



Droplet hysteresis investigation on non-wetting striped textured surfaces: A lattice Boltzmann study



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HIGHLIGHTS

- Simulation based on a newly proposed high-density-ratio lattice Boltzmann model.
- Hysteresis is found to be eliminated through vibrating the substrate.
- The droplet dynamic behaviors on textured surfaces are captured.

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ABSTRACT

The Cassie–Baxter model is widely used to predict the apparent contact angles on textured super-hydrophobic surfaces. However, it has been challenged by some recent studies, since it does not consider contact angle hysteresis and surface structure characteristics near the contact line. The present study is to investigate the contact angle hysteresis on striped textured surfaces, and its elimination through vibrating the substrate. The two-phase flow is simulated by a recently proposed lattice Boltzmann model for high-density-ratio flows. Droplet evolutions under various initial contact angles are simulated, and it is found that different contact angles exist for the same textured surface. The importance of the contact line structure for droplet pinning is underlined via a study of droplet behavior on a composite substrate, with striped textured structure inside and flat structure outside. A “stick–jump” motion is found for the advancing contact line on the striped textured surface. Due to hysteresis, the contact angles after advancing are not consistent with the Cassie–Baxter model. The stable equilibrium is obtained through properly vibrating the substrate, and the resulted contact angles are consistent with Cassie’s predictions.

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1. Introduction

Wetting of fluid on a solid surface is a fundamental topic in science and engineering. It is well known that microtextured or nanotextured hydrophobic surfaces can become super-hydrophobic [1,2], which exhibit high apparent contact angles, enhanced transport properties and the ability of self-cleaning. Such super-hydrophobic surfaces were widely found in nature, and examples include the water-proof legs of water striders [3], the wings of butterflies [4] and the leaves of plants such as lotus and cabbage [5]. With the rapid development of micro- and nano-fabrication technology, super-hydrophobic

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surfaces have been of great promise for the lab-on-a-chip, microfluidic devices, and fuel cell chips [6–9]. However, due to complex interfacial dynamics between fluids and solid surface, the mechanisms involved in these super-hydrophobic structures are not fully comprehended, which hinder device design and optimization.

In contrast, the physics of liquid droplet behavior on flat homogeneous surfaces is well understood. The contact angle θ_{flat} that a droplet of a certain liquid forms in contact with an ideally flat, homogeneous, and rigid surface is expressed by Young's law:

$$\cos \theta_{\text{flat}} = \frac{\gamma_{\text{SG}} - \gamma_{\text{SL}}}{\gamma_{\text{LG}}}, \quad (1)$$

where γ_{SG} , γ_{SL} , and, γ_{LG} represent the interfacial free energy per unit area of the solid–gas, and solid–liquid and liquid–gas interfaces, respectively. In this paper, the subscripts 'S', 'L' and 'G' denote solid phase, liquid phase and gas phase, respectively. Note that θ_{flat} can affect droplet dynamic behavior on flat surfaces [10].

Wenzel [11] made the first attempt to understand the effect of roughness on surface wettability. He identified that the natural tendency of a material (hydrophilic or hydrophobic) is enhanced by the presence of textures. Wenzel's interpretation of this phenomenon is based on an increase in the surface area of a material due to its roughness. The apparent contact angle θ_{Wenzel} on a rough surface is given by Ref. [11]

$$\cos \theta_{\text{Wenzel}} = r \cos \theta_{\text{flat}}, \quad (2)$$

where r is the surface roughness factor, defined as the ratio of the actual area (including the asperities) of the rough surface to the apparent area. However, when the air bubbles are entrapped inside the grooves, underneath the liquid (heterogeneous wetting), the solid surface is partially wetted by the liquid, and Wenzel's model turns out not to be applicable. For heterogeneous wetting cases, Cassie and Baxter [12] proposed a model to relate the apparent contact angle θ_{Cassie} to the rough surfaces, and it is expressed by

$$\cos \theta_{\text{Cassie}} = f \cos \theta_{\text{flat}} - (1 - f), \quad (3)$$

where f is the fraction of solid surface area wet by the liquid. The Cassie–Baxter model is widely used because of its capability in describing heterogeneous surfaces. However, it has been challenged by some successive studies, which are manifested in two aspects: the model does not consider the contact angle hysteresis [13,14], which naturally exists in the flow physics; it is not capable of dealing with a composite substrate [15], where the local areal fraction near the contact line differs from the overall one. Discrepancies have arisen in the literature regarding the understanding of contact angle on the textured surfaces. Extrand [16] argued that the three-phase structure at the contact line controls the contact angle rather than the liquid–solid interface beneath the droplet. Gao and McCarthy [17] attributed the difference between their experiment and the Cassie–Baxter model to the distortion of triple contact line. While Choi et al. [13] observed that along the stripe direction of a textured surface, both advancing and receding contact angles match the predictions from the Cassie–Baxter model despite the severe distortion of triple contact line. They proposed a differential texture parameter to predict metastable states of system; thus the advancing and receding contact angles on textured surfaces are determined.

An experimental study of micro-droplet behavior on textured surfaces is challenging because of a large span of length- and time-scales involved. In the last two decades, the lattice Boltzmann method (LBM) has developed into a promising numerical alternative for simulating fluid flows and transport problems. The fundamental idea of the LBM is to construct simplified kinetic models that incorporate the essential physics of microscopic or mesoscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations [18,19]. Its kinetic nature provides many of the advantages of molecular dynamics, including clear physical pictures, easy implementation of boundary conditions, simplicity of programming, and ability of incorporating microscopic interactions, [20,21] which make the LBM particularly suitable for simulating multiphase flows. Several lattice Boltzmann models have been proposed for multiphase and multi-component flows, including the color model [22], the interparticle-potential model [23], the free-energy model [24], and the mean-field model [25]. These models have been applied to study the contact line motion [26–28], droplet morphology [29–32], and droplet stability [33,34] on textured surfaces. However, less attention has been paid to the contact angle hysteresis phenomenon on textured surfaces. Also, these models are limited to the multiphase flows with small density ratio due to numerical instability. Recently, a multiphase lattice Boltzmann model with density ratio up to 1000 was proposed by Lee and Liu [35], which is built upon the diffuse-interface theory and uses a stable numerical discretization scheme for the continuous Boltzmann equation.

In this paper, the multiphase model proposed in Ref. [35] is adopted to investigate droplet properties on striped textured surfaces. The capability of the model is first verified by recovery of the Cassie and Wenzel states for a droplet on a textured surface. The contact angle hysteresis phenomenon is then demonstrated by droplet evolutions on a striped textured surface under various initial contact angles. Finally, we suggest a strategy to eliminate the contact angle hysteresis. The obtained results can help in understanding the droplet behavior on textured surfaces.

2. Numerical method

The computational method adopted in this study is based on the model proposed by Lee and Liu [35], and only a brief description of this model is given in this section. In this method, we incorporate the gravity effect following our previous

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