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Thermodynamic analysis on wetting properties of a droplet on a solid surface with engineered trapezoidal microarchitecture

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ABSTRACT

The wetting properties of a hydrophobic solid surface containing an engineered trapezoidal microarchitecture have been investigated based on a 3-D thermodynamic model. The three-phase contact line tension is introduced in the present approach for a droplet in the composite state, and the relationship between surface topology and superhydrophobicity is established. It is demonstrated that both trapezoid base angle and base spacing have great influence on the wetting transition between composite and non-composite states. Some recommendations are made for fabricating ideal superhydrophobic surfaces with optimal geometries. The validity of the present theoretical results has also been verified by comparing our theoretical predictions and experimental data available in the literature. The developed model in this paper sheds lights on the wetting properties of advanced materials with engineered microarchitecture.

1. Introduction

Optimal design for solid surfaces with controllable wettability has been an important topic for micro/nanofabrication in recent years [1,2]. Particularly, superhydrophobic surfaces with large water contact angle (CA) and small contact angle hysteresis (CAH) have attracted significant attention from both scientific research and practical applications [3,4]. It is well-recognized that the combination of low surface energy and high surface roughness of a surface is the main reason for the superhydrophobicity [5,6]. According to previous research studies, a droplet on a superhydrophobic solid surface usually traps air between the rough structures and water [7,8]. The water CA of air is 180°; an increased roughness could result in an increased liquid-air contact area and a decreased solid-liquid contact area, which implies that hydrophobicity strongly depends on surface roughness. As a result, it is of great significance to design optimal geometry or analyze the correlation between the surface roughness and wetting behavior for superhydrophobic surface.

Although the manufacturing process of superhydrophobic surfaces with ideal surface geometries has been widely investigated [9–11], studies on the theoretical analysis of superhydrophobic surfaces are still challenging because of the significant deviation of theoretical predictions from experimental measurements. So far, analyses on the wetting behavior of superhydrophobic surfaces are commonly based on two simple models. In Cassie's state [12], droplet traps air beneath the liquid, while in Wenzel's state [13], droplet penetrates the asperities or microarchitecture of solid surface. The free energy (FE) determines the final stable state according to the lowest principle of energy. Therefore, thermodynamic method is considered as a powerful tool in analyzing superhydrophobicity. Considerable efforts have been made to investigate the wettability of solid surfaces using the thermodynamic analysis. For example, Nosonovsky and Bhushan [14] proposed a comprehensive analytical model to investigate the relationship between local roughness and CA with various roughness distributions taken into consideration, the results were verified by experimental measurements for the water CA of a lotus leaf surface. Bell et al. [15] employed a thermodynamic model for analyzing the effect of gravity on wetting properties of solid surfaces with two-dimensional asperities. The model predictions are in good agreements with experimental observations. Marmur [16] used a theoretical thermodynamic model to study the transition between composite and non-composite wetting states based on Wenzel and Cassie equations, and added a new condition necessary for the existence

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of Wenzel wetting state. Patankar [17] proposed a methodology to determine the possibility of a transition from a Cassie to a Wenzel drop on a square-pillar textured surface using the energy balance.

The previously reported studies for the theoretical analysis of the wetting properties of solid surfaces are sophisticated; nevertheless, theoretical models of FE barrier (FEB) caused by various meta-stable wetting states were not presented in these previous works. It is found that only apparent CA is not enough for characterizing superhydrophobicity, CAH is also necessary for describing superhydrophobicity [18–20]. To date, the commonly used approach for thermodynamically predicting the CA and CAH is to calculate the FE and FEB as a result of droplet movement. Li et al. [21,22] built a two-dimensional (2-D) model to thermodynamically analyze the wetting behavior of a superhydrophobic surface. The model can deal with the effect of geometrical parameters on CA, CAH, and the transition between composite and non-composite states. Long et al. [23] employed a 2-D regular surface model to study contact angles on rough and heterogeneous surfaces. Tie et al. [24] systematically investigated the wettability of various orientations of different parallel grooved surfaces. However, the above mentioned studies are mainly based on a 2-D model by analyzing the system along a specific plane. Such method simplifies the mathematical treatment, but it has its own limitations for representing the more practical 3-D microarchitectures [21,25]. In addition, it has been demonstrated that the movement of three-phase contact lines contributes primarily to CAH [26]. The three-phase contact line is represented by points in a 2-D model because of the simplification; as a result, 2-D model cannot deal with the conditions with the properties of three-phase contact line being taken into considerations. Hence, it is necessary to build a 3-D model to investigate the wetting behavior of superhydrophobic surface from both CA and CAH perspectives.

Recently, we proposed a thermodynamic approach using a 3-D model and successfully made relationship between geometrical parameters and superhydrophobicity including CA, CAH, and the transition between different wetting states according to the FE change as a result of three-phase contact line moving [25,27]. Herein, we extend our 3-D thermodynamic analysis to a superhydrophobic surface with trapezoid microstructures since such surface possesses special wetting properties and attracts much attention from both experimental and theoretical studies on engineered microarchitected materials [28,29]. The present study mainly focusses on the effects of trapezoid base angle and base spacing on the superhydrophobicity and the effect of geometrical features of asperities on the wetting behavior of a Cassie droplet.

2. Thermodynamic analysis

2.1. Definition of the trapezoid microarchitecture

A typical 3-D trapezoidal microarchitecture is shown in Fig. 1. The trapezoid base width a, base spacing b, and top width c are defined in Fig. 1a, and the trapezoid base angle α is shown in Fig. 1b. The trapezoid height h can be derived geometrically as:

$$h = \frac{\sqrt{2}(a-c)\tan\alpha}{2} \quad (1)$$

Similarly, the side length of trapezoidal microarchitecture l can be obtained as:

$$l = \frac{\sqrt{2}(a-c)}{2\cos\alpha} \quad (2)$$

When a droplet is placed on an ideal, smooth, and rigid solid surface, the CA can be expressed by the classical Young's equation [30]

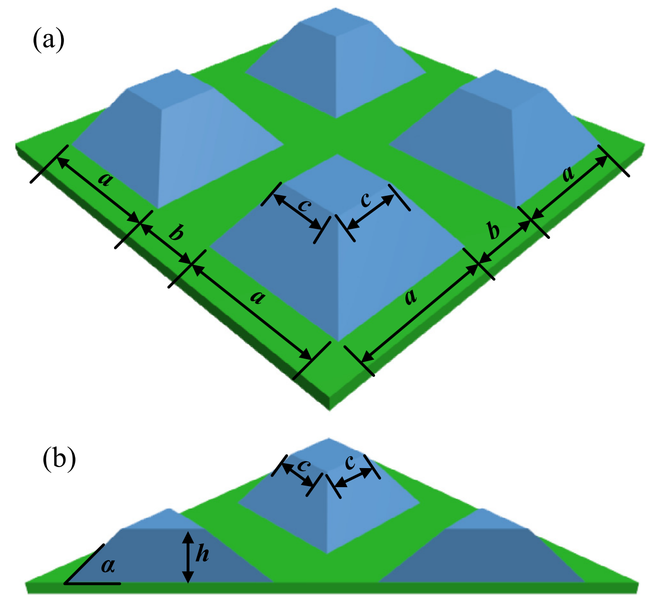

Fig. 1. Definition of the trapezoidal microarchitecture.

$$\gamma^{la}\cos\theta_Y = \gamma^{sa} - \gamma^{ls} \quad (3)$$

where γ^{la}, γ^{sa}, and γ^{ls} represent the liquid-air, solid-air, and liquid-solid interface tensions, respectively; θ_Y is the Young's CA or intrinsic CA. Since our interest is focused on superhydrophobic surfaces, θ_Y will be confined in this paper to be larger than 100° and smaller than 180°. Since asperities exist in the practical solid surfaces, a droplet on a solid surface would stays in two kinds of wetting states which are specifically discussed in the present study. When droplet traps air between solid and liquid, droplet stays in the composite state [12] (see Fig. 2a); while when droplet penetrates into asperities of a solid surface, droplet is in non-composite state [13] (see Fig. 2b). In our 3-D model, the roughness ratio r of the superhydrophobic surface with trapezoidal microarchitecture can be expressed as:

$$r = \frac{2(a+c)\sqrt{l^2 - \left(\frac{a-c}{2}\right)^2} + b^2 + 2ab + c^2}{(a+b)^2} \quad (4)$$

The surface fraction f of solid and liquid interface can be written as:

$$f = \frac{c^2}{(a+b)^2} \quad (5)$$

2.2. Thermodynamic analysis

Some assumptions are made in the thermodynamic analysis. First, the gravity is neglected when the droplet size is small enough (millimeter scale) but sufficiently larger than the scale of surface asperities. The influence of gravity is commonly indicated by the

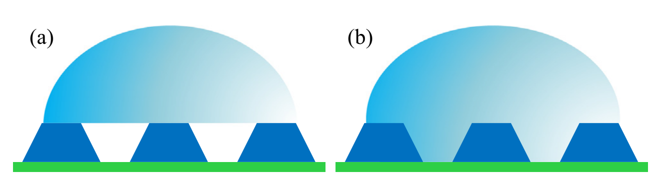

Fig. 2. Two wetting states of a droplet on a microarchitected solid surface. (a) Composite state. (b) Non-composite state.