



Numerical Study of the Wetting Dynamics of Surfaces Textured by Femtosecond Laser: Beyond Classical Wenzel and Cassie-Baxter Model

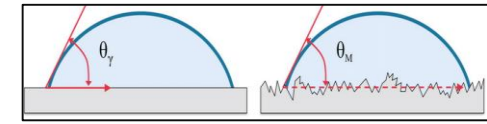
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European Materials Research, E-MRS

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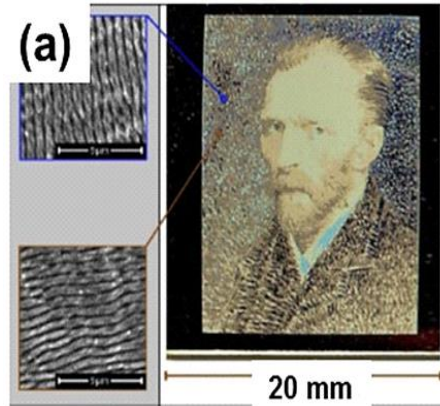
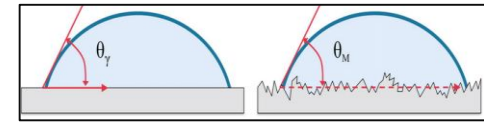
Present Outline



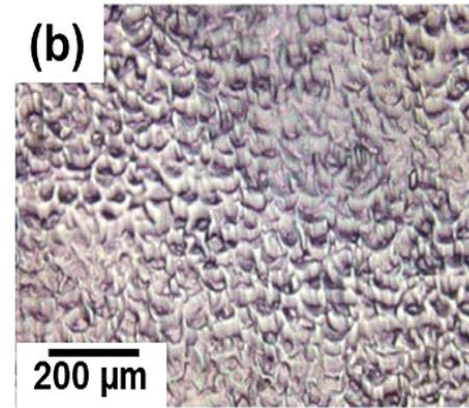
- 1 Motivation
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Motivation

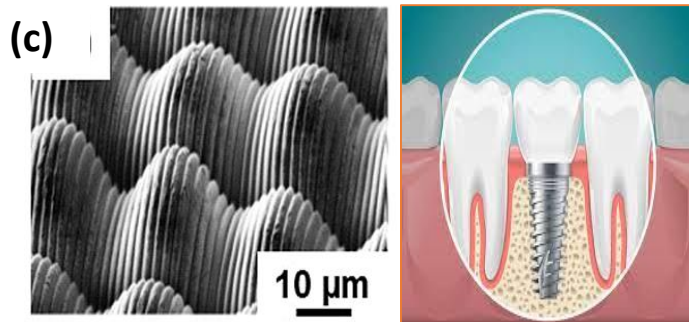
Functionalities of laser-induced nanostructures



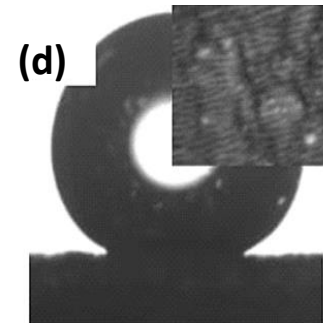
(a) Structural colors and optical marking



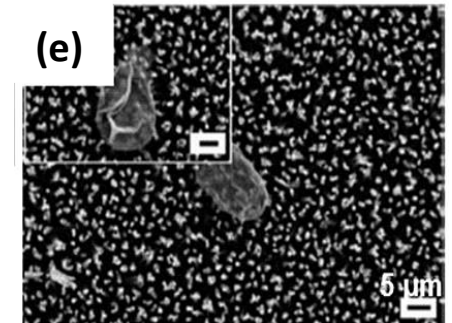
(b) Plasmonic colors



(c) Hierarchical structures



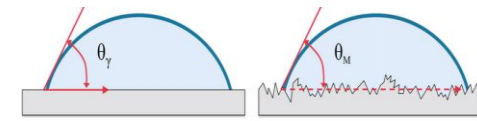
(d) Superhydrophobic contact properties originating in hierarchical topographies



(e) Bactericide properties of nanostructured surfaces

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

Challenge



Wettability of laser textured surfaces

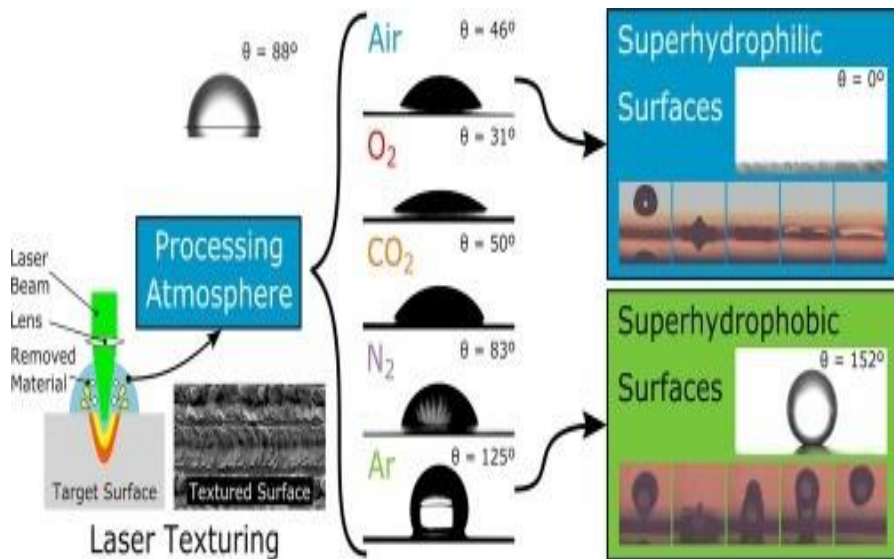
[1] Changes over time

[2] Changes from superhydrophilic to superhydrophobic

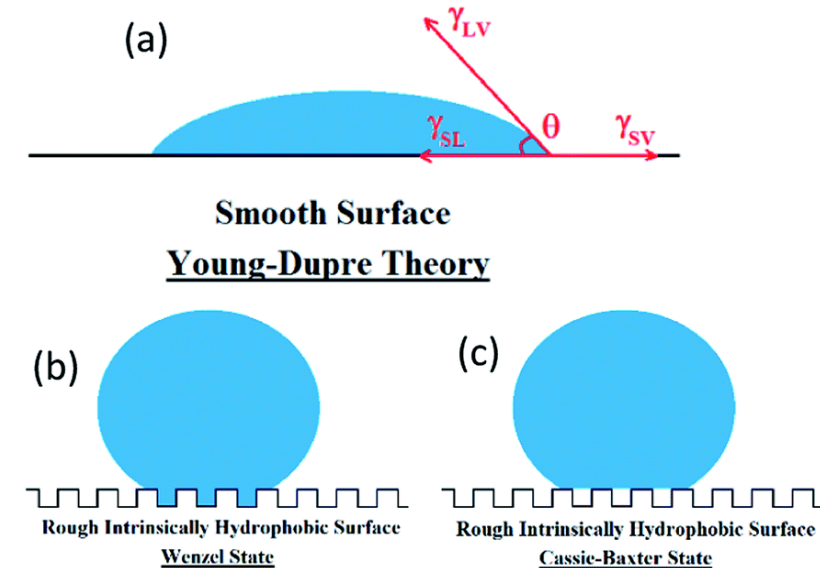
[3] The existing wetting models is difficult to account for this wetting mechanism;

- Wenzel and Cassie-Baxter

Alternate hydrophobic and hydrophilic properties



Existing wetting model

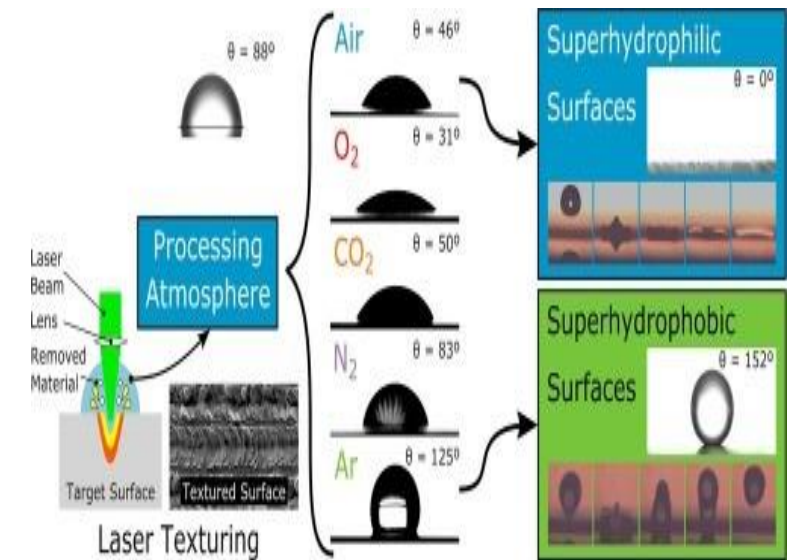
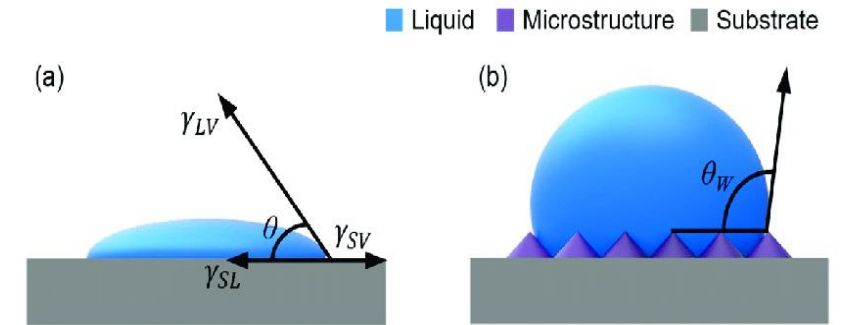
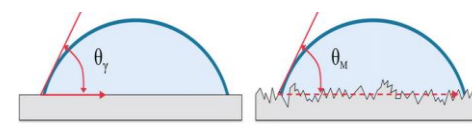


P. Bizi-bandoki et al. Time dependency of the hydrophilicity... Appl. Surf. Sci., 273 (2013), pp. 399-407

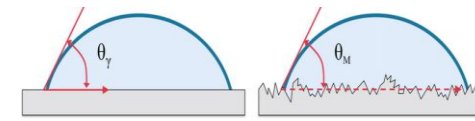
Objective

[1] Develop a more realistic wettability model accounting for the changes in surface structure and wettability.

[2] Chemical surface alterations such as oxidation and/or molecule adsorption causes the wettability of lasertextured surfaces alternates over time.



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

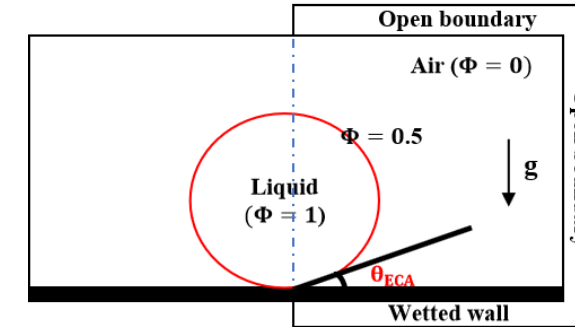
Level Set Method **(Interface Tracking Method)**

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

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

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

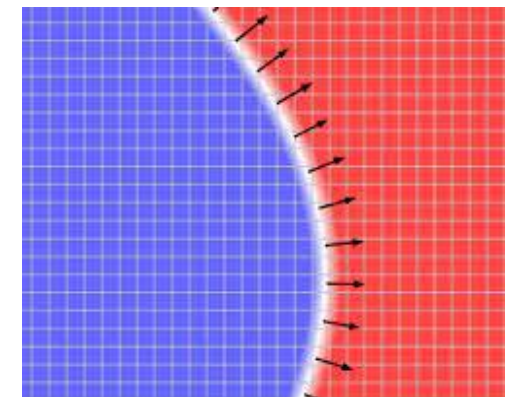
Simulation Set-up



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.



Model Validation

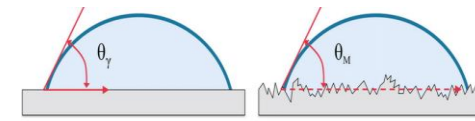
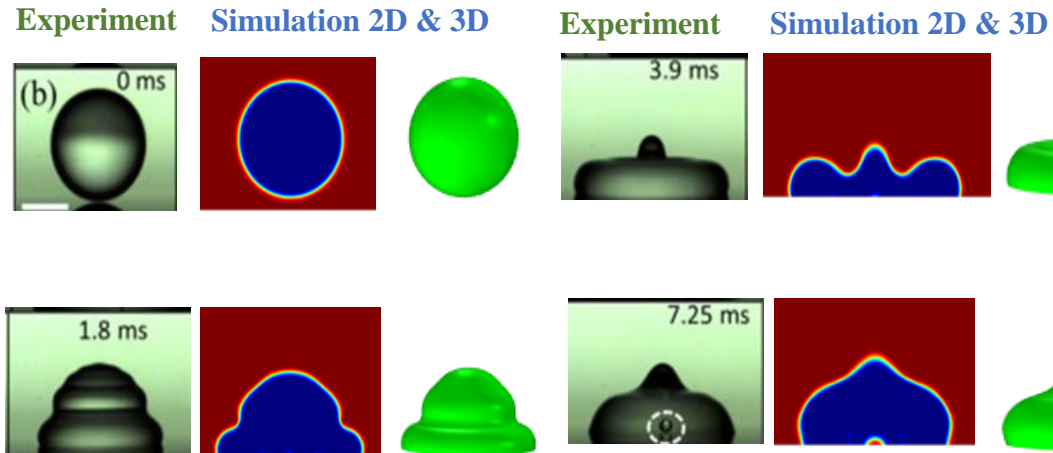
Water Droplet on Glass

Properties

Diameter of droplet = 2 mm

Impact velocity = 0.52 m/s

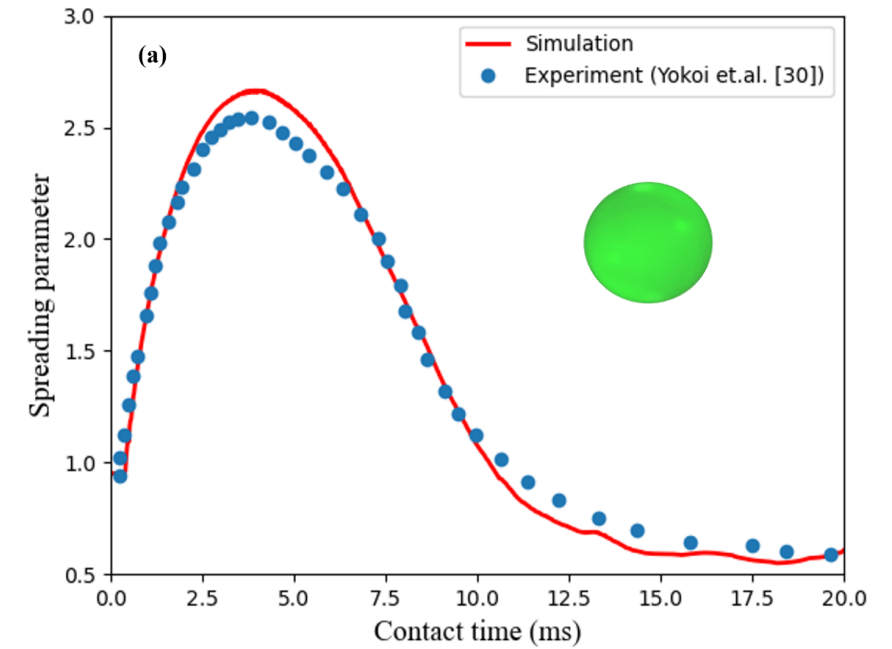
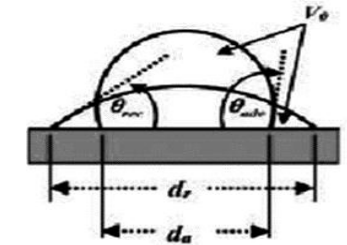
Equili. Contact Angle = 106°



Spreading Parameter

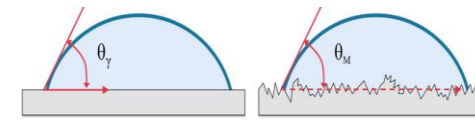
Spreading Parameter $\beta^* = \frac{d_a}{D}$

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

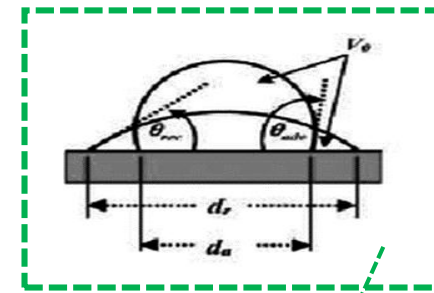
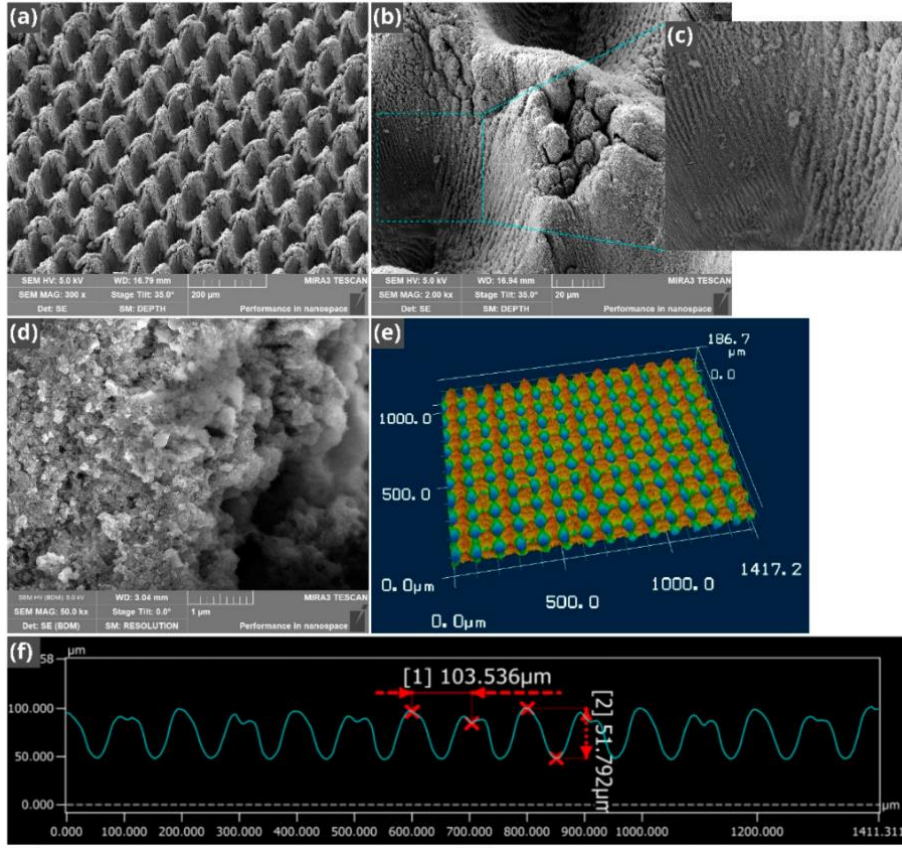


Omeje, Ilemona S., et. al. Applied Surface Science Advances 9 (2022).

CFD Results: Hierarchical Reliefs

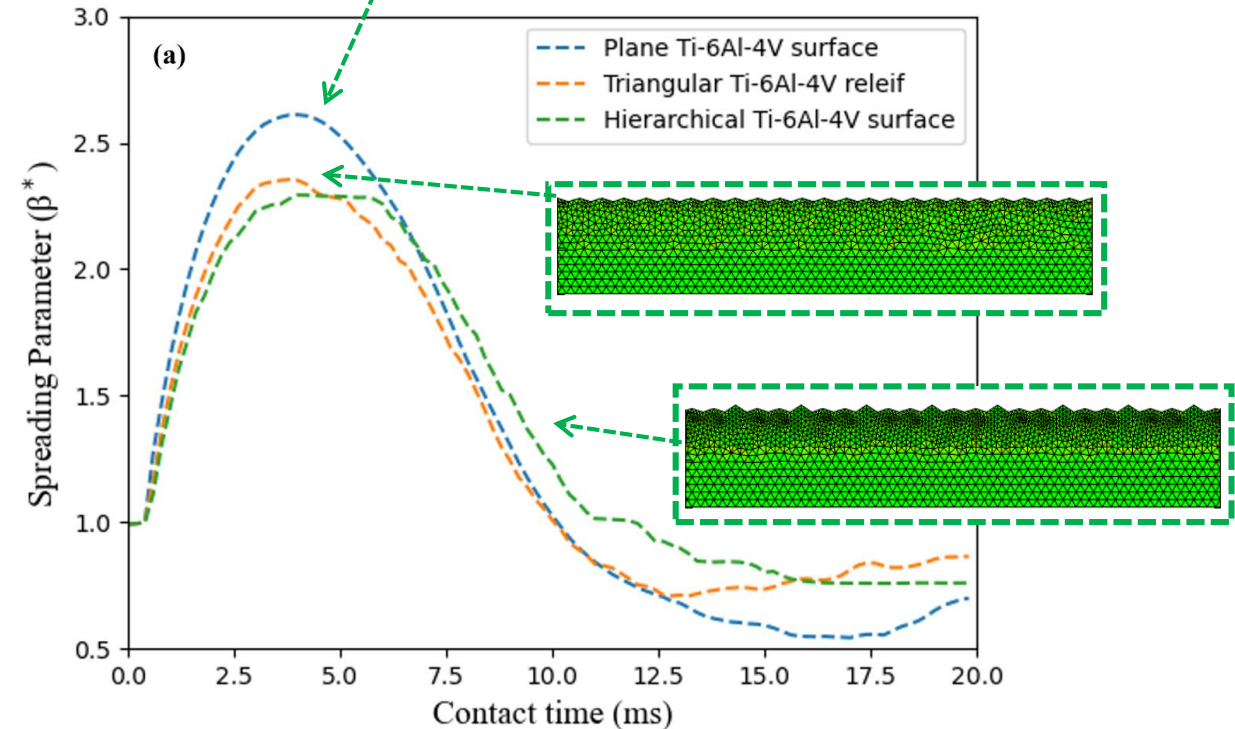


Surface of Superwicking Ti-6Al-4V Alloy Material Fabricated by Femtosecond Laser



Spreading Parameter

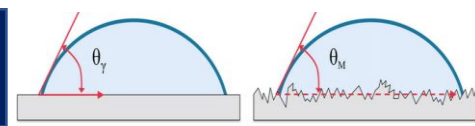
Spreading Parameter $\beta^* = \frac{d_a}{D}$
 Here d_a = diameter of droplet
 D = Initial diameter of droplet



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

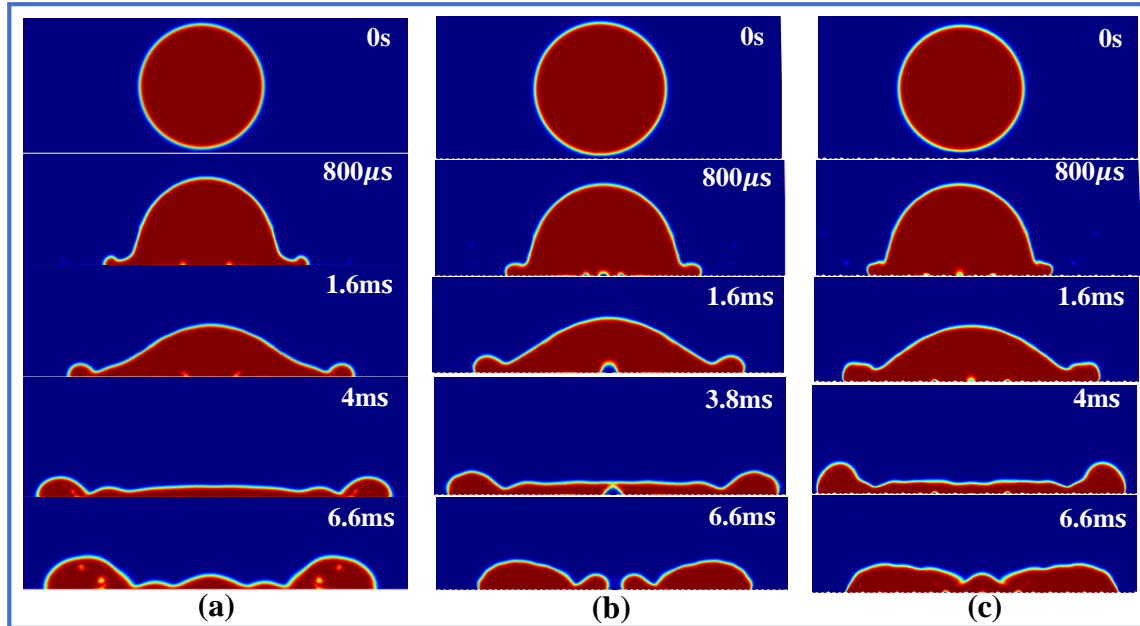
Omeje, Ilemona S., et al. Applied Surface Science Advances 9 (2022).

CFD Results: Effect of Velocity and Viscosity



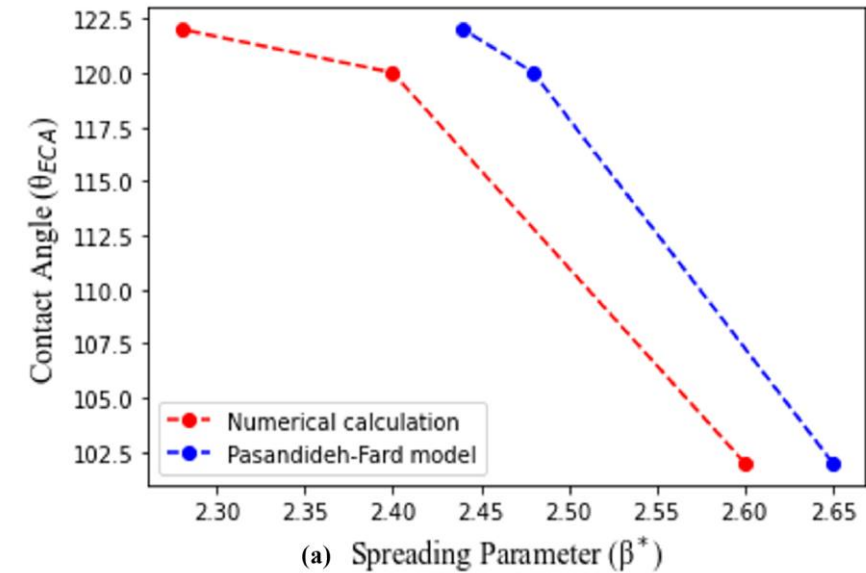
Snapshot of water impact on (a) **solid**, (b) **triangular**, and (c) **hierarchical Ti-6Al-4V alloy surface** at different time scale

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

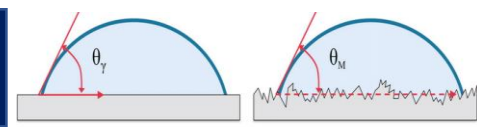


Maximum β^* of the current study and that of the analytical solution.

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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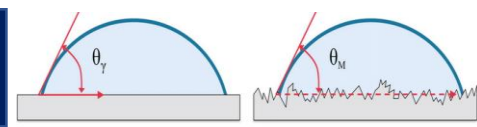


Summary

- 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**