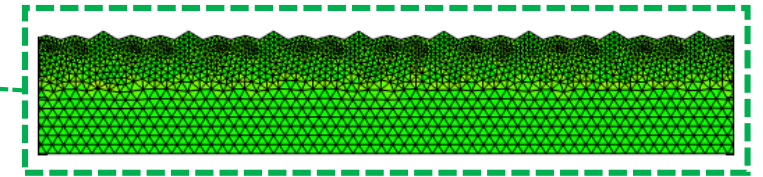
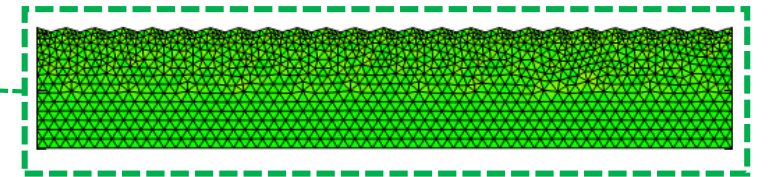
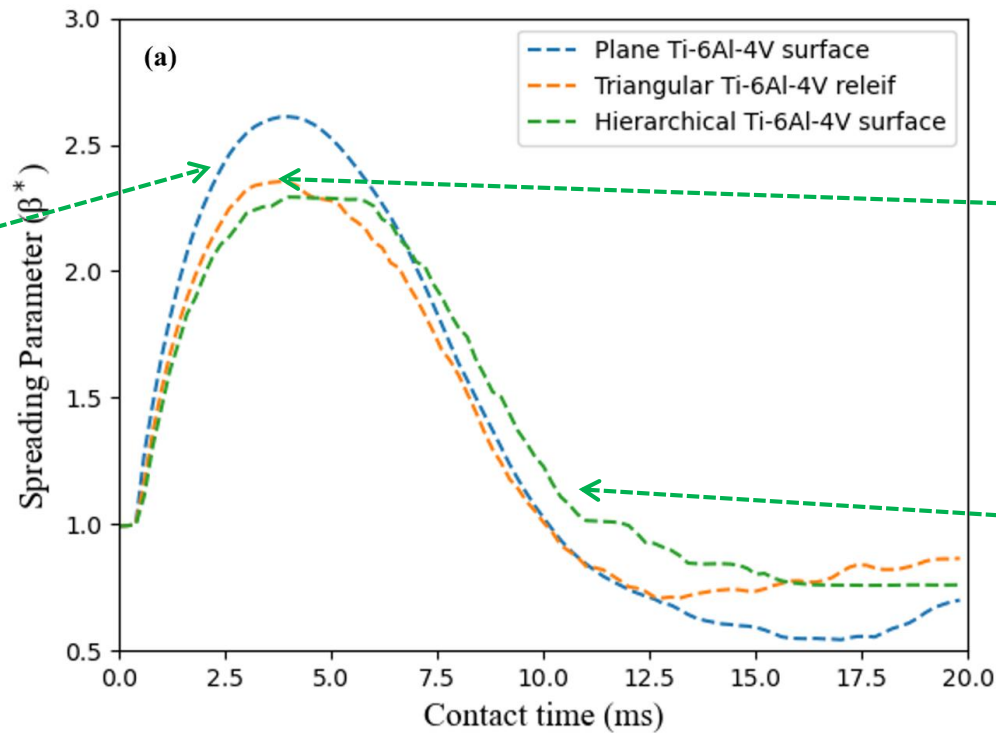
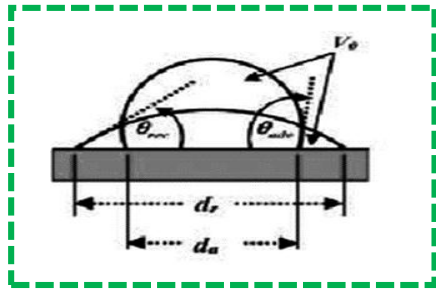
**Explore the spreading parameter**

# CFD Results: Hierarchical Reliefs



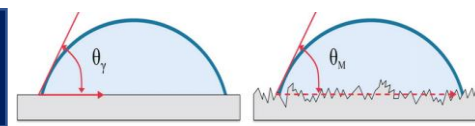
## Spreading Parameter

**Spreading Parameter  $\beta^* = \frac{d_a}{D}$**   
Here  $d_a$  = diameter of droplet  
 $D$  = Initial diameter of droplet



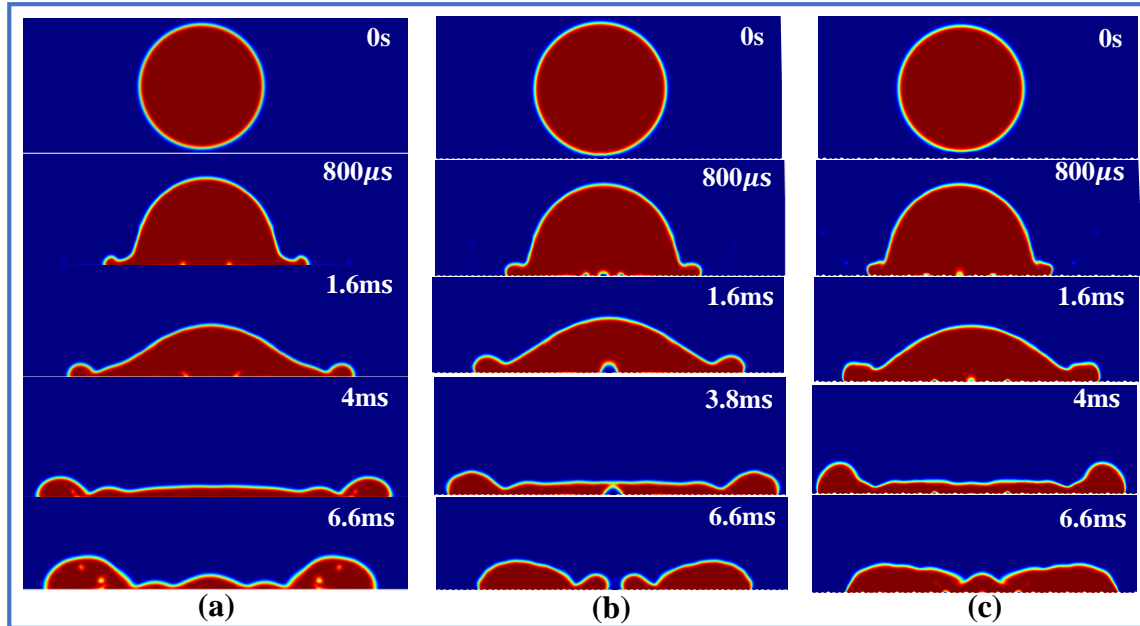
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# CFD Results: Effect of Velocity and Viscosity



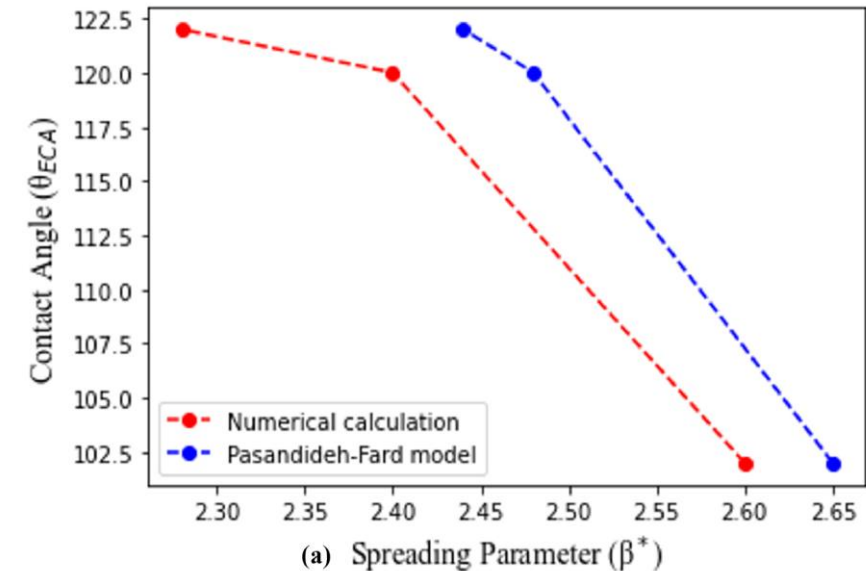
Snapshot of water impact on (a) **solid**, (b) **triangular**, and (c) **hierarchical Ti-6Al-4V alloy surface** at different time scale

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



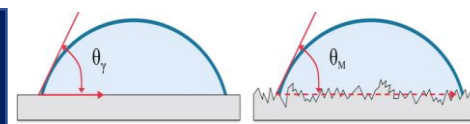
Maximum  $\beta^*$  of the current study and that of the analytical solution.

Surfaces	Max. $\beta^*$ (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

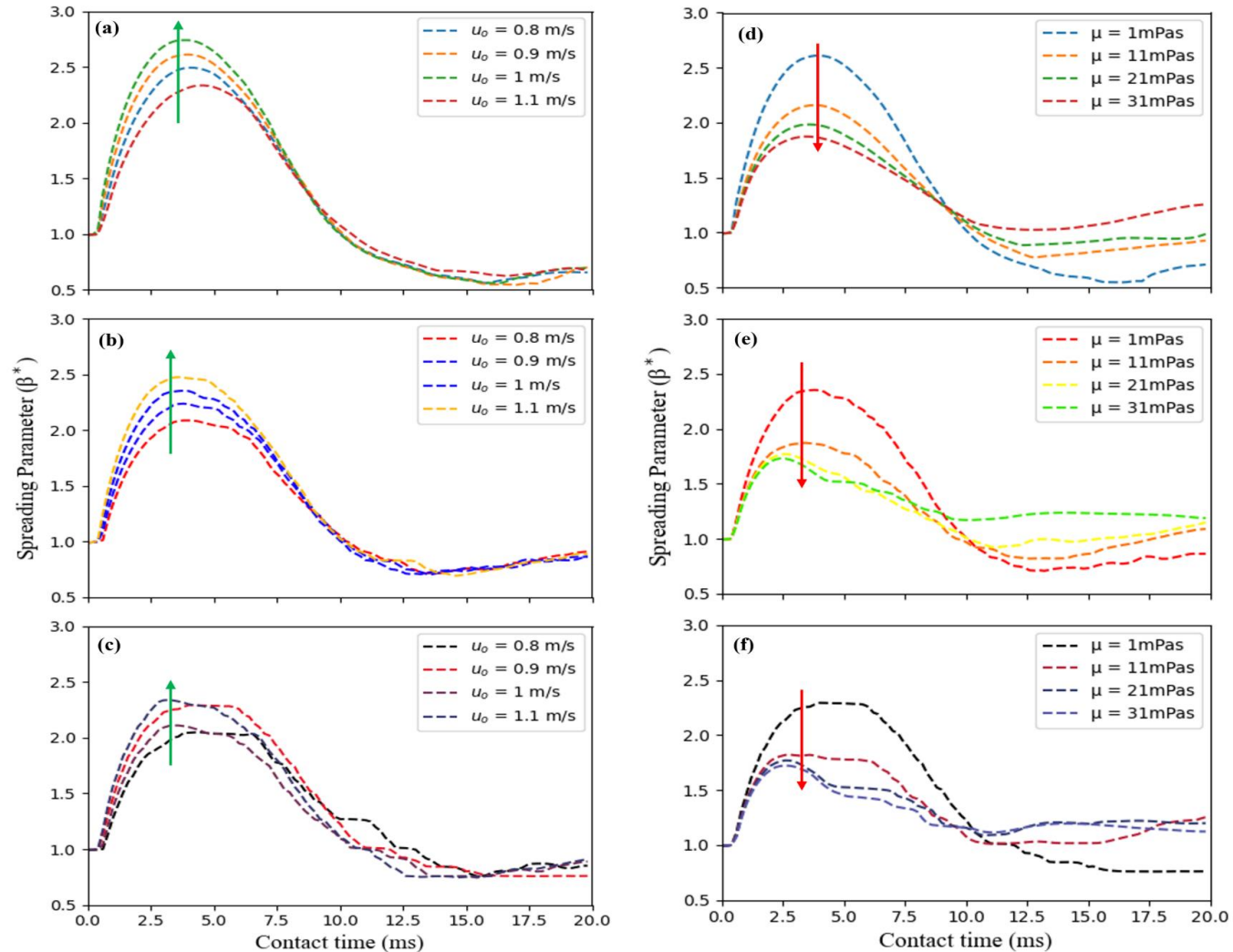


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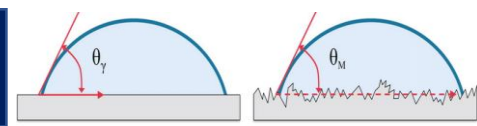
# CFD Results: Effect of Velocity and Viscosity



## Effect of velocity and viscosity of droplet



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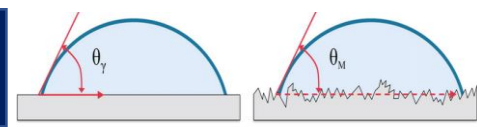


## Summary

- 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**