



## Article

## Wetting transition energy curves for a droplet on a square-post patterned surface

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## ABSTRACT

Due to the property of water repulsion, biomimetic superhydrophobic surfaces have been widely applied to green technologies, in turn inducing wider and deeper investigations on superhydrophobic surfaces. Theoretical, experimental and numerical studies on wetting transitions have been carried out by researchers, but the mechanism of wetting transitions between Cassie–Baxter state and Wenzel state, which is crucial to develop a stable superhydrophobic surface, is still not fully understood. In this paper, the free energy curves based on the transition processes are presented and discussed in detail. The existence of energy barriers with or without consideration of the gravity effect, and the irreversibility of wetting transition are discussed based on the presented energy curves. The energy curves show that different routes of the Cassie-to-Wenzel transition and the reverse transition are the main reason for the irreversibility. Numerical simulations are implemented via a phase field lattice Boltzmann method of large density ratio, and the simulation results show good consistency with the theoretical analysis.

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## 1. Introduction

Surface roughness, which can be found in the form of micro or hierarchical structures in nature, has been widely investigated for its enhancement to hydrophobicity [1–4]. Through mimicking natural superhydrophobic surfaces including plant leaves and animals such as lotus leaves, rice leaves and water strider legs, manmade superhydrophobic surfaces via various of methodologies have been presented and applied in industrial applications, for instance, coating, self-cleaning surfaces, microfluidic devices with surface-tension-induced drop motion and so forth [5,6]. Among all the natural water-repellence examples, lotus leaves are the most impressive for their superhydrophobic characteristic which is also known as “lotus effect”. Due to the micrometre order length scales of the micro posts on the surfaces, the apparent contact angle (APCA) of lotus leaves is approximately 160° while the hysteresis angle is just about 4° [7].

As the wetting phenomena have been investigated over the past decades, significant progress on theoretical models has also been achieved with considerable attention. The starting point of wetting on an ideal rigid, flat and homogeneous surface is characterized by the well-known Young’s Equation [8]:

$$\cos \theta_Y = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}}, \quad (1)$$

where  $\sigma$  is the surface tension which represents the energy per unit area of the interface between solid/gas, solid/liquid or liquid/gas, and  $\theta_Y$  is the Young’s contact angle. Young’s Equation reveals the relationship between surface tensions and contact angle in the ideal situation, however, it cannot be applied to most real surface conditions due to the existence of surface roughness. For the surface roughness, a new correlation where the apparent contact angle is related to surface roughness was presented by Wenzel [9]:

$$\cos \theta_w = r \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}}, \quad (2)$$

which is also normally written as the following reformed equation:

$$\cos \theta_w = r \cos \theta_Y, \quad (3)$$

where  $r$ , the roughness parameter corresponding to the “roughness factor”, which is also referred to as roughness area ratio, denotes as the ratio of the actual surface area with respect to the projected structure surface, and  $\theta_w$  is the Wenzel’s angle. The Wenzel equation is associated with the homogeneous wetting states, where the grooves caused by the surface roughness are penetrated with water. Apart from the homogeneous wetting state, there is another stable state, the heterogeneous wetting state, and the corresponding equation to the heterogeneous wetting regime was proposed by Cassie and Baxter [10]:

$$\cos \theta_{CB} = f \cos \theta_Y + f - 1. \quad (4)$$

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If the roughness ratio,  $r_f$ , the ratio of the actual wetted area over the projected area is considered, Eq. (4) can be modified to the following form [11]:

$$\cos \theta_{CB} = r_f f \cos \theta_Y + f - 1, \quad (5)$$

where  $f$  is the area fraction on the horizontal projected plane of the liquid-solid contact area over the total area of solid-liquid and liquid-gas contact. Eq. (5) would become the same form with Wenzel's equation when  $f = 1$  and  $r_f = r$ . By equating Eqs. (3) and (5), the critical contact angle theoretically used to separate the two wetting states can be calculated as [12]:

$$\cos \theta_C = \frac{1-f}{r_f f - r}. \quad (6)$$

It should be noted that when  $\theta_C > 90^\circ$ , both two wetting states exist. Then the homogeneous wetting state is preferable only if  $\theta_Y < \theta_C$ , otherwise the droplet stays at a heterogeneous wetting state, theoretically [13]. However, it has been observed that, even the Young's angle is smaller than the critical angle, the Cassie-Baxter wetting state can exist, which means that Wenzel and Cassie-Baxter states may stay on the same specific surface at the same time [14–17].

Bormashenko [18,19] reviewed the main experimental and theoretical approaches to wetting transitions in 2010 and 2015 respectively. Experiments to study the wetting transitions were implemented by giving external factors such as pressure [20], initial velocity [21], evaporation of droplets [22], vibration [23], and electric field [24,25]. And the role of gravity in wetting transitions was also discussed [11]. Patankar [11] and Zu et al. [26] theoretically analyzed the wetting transition from Cassie-Baxter state to Wenzel state from the free energy point of view, and the energy barrier was discussed both in their work. Whyman and Bormashenko [27] theoretically investigated the interfacial free energy and discussed the irreversibility of Cassie-to-Wenzel transition. Ren [28] computed the transition states, the energy barriers and the minimum energy paths for Cassie-to-Wenzel transition using the string method. Pashos et al. [29,30] developed a numerical method to investigate the minimum energy paths and the free energy changes were presented in their work. Prakash et al. [31] studied the spontaneous recovery of superhydrophobicity on nanotextured surfaces using molecular simulations. Bico et al. [32] and Bormashenko et al. [33] studied the Cassie impregnating state apart from the Cassie-Baxter state and Wenzel state, and Gibbs free energy curves of the three wetting states were presented. In their work, the impregnating state was observed via vibration so that the liquid can impregnate the grooves outside of the droplet/solid interface. In this paper, we focus on the transition between the more regular Cassie-Baxter and Wenzel wetting states.

Wenzel's equation and Cassie and Baxter's equation can describe the stable wetting states on real rough surfaces to a great extent when the droplet size is much larger than the typical roughness scale. Nevertheless, there are still points of the theory of wetting states which are not fully understood. For instance, when a droplet stays in a stable wetting state, and how the transition between the two wetting states occurs [13]. It is crucial to understand the mechanism of wetting transition process for the design and manufacturing of devices with highly stable superhydrophobic surfaces. This paper focuses on the wetting transition process as well as the different wetting states on the simplest model, the square-post patterned surface from the free energy point of view.

## 2. Theoretical analysis

In the present study, the substrate patterned by square posts as the roughness surface is considered as shown in Fig. 1, where  $a$ ,  $b$

and  $h$  are the post width, post spacing, and post height respectively. It should be pointed out that the droplet size scale is much larger than the size scale of micro posts in the theoretical analysis. Under this assumption, the theoretical analysis can be conducted based on a single unit of patterned substrate with periodical pattern and the Wenzel and Cassie-Baxter equations can be used for the calculation of the apparent contact angles. In the presented pattern,  $r_f$  equals to 1.

### 2.1. The model of net free energy

All the parameters needed for the following theoretical analysis are presented in Fig. 2 in three typical wetting state cases. Firstly, considering a droplet staying steady on a flat ideal surface as shown in Fig. 2a, the equilibrium free energy can be calculated as [13]

$$E_Y = S(\sigma_{SL} - \sigma_{SG}) + S' \sigma_{LG}, \quad (7)$$

where  $S$  and  $S'$  represent the solid/liquid interface area and the liquid/gas interface area respectively. Similarly, the equilibrium free energy equations for Cassie-Baxter and Wenzel states are

$$E_{CB} = S_{CB}(\sigma'_{SL} - \sigma_{SG}) + S'_{CB} \sigma_{LG}, \quad (8)$$

$$E_W = S_W(\sigma'_{SL} - \sigma_{SG}) + S'_W \sigma_{LG}, \quad (9)$$

where  $\sigma'_{SL}$  is the equivalent free energy per unit area of the solid/liquid interfaces for both of the two states, while  $S_{CB}$  and  $S_W$  both represent the projected horizontal areas. Considering the equivalent surface tension, Young's equation can be applied into the heterogeneous and homogeneous wetting states:

$$\cos \theta_{CB} = \frac{\sigma_{SG} - \sigma'_{SL}}{\sigma_{LG}}, \quad (10)$$

$$\cos \theta_W = \frac{\sigma_{SG} - \sigma'_{SL}}{\sigma_{LG}}. \quad (11)$$

By combining the above equations, the free energy equations for Cassie-Baxter and Wenzel states can be expressed as

$$E_{CB} = S_{CB}[f(\sigma_{SL} - \sigma_{SG}) + (1-f)\sigma_{LG}] + S'_{CB} \sigma_{LG}, \quad (12)$$

$$E_W = S_W r(\sigma_{SL} - \sigma_{SG}) + S'_W \sigma_{LG}. \quad (13)$$

### 2.2. Cassie-to-Wenzel wetting transition

#### 2.2.1. Without gravity effects

Usually, the transition process from Cassie-Baxter state to Wenzel state can be easily observed, however, the reverse process is hard to be achieved. Thus it is generally agreed that the wetting transition from Cassie-Baxter state to Wenzel state is irreversible

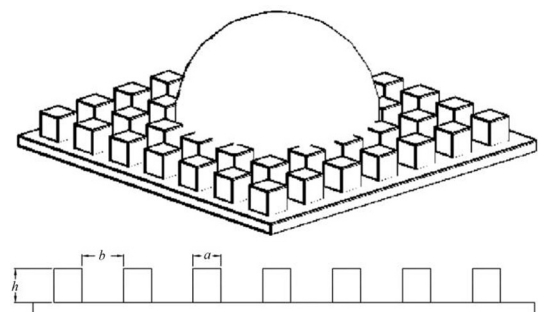


Fig. 1. Structure of the micro roughness surface.

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