



HAL
open science

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

Ilemona Omeje, Patrick Ganster, Tatiana Itina

► To cite this version:

Ilemona Omeje, Patrick Ganster, Tatiana Itina. Multiscale Simulation of laser textured surface wettability: toward understanding the role of surface oxidation and molecular adsorption. 10th International Conference on Multiscale Materials Modeling, Baltimore, USA, MMM, Oct 2022, Baltimore, United States. ujm-04249988

HAL Id: ujm-04249988

<https://ujm.hal.science/ujm-04249988>

Submitted on 20 Oct 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



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

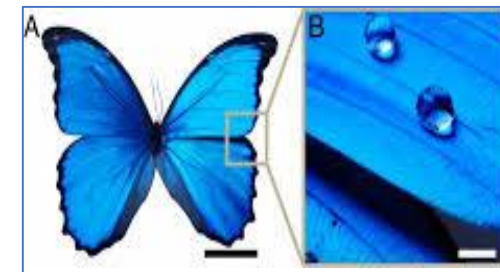
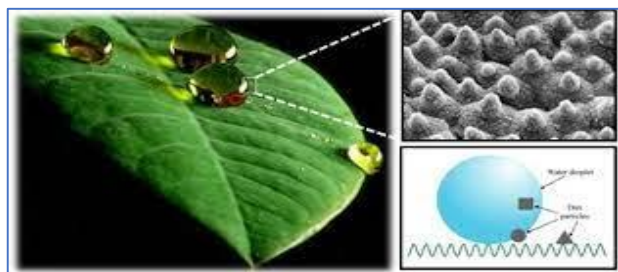
Ilemona S. Omeje¹, Patrick Ganster² and Tatiana Itina¹

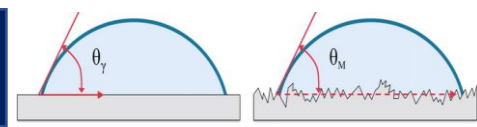
¹*Laboratoire Hubert Curien, UMR 5516, Université de Lyon/Université Jean Monnet, Saint-Etienne, France*

²*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

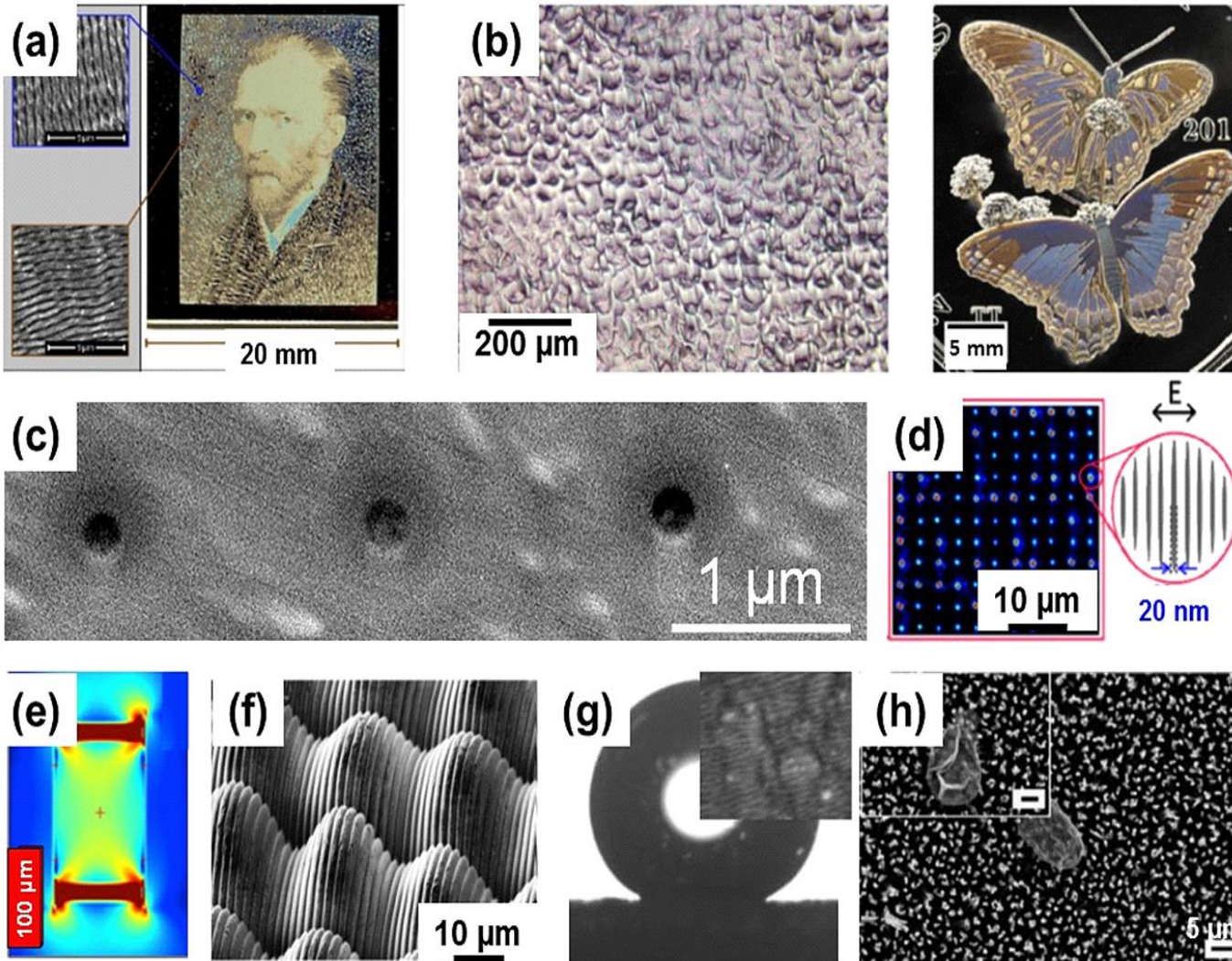
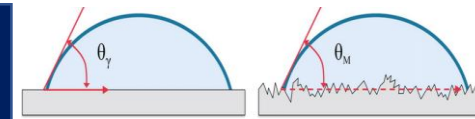
4 CFD Approach

5 Model Validation

6 CFD Results

7 Summary and Future Work

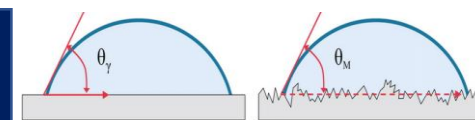
Motivation



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>



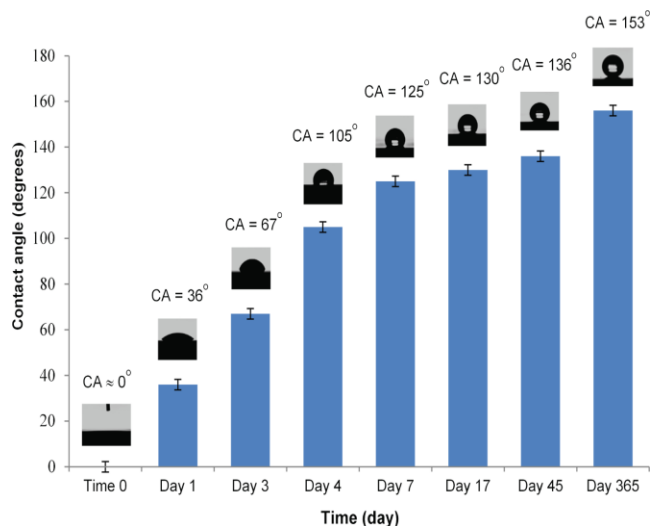
Challenge Wettability of laser textured surfaces

- Changes over time

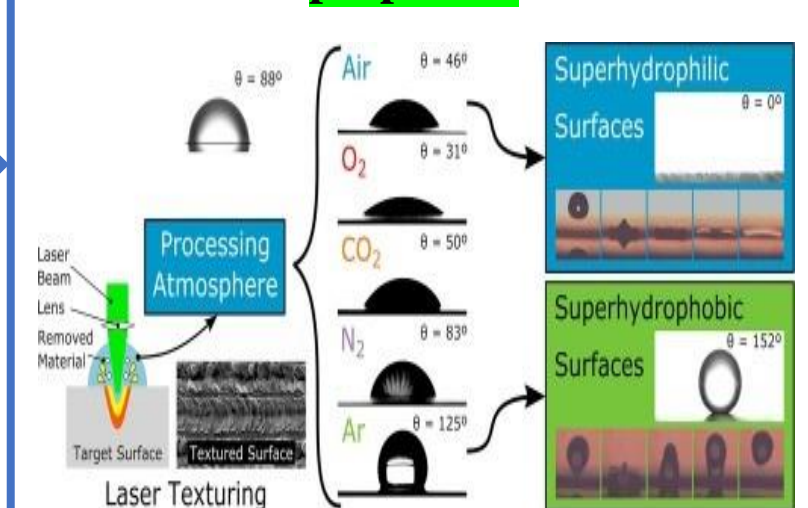
- Changes from superhydrophilic to superhydrophobic

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

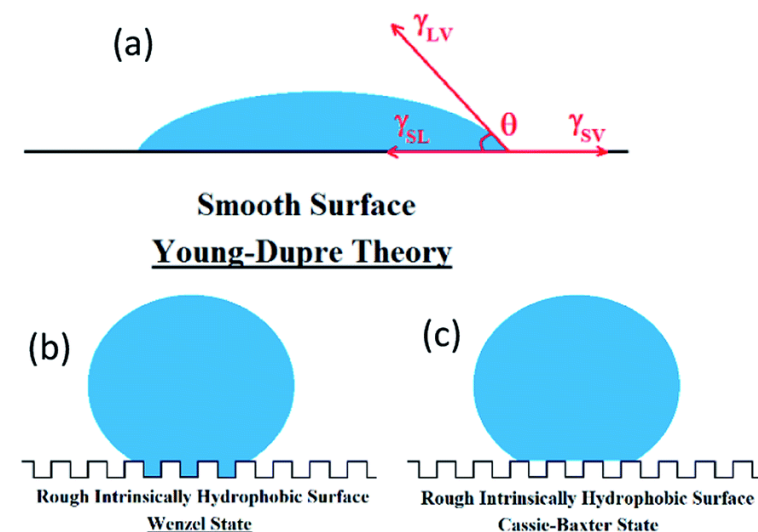
Wettability changes with time



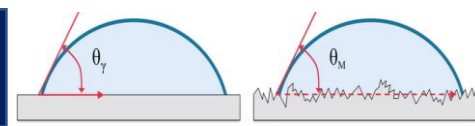
Alternate hydrophobic and hydrophilic properties



Existing wetting model



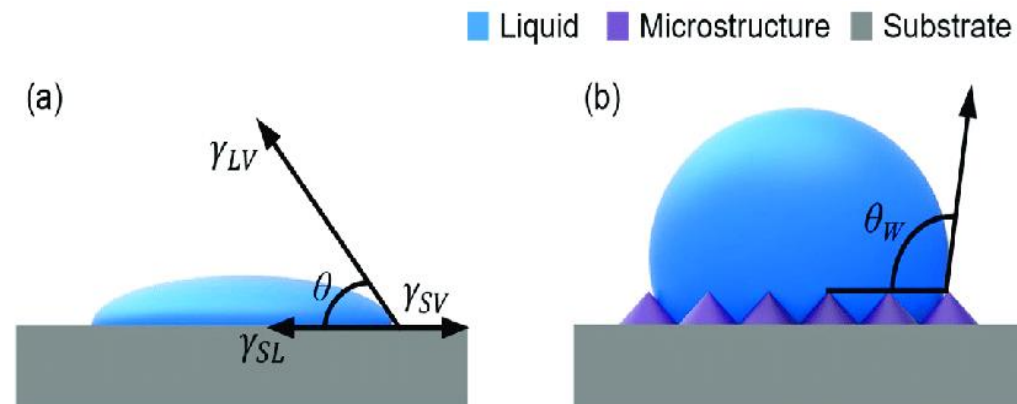
P. Bizi-bandoki et al. Time dependency of the hydrophilicity... Appl. Surf. Sci., 273 (2013), pp. 399-407



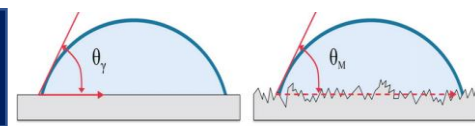
Develop a more realistic wettability model accounting for the changes in surface structure and wettability

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

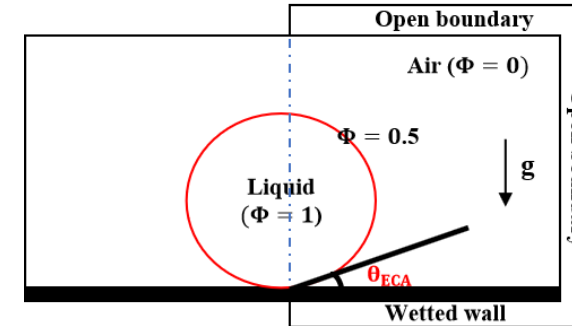
Level Set Method (Interface Tracking Method)

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

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

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

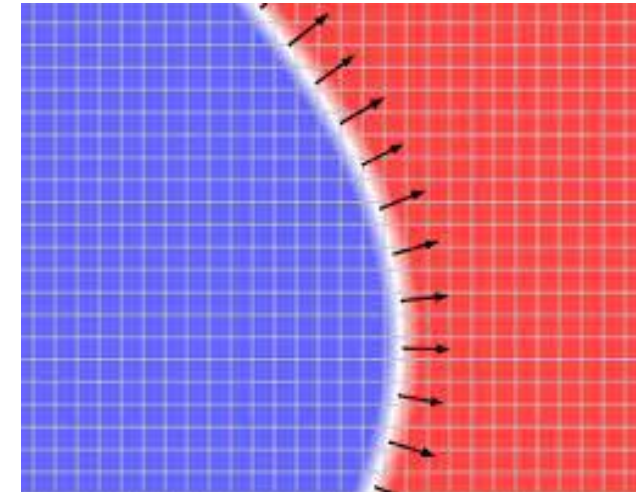
Simulation Set-up

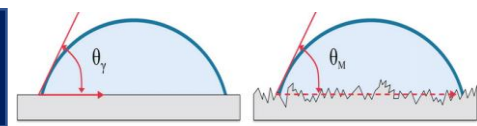


Schematic diagram of 2D axisymmetric setup

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.





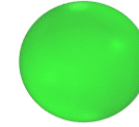
Water Droplet on Glass

Properties

Diameter of droplet = 2 mm

Impact velocity = 0.52 m/s

Equili. Contact Angle = 106°

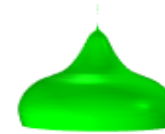
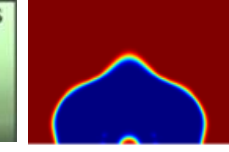
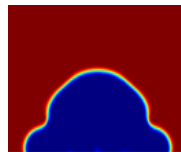
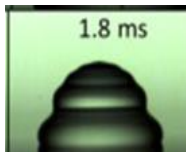
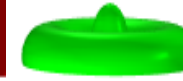
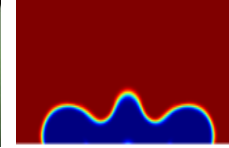
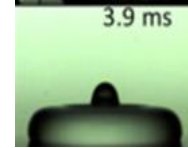
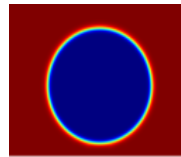
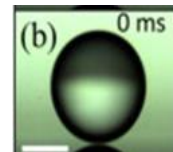


Experiment

Simulation 2D & 3D

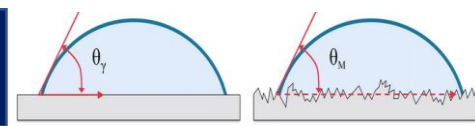
Experiment

Simulation 2D & 3D



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

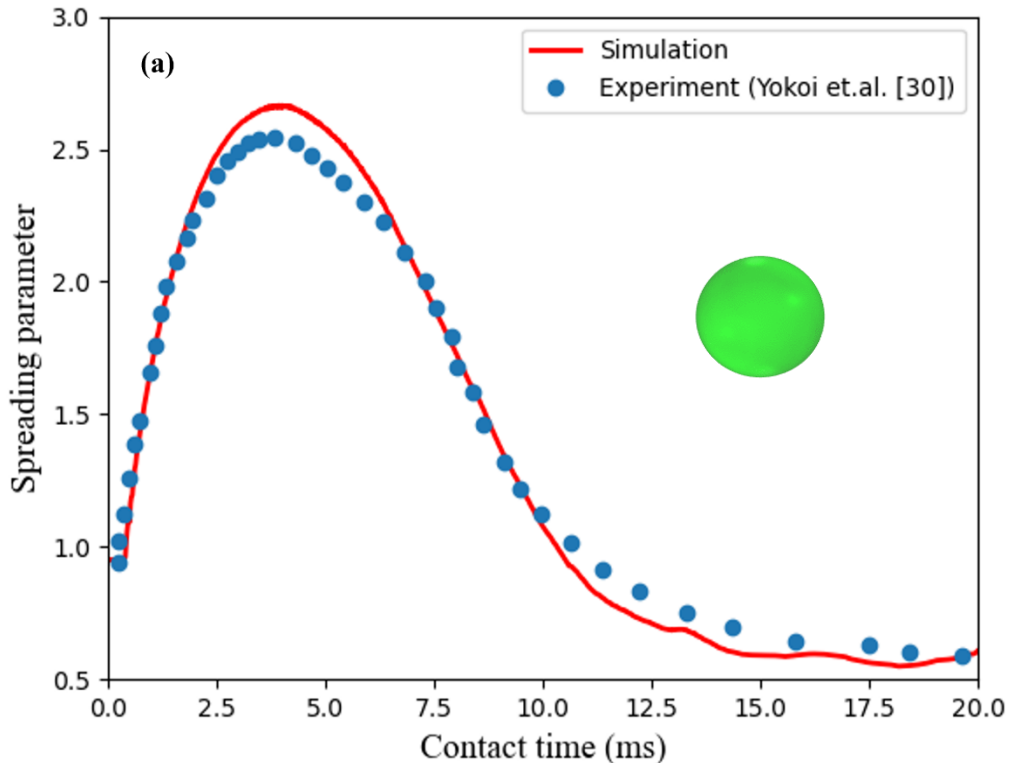
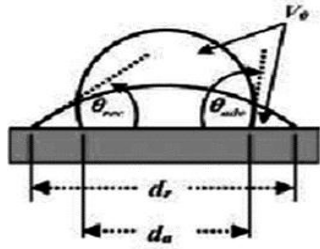
Model Validation: Spreading Parameter



Spreading Parameter

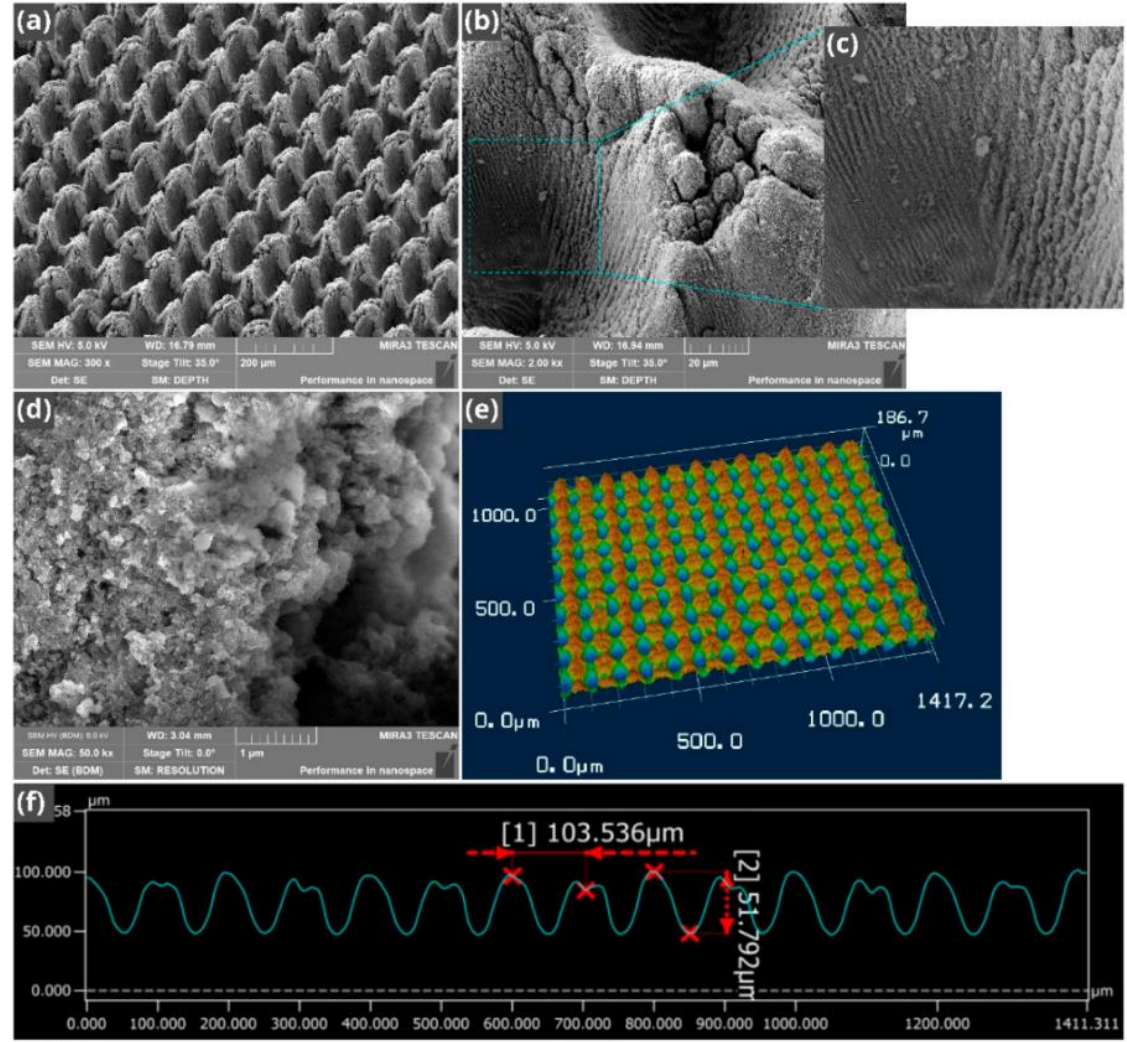
Spreading Parameter $\beta^* = \frac{d_a}{D}$

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

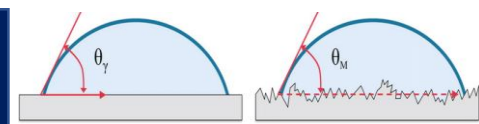


Omeje, Ilemona S., et. al. Applied Surface Science Advances 9 (2022).

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

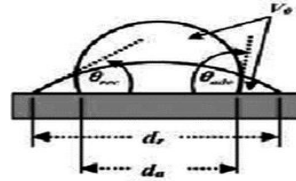


<https://doi.org/10.3390/nano11040899>

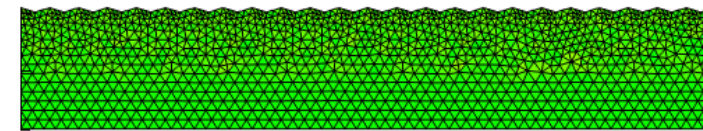
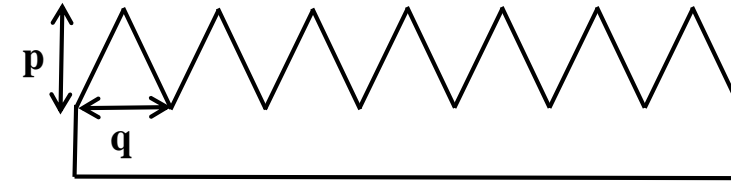


Performed wettings studies:

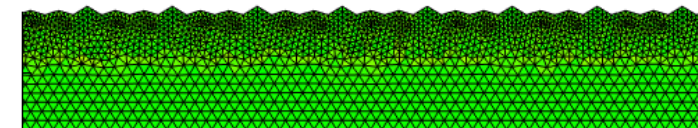
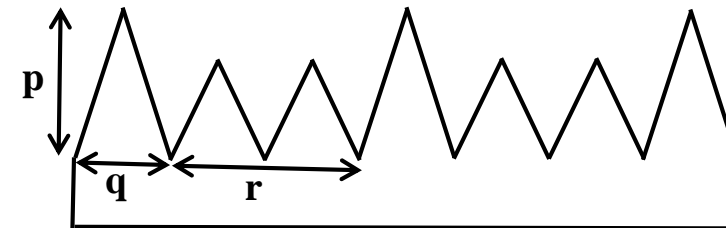
1. Plain **Ti-6Al-4V Surface**



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

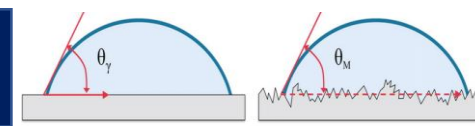


3. One with 2 periods and height



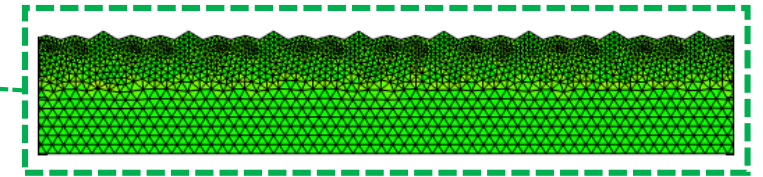
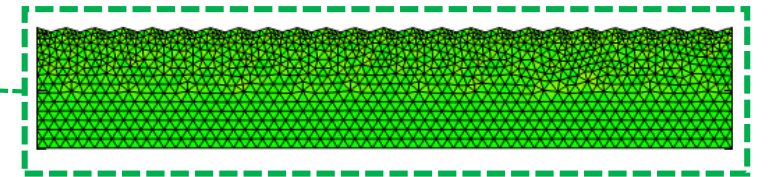
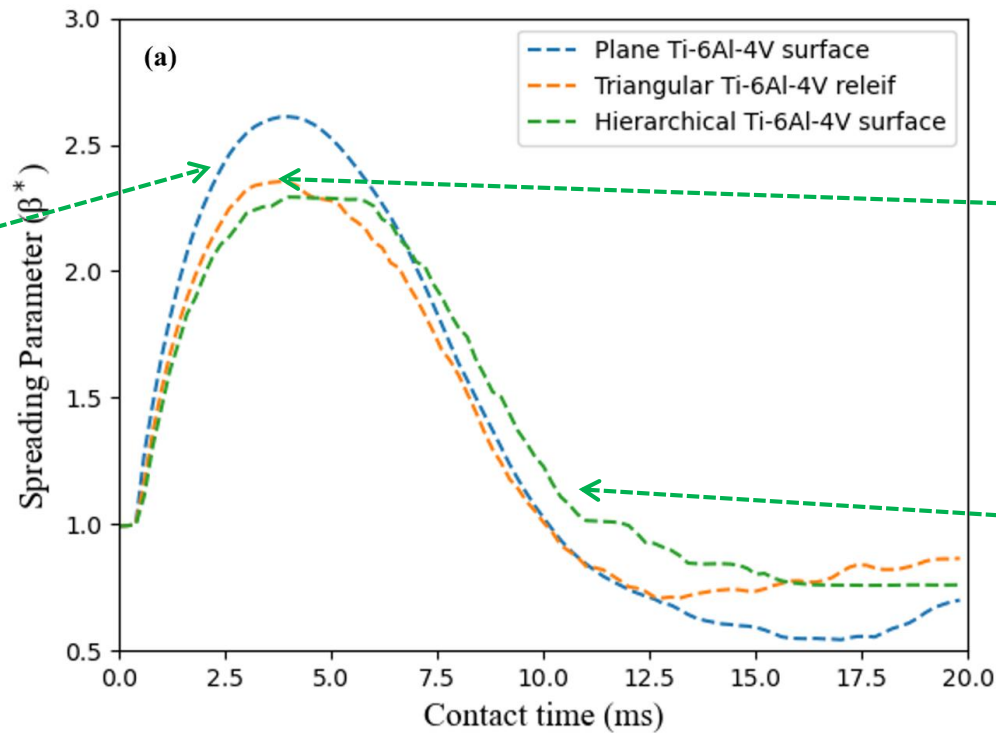
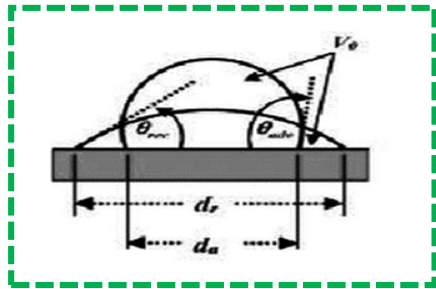
Explore the spreading parameter

CFD Results: Hierarchical Reliefs



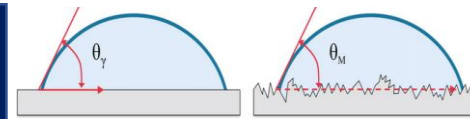
Spreading Parameter

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



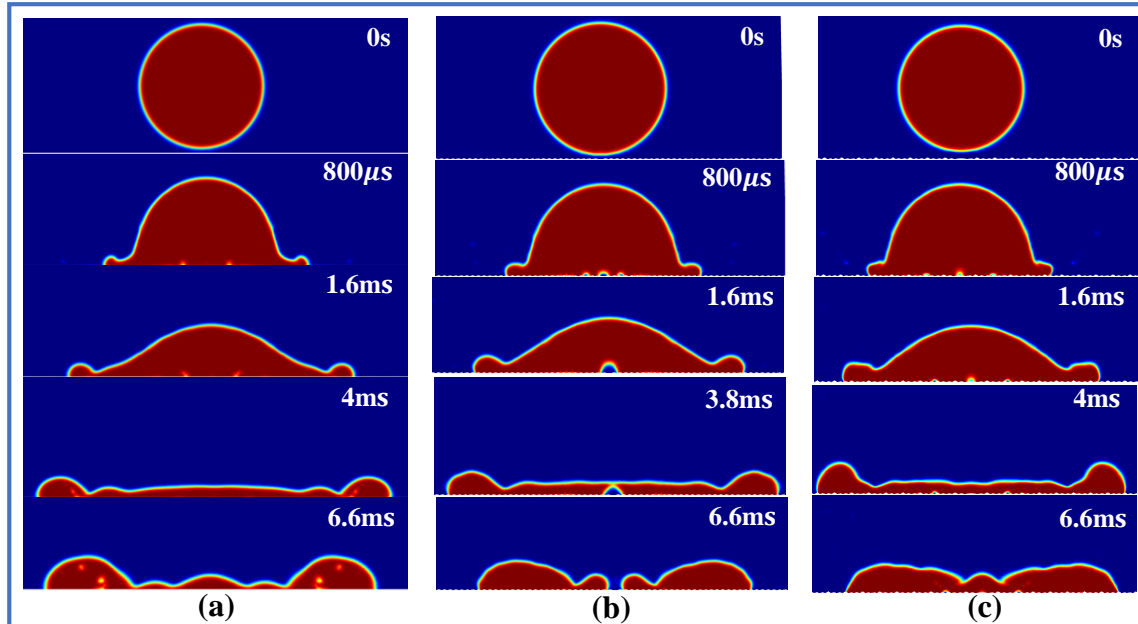
Omeje, Ilemona S., et al. Applied Surface Science Advances 9 (2022).

CFD Results: Effect of Velocity and Viscosity



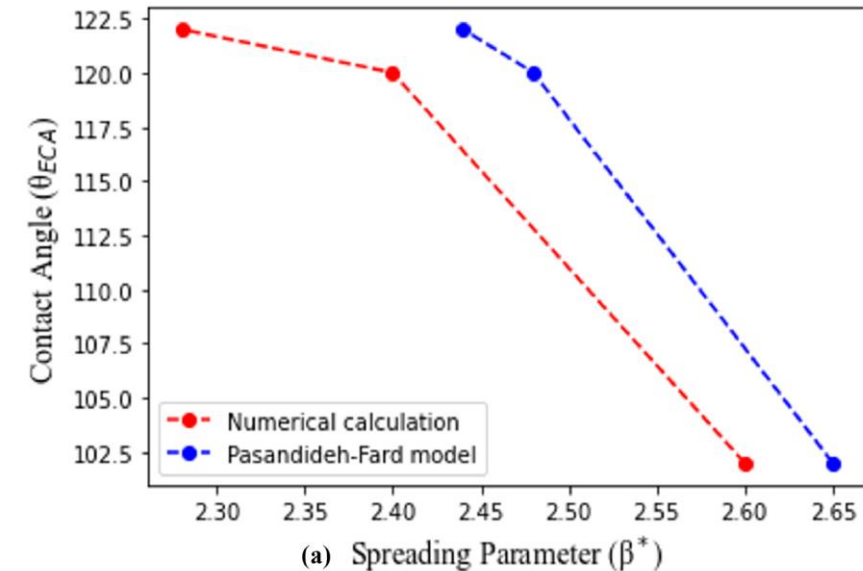
Snapshot of water impact on (a) **solid**, (b) **triangular**, and (c) **hierarchical Ti-6Al-4V alloy surface** at different time scale

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



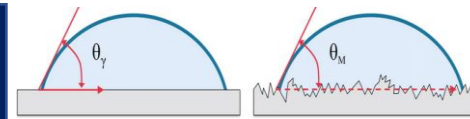
Maximum β^* of the current study and that of the analytical solution.

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

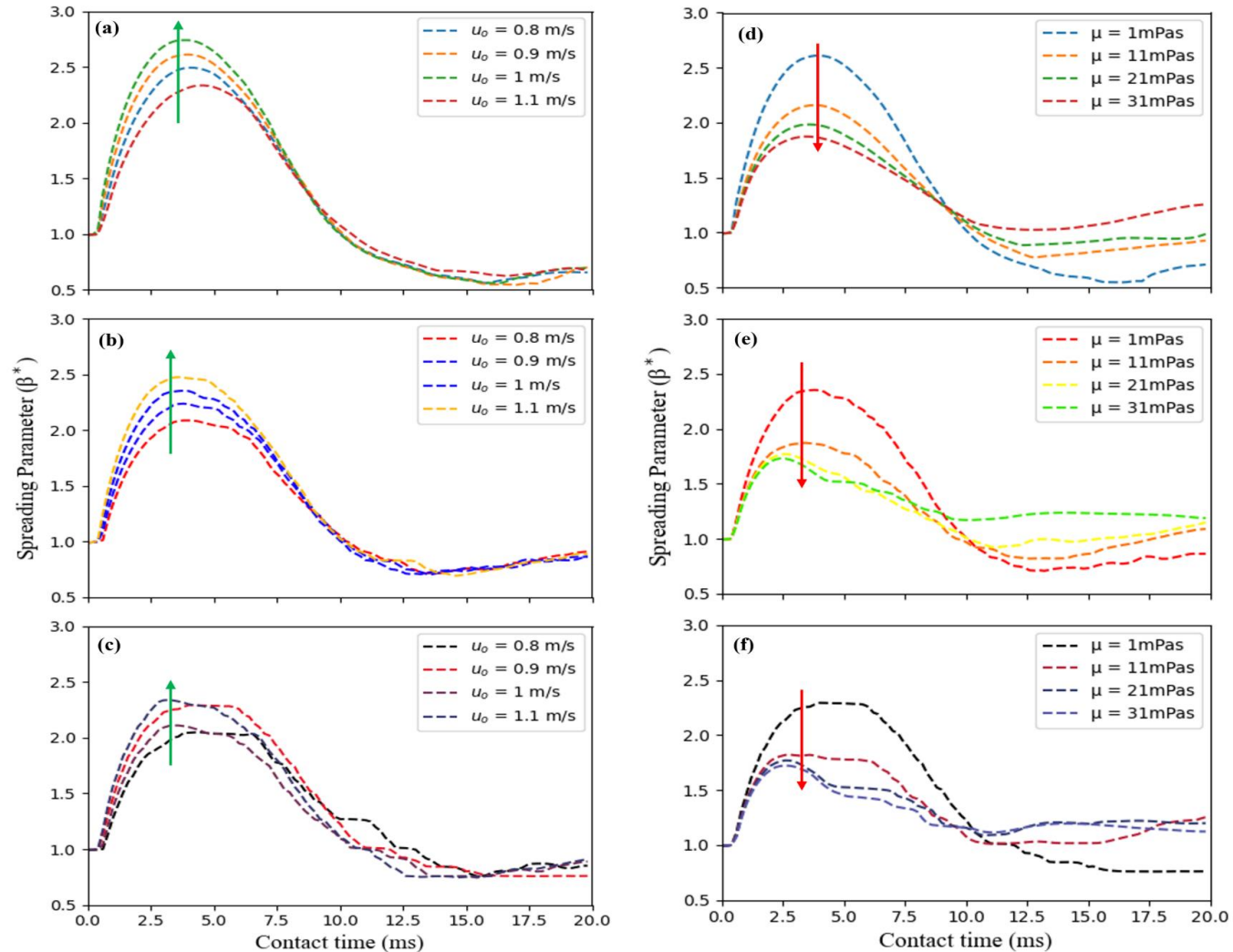


Omeje, Ilemona S., et. al. Applied Surface Science Advances 9 (2022).

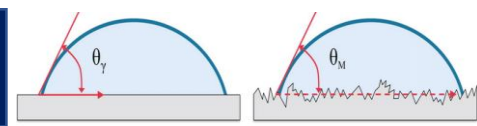
CFD Results: Effect of Velocity and Viscosity



Effect of velocity and viscosity of droplet



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

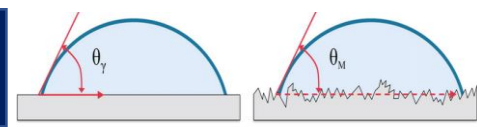


Summary

- 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**