Electronic Supplementary Material (ESI) for Soft Matter

Enabling efficient energy barrier computations of wetting transitions on geometrically patterned surfaces

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Supplementary Information

Contents

1. Axisymmetric droplets

In this section, we present computations of the equilibrium of axisymmetric droplets wetting solid surfaces textured with concentric rings. The mathematical formulation of the augmented YL equation, governing the surface shape of axisymmetric droplets, is presented below.

The droplet surface is conveniently defined in spherical coordinates (r, θ). When axial symmetry is considered around the y-axis, the problem is one-dimensional. The parameterization of the spherical coordinates (r, θ) is performed in terms of the arc-length, s, of the intersection of the droplet surface with the xy-plane (see Fig. SI 1), (i.e., $r \equiv r\,(s)$, $\theta \equiv \theta\,(s)$).

The local mean curvature of the droplet surface reads:

$$C = \frac{1}{r sin\theta \sqrt{r^2 {\theta_s}^2 + {r_s}^2}} \left[2r\theta_s sin\theta - r_s cos\theta + r sin\theta \frac{\partial}{\partial s} arctan\left(\frac{r\theta_s}{r_s}\right)\right] \qquad \text{(SI-1)}$$

$$\theta_s \equiv \frac{\partial \theta}{\partial s},\ r_s \equiv \frac{\partial r}{\partial s}$$

The unknown functions, $r(s)$ and $\theta(s)$, are determined by solving the augmented Young-Laplace equation (eq. (1)) and the dimensionless arc-length differential equation:

$$\left(\frac{dr}{ds}\right)^2 + r^2\left(\frac{d\theta}{ds}\right)^2 = 1. \tag{SI-2}$$

Due to the incompressibility of the liquid, the volume remains constant at any drop deformation:

$$\int_0^{s_{max}} r^3 sin\theta \frac{\partial\theta}{\partial s} ds = 2. \tag{SI-3}$$

The characteristic length is R_o, the radius of a sphere the volume of which is equal to the droplet volume.

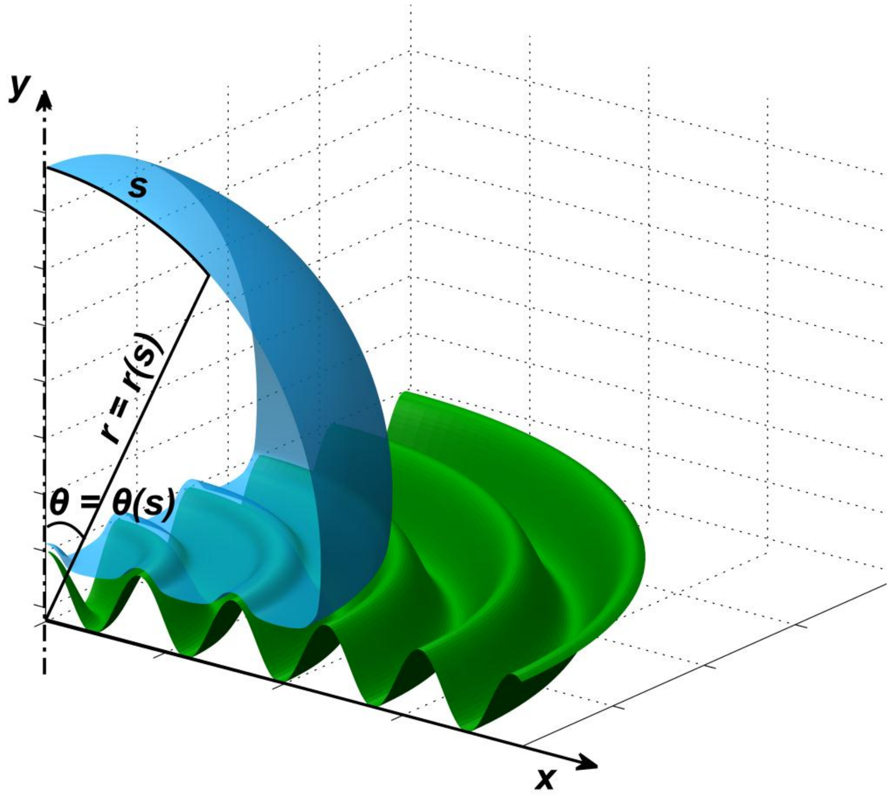

Fig. SI 1 Axisymmetric liquid droplet on a ring-patterned surface.

The maximum arc-length, s_{max}, of the droplet surface is unknown and is computed by accounting for the following algebraic equation:

$$\theta = 0 \text{ at } s = s_{max}. \tag{SI-4}$$

Moreover, the following boundary conditions are accounted for:

$$\frac{\partial r}{\partial s} = 0 \text{ at } s = 0 \text{ and at } s = s_{max}, \tag{SI-5}$$

$$\theta = 0 \text{ at } s = 0. \tag{SI-6}$$

The Neumann-type boundary conditions (eq. (SI-5)) impose the axial symmetry around the *y*-axis and the Dirichlet-type boundary condition singles out the arc-length equation solution (eq. (SI-2)).

1.1. Single-pillar structured surface

We first test the validity of the augmented YL equation by comparing its predictions with results obtained from the conventional YL equation for an axisymmetric droplet wetting a single-pillar structured solid surface; the pillar intersection with the vertical *xy*-plane is given by eq. (16).

The bifurcation diagram in Fig. SI 2 depicts the dependence of the dimensionless droplet height on the material wettability (θ_Y).

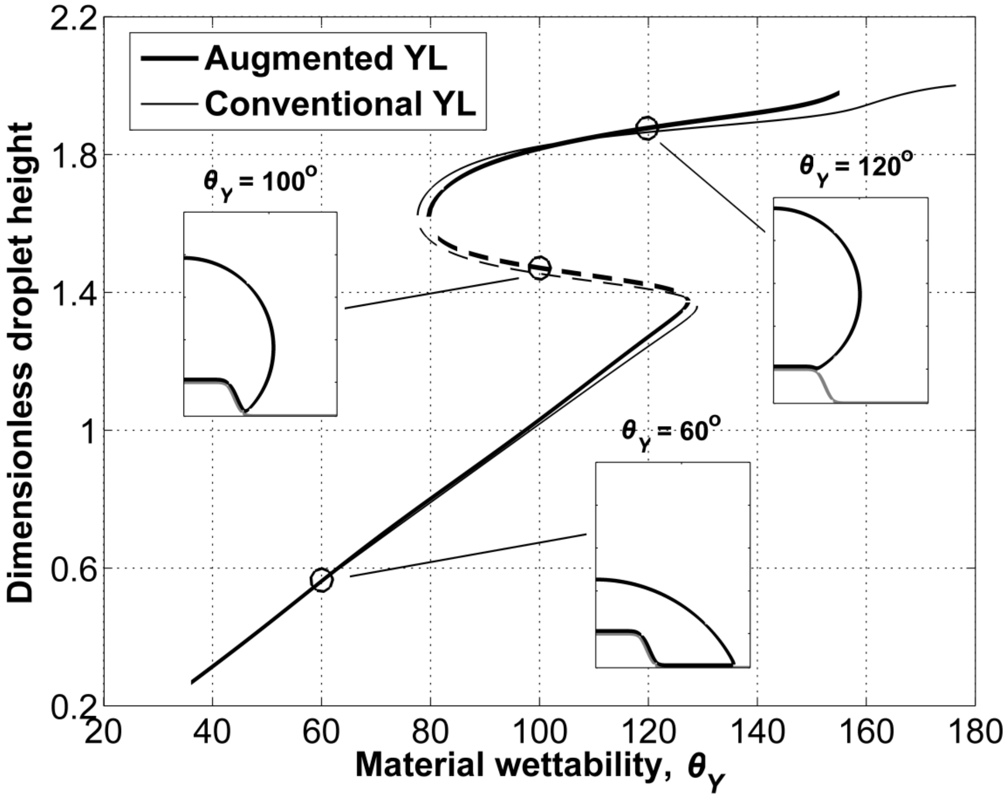

Fig. SI 2 Dependence of the droplet height on the material wettability (θ_Y) for a single-pillared solid surface structure (eq. (16) with p_1 = 0.6, p_2 = 10, p_3 = 5).

It is observed that both the augmented and the conventional YL equations produce nearly identical results. Furthermore the transition between the upper and the lower stable branch is hysteretic, similar with the case of a cylindrical droplet wetting a single-striped surface (see Fig. 6).

The augmented YL equation can also be applied for the computation of axisymmetric droplets wetting solid surfaces decorated with concentric rings.

1.2. Concentric rings-patterned surface

The proposed methodology is applied to a spherical droplet wetting the axisymmetric patterned solid surface depicted in Fig. SI 1. The intersection of this solid surface with the vertical *xy*-plane is given by eq. (17).

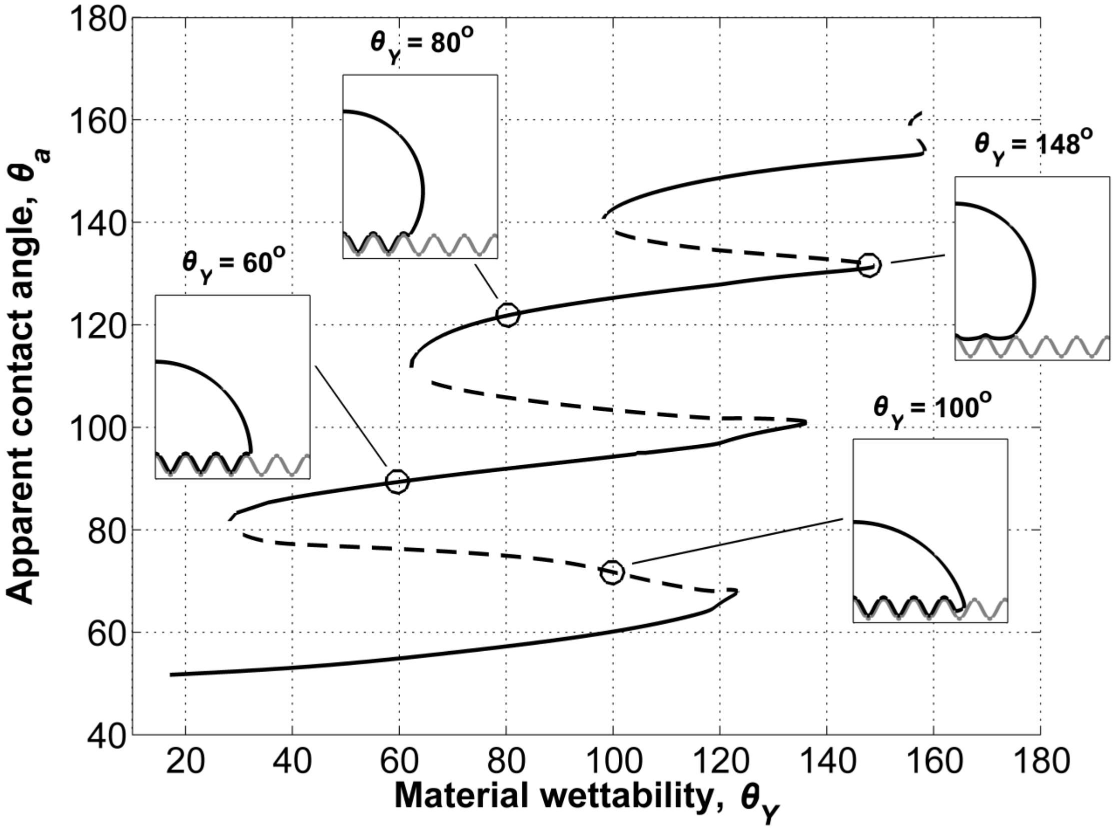

Fig. SI 3 Dependence of the droplet height on the material wettability (θ_Y) for a concentric rings-patterned solid surface (eq. (17) with p_4 = 8, p_5 = 2).

The dependence of the apparent contact angle, θ_a, as a function of the material wettability, θ_Y, is depicted in Fig. SI 3. One can observe that the solution space of the axisymmetric droplet is similar to the one of a cylindrical droplet, sitting on a patterned solid surface.

2. Arbitrary shaped corrugations

The augmented YL equation can be trivially extended to any kind of corrugations. In this section, we present a computed equilibrium solution of a cylindrical droplet wetting a solid surface which is decorated with mushroom shaped stripes (see Fig SI 4).

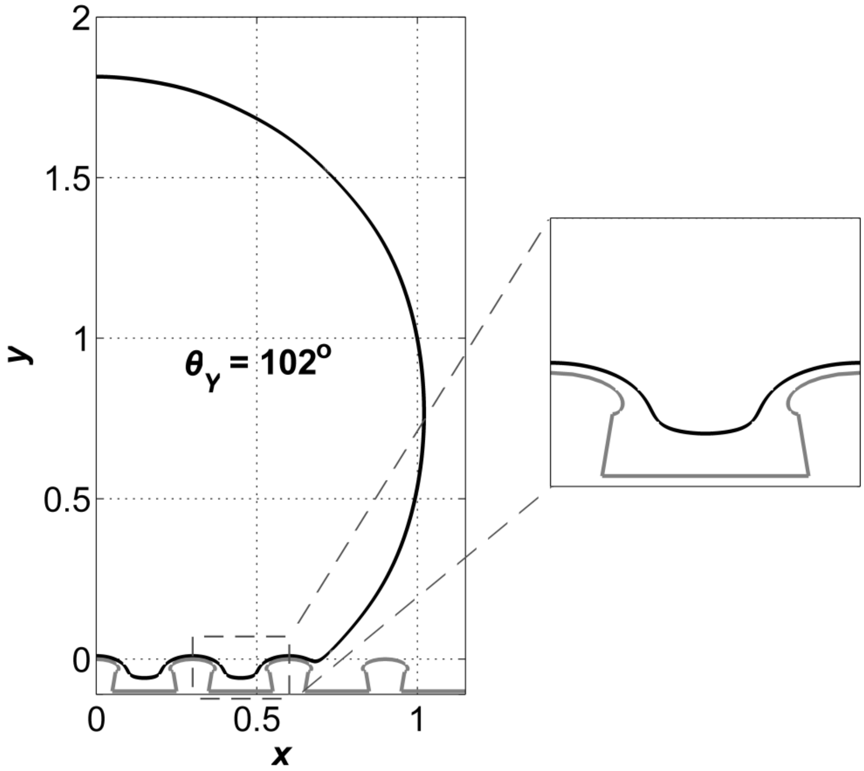

Fig. SI 4 Equilibrium solution of a cylindrical droplet wetting a mushroom-like striped surface. The material wettability corresponds to $\theta_Y = 102^o$. The inset shows a magnified view of the cross-section of each mushroom-shaped stripe.

Mushroom-shaped structures are commonly used in solid surfaces that demonstrate increased robustness of the Cassie type wetting states [1]. A correlation of their geometric structural properties with the apparent wetting behavior can be systematically studied using the proposed augmented YL methodology.

3. Eikonal equation

The disjoining pressure, p^{LS}, is a function of the Euclidean distance from the solid boundary. For structured surfaces (see Fig. SI 5), this distance is computed solving the Eikonal equation, which reads:

$$|\nabla\delta(x,y)| = 1,\ \ x,y \in \Phi, \tag{SI-7}$$

$$\delta(x,y) = 0,\ \ x,y \in \partial S, \tag{SI-8}$$

where Φ denotes the two-dimensional computational domain and ∂S is the solid surface boundary.

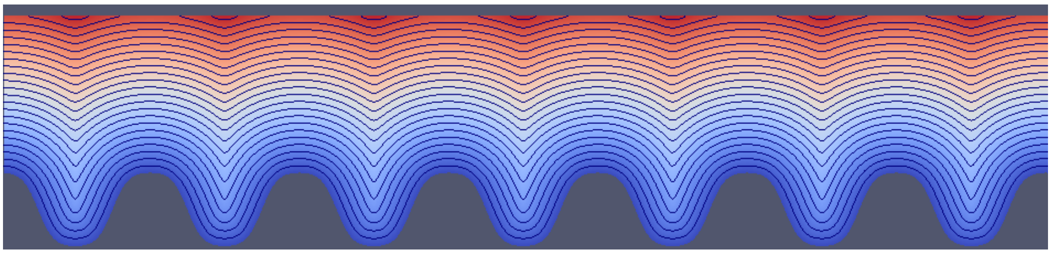

Fig. SI 5 Contour lines of constant distance, δ, from the solid boundary obtained from the Eikonal equation solution. The topography of the solid surface is given by eq. (18).

The equation is solved with the vanishing viscosity method [2]. The distance, δ, of a point located at the droplet surface from the solid boundary is interpolated from the solution of the Eikonal equation. Thus, the Eikonal equation is solved only once for a particular solid surface geometry.

References

1. S. M. Kang, S. M. Kim, H. N. Kim, M. K. Kwak, D. H. Tahk and K. Y. Suh, *Soft Matter*, 2012, 8, 8563-8568.
2. M. G. Crandall, in *North-Holland Mathematics Studies*, eds. D. C. Alan Bishop and N. Basil, North-Holland, 1982, vol. Volume 61, pp. 117-125.