

## Numerical Study on Size Effects in the Wettability of Textured Surfaces

Zhiru Yang <sup>a</sup>, Dezheng Le <sup>b</sup> and Yang Zhou <sup>c</sup>

School of Mechanical Engineering, Jiangsu University, Zhenjiang 212013, China.

<sup>a</sup>wan\_009@126.com, <sup>b</sup>xxzj\_009@126.com, <sup>c</sup>yzr\_009@sina.cn

### Abstract

**Superhydrophobic surfaces have attracted a great deal of attention due to their excellent water resistance performs. In this study, Ansys Fluent software is employed to simulate the droplet on the micro-textured surfaces with different structural parameters to explore the effect of the micro-textured structure parameters on the surface hydrophobic properties. The simulation results show that the hydrophobic properties of the surface of the material with the micro-texture are significantly improved and fully accord with the characteristics of the Cassie wetting model. It is also found that the relatively small micro-texture size and the larger micro-texture density are more favorable to obtain surface superhydrophobic properties.**

### Keywords

**Textured surface; size characteristic; droplet; wetting; contact angle.**

### 1. Introduction

Hydrophobicity is widely used in nature and engineering applications [1, 2]. The hydrophobic property of the surface largely determines the application of the material [3]. The microstructure of the solid surface is one of the important factors that affect the wettability of the surface. In nature, there are lots of plants and animals show superhydrophobic properties [4, 5]. Studies have shown that micro-scale or nano-scale texture can significantly improve the surface water repellency. Generally speaking, droplets show both Wenzel and Cassie on the textured surface. In the Wenzel state, the droplets can immerse themselves in the rough structure and wet the entire rough surface [6]. In the Cassie state, droplets form an arch bridge between the air microcolumns without infiltrating the microstructure [7]. Cassie and Baxter proposed the Cassie-Baxter equation based on the difference of the area fractions of the solid-liquid interface and the gas-liquid interface when the droplets were infiltrated, and thus the different surface energies [8]. Through this equation, it can be seen that the size features of the surface micro-texture have a significant effect on the surface hydrophobicity of the material. In this regard, the current researchers using different processes in the metal, ceramic and polymer materials such as surface preparation of micro-textured surfaces with different geometrical and structural characteristics, and to achieve the superhydrophobic surface preparation [9], but the experimental study can only quantitative research of the relationship between the microstructure and contact angle, it is difficult to observe the solid-liquid-gas contact state. Therefore, by simulating the contact between droplet and textured surface in the process of droplet, the main structural parameters including the influence of the size of micro-dimples and the density of micro-dimples on the static contact angle, that is, the surface hydrophobicity, are studied and combined with the theory of wetting Discussion, designed to provide theoretical support for the design of related equipment.

## 2. Numerical Methods

### 2.1 Model Setup.

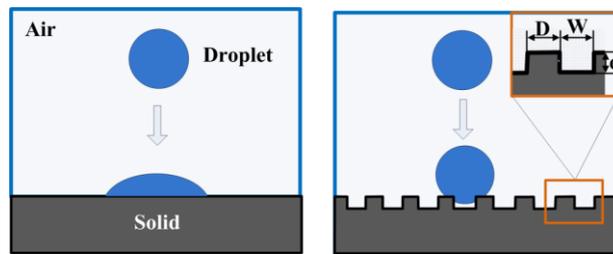


Fig. 1 Schematic of the physical model.

In the simulation, the liquid phase is set as water, and its specific physical parameters are: density  $\rho = 1000 \text{ kg / m}^3$ , viscosity  $\mu = 1 \times 10^{-3} \text{ Pa} \cdot \text{s}$ , and surface tension  $\sigma = 7.35 \times 10^{-2} \text{ N / m}$ . Set the acceleration of gravity  $g = 9.8 \text{ m}^2 / \text{s}$ , and its direction is vertical down, the initial shape of the droplet spherical diameter is 2 mm. A two-dimensional model was created using preprocessing software workbench. The simulated area was an  $8 \times 10 \text{ mm}$  symmetric 2-dimensional area. The texture dimensions are:  $W = 60 \text{ }\mu\text{m}$ ,  $D = 60 \text{ }\mu\text{m}$ ,  $d = 20 \text{ }\mu\text{m}$ . In the process of simulation, the shape of gas-liquid free interface changes obviously. The uniform grid of quadrilateral is used to divide the quadrilateral grid into a total of 40,000 to 45,000 quadrilateral grids. ANSYS12 FLUENT was used for numerical calculation and post-processing. The solver used in the numerical model was pressure based implicit algorithm, multiphase flow model was VOF model, and pressure-velocity coupling method was Fractional Step method. The wall of the lower boundary of the simulation area is set as the wall with hydrophilic property, the contact angle of the wall is set to be  $70^\circ$ , and the rest of the boundaries are set as the pressure inlet boundary and the pressure is zero. The boundary of the wall is free of slip boundary conditions, is the velocity components are all zero.

### 2.2 Boundary Conditions and Parameters.

The structural features of the micro-texture also have an influence on the spreading and static contact angle of the droplet, thereby exploring the structural change of the micro-texture, including the areal density and the size of the droplet, in order to explore the transition of the wetting state And the impact of the speed of the relationship. In this paper, we mainly simulate the process of liquid droplet textured surface to study the influence of the microstructure texture on the static contact angle of the droplet, that is, the hydrophobic property of the surface. The structural parameter design is shown in Table 1. The process of droplet simulation is mainly controlled by the droplet in the vicinity of the texture surface free fall, to ensure that the critical speed approaches 0 m/s, and when the droplet is stable, steady-state contact angle calculation.

Table 1 Geometrical parameters of micro texture

Samples	G1	G2	G3	G4	G5	G6	G7	G8	G9
W / $\mu\text{m}$	40	40	40	60	60	60	80	80	80
D / $\mu\text{m}$	20	40	60	30	60	90	40	80	120
d / $\mu\text{m}$	20	20	20	30	30	30	40	40	40

## 3. Results and Discussion

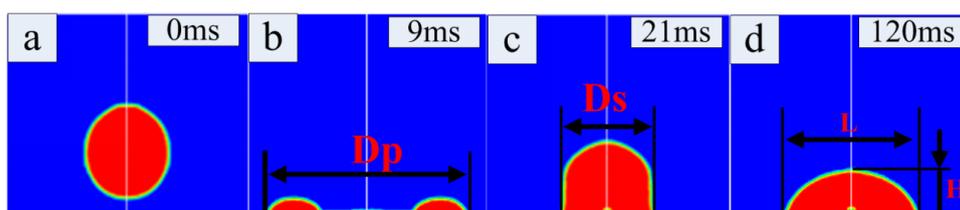


Fig. 2 Process of droplet impact on the surface.

When the drop has a certain velocity impacting the surface of the material, the dynamic process of the droplet generally goes through four stages, as shown in Figure 2. Droplets drop at a certain height

(Figure 2a). Droplets with larger kinetic energy gradually spread due to inertia when they contact the surface, until they reach the maximum spreading diameter (Figure 2b), begin to retract under inertia and reach a minimum Shrink the diameter (Figure 2c) and then circulate the above process and finally stabilize (Figure 2d). Shown in Figure 2 for the static contact angle calculation diagram, in which independent variable H can be calculated by the number of grid calibration (single grid side length of 0.05mm); argument L by observing the contact line contains the number of dimples Calibration. The contact angle is then calculated according to the equation:  $\theta = 2 \tan^{-1} (2H / L)$ .

In the simulation, assuming that the solid wall is not modified or textured with low surface energy, the solid contact angle of the solid wall in the contact area of the droplet is  $70^\circ$ , at which point there is a great adhesion between the drop and the surface. Figure 3 shows the simulated contact angle  $\theta$  and theoretical contact angle  $\theta_c$  versus A, where A represents the dimples dimensionless surface density.

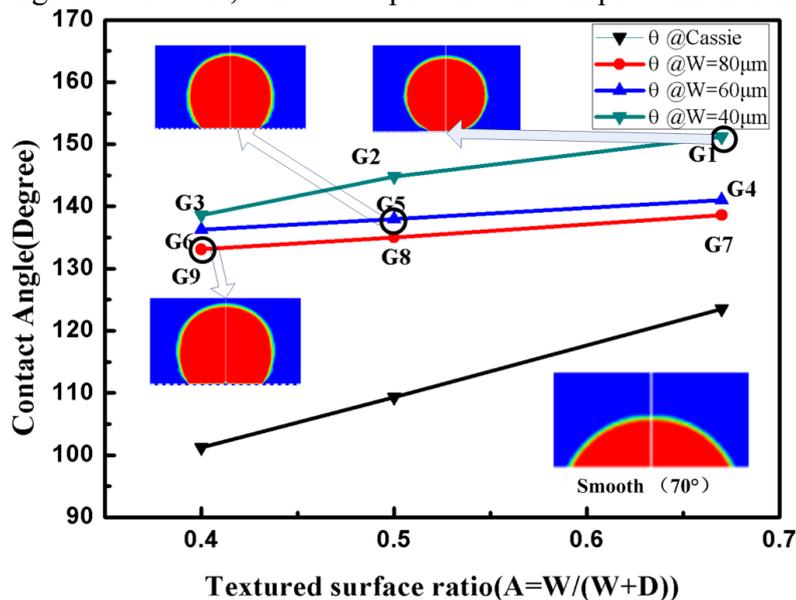


Fig. 3 Contact angle of textured surface under set conditions.

Figure 3 shows the contact angle of textured surface with different areal densities and dimple diameters. The values of contact angles  $\theta$  and  $\theta_c$  change with respect to A, and A represents the texture density of the dimples. Where  $\theta$  and  $\theta_c$  denote the calculated and theoretical values of the contact angles respectively. The calculated value  $\theta$  increases with A and is proportional to A, and the calculated and theoretical values remain similar to the trend of growth; however, it should be noted The result is that the difference between  $\theta$  and  $\theta_c$  is about  $30^\circ$ , Mainly due to the fact that the surface properties dominate the overall process where the drop velocity V approaches zero, where the droplet does not have enough kinetic energy Further spreading, at which point the movement of the line of contact is limited by the raised portion of the textured surface, the adhesion of the contact surface prevents movement of the line of contact, allowing the droplet to maintain a higher contact angle on the textured surface. Therefore, the simulated contact angle of the highly wettable material surface is greater than the corresponding theoretical contact angle.

Figure 4 shows the variation of surface contact angle with dimple diameter with different micro-texture surface densities. Under different micro-textured surface densities, the contact angle  $\theta$  value changes with respect to the dimple size. From the figure, the static contact angle of droplets on the wall surface with dimple surface density of 66% and dimple diameter of  $40 \mu\text{m}$  is calculated. The contact angle was calculated to be  $151.2^\circ$  to achieve superhydrophobicity. When the dimple diameter increased to  $60 \mu\text{m}$  and  $80 \mu\text{m}$  respectively, the static contact angles of the corresponding droplets are  $141^\circ$  and  $138.6^\circ$ , respectively. The static contact angle decreases with the increase of the dimple diameter, and the same is obtained when the areal density is 50% and 40%, respectively. But the surface remains highly hydrophobic. The above results indicate that the relatively small micro-texture contributes more to the hydrophobic properties of the material surface, which is still related to the

solid-liquid real contact area, such as G1, G4 and G7, the surface density of micro dimples remains at 66%. Theoretically, the solid-liquid contact area remains constant, but when the drop is in contact with the solid, it is more likely to dip into the relatively large dimple, effectively increasing the real contact area of the solid-liquid as it contacts the inner wall of the dimple, But Cassie wetting equation can be found, when the solid-liquid contact area increases, the contact angle will decline, but because the droplets are dropping in a drop manner, increasing the size of the dimple only less liquid Drop in, so the contact angle decreased slightly, the surface remains highly hydrophobic (minimum 133.1 °).

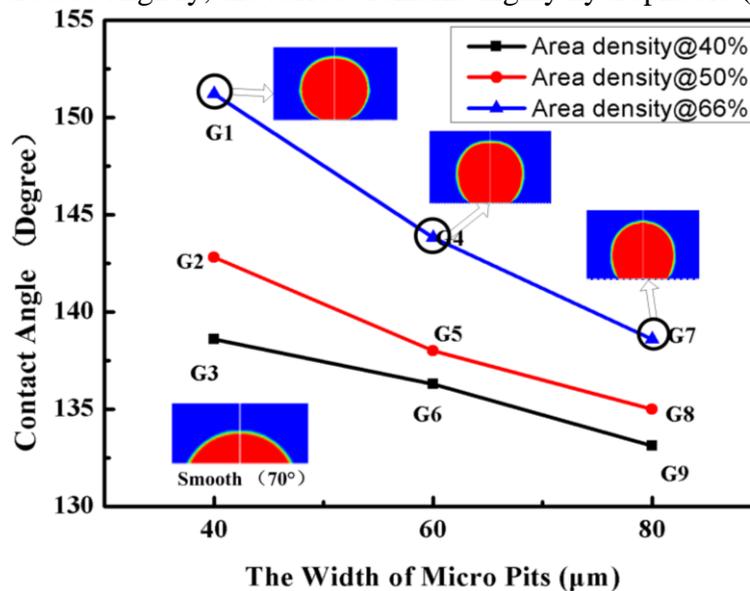


Fig. 4 Surface contact angle vs. micro-texture surface densities.

#### 4. Conclusion

In this paper, Ansys Fluent software is employed to fabricate microstructures with different structural features on the proposed smooth surface with hydrophilic character ( $CA = 70^\circ$ ) to study the effects of dimple diameter and dimple surface density on the surface hydrophobicity. Through the numerical results, the following conclusions are drawn:

- (1) Preparation of micro-texture on a smooth surface can achieve surface wetting transitions, resulting in surfaces with superhydrophobic properties. It is found that the variation of contact angle has a uniform variation. And the static contact angle of the surface drops gradually increases with the increase of micro-texture density.
- (2) The textured surfaces with dimples in the range of 40 - 80  $\mu\text{m}$  are highly hydrophobic or superhydrophobic. When the dimple diameter is reduced, the static contact angle of the micro-textured surface decreases but the hydrophobicity remains high.

#### Acknowledgements

This work was financially supported by the National Natural Science Foundation of China via grant number 51505194, the Natural Science Foundation of Jiangsu Province via grant number BK20150517 and the Senior Talent Start-up Foundation of Jiangsu University via grant number 15JDG033.

#### References

- [1] A. Marmur. Wetting on hydrophobic rough surfaces: To be heterogeneous or not to be?, *Langmuir*, Vol. 19(2003), No.20, p. 8343-8348.
- [2] Z. Zhang, M. Ha and J. Jang. Contrasting water adhesion strengths of hydrophobic surfaces engraved with hierarchical grooves: lotus leaf and rose petal effects, *Nanoscale*, Vol. 9(2017), No. 42, p. 16200-16204.

- 
- [3] L. Feng, S. Li, Y. Li, et al. Super-hydrophobic surfaces: From natural to artificial, *Advanced Materials*, Vol. 14(2002), No. 24, p. 1857-1860.
- [4] K. Golovin, M. Boban, J. M. Mabry, et al. Designing Self-Healing Superhydrophobic Surfaces with Exceptional Mechanical Durability, *Acs Applied Materials & Interfaces*, Vol. 9(2017), No. 12, p. 11212-11223.
- [5] J. Quek, C. Magee and H. Low. Physical Texturing for Superhydrophobic Polymeric Surfaces: A Design Perspective, *Langmuir*, Vol. 33(2017), No. 27, p. 6902-6915.
- [6] E. Bormashenko, Y. Bormashenko, G. Whyman, et al. Micrometrically scaled textured metallic hydrophobic interfaces validate the Cassie-Baxter wetting hypothesis, *Journal of Colloid and Interface Science*, Vol. 302(2006), No. 1, p. 308-311.
- [7] C. Lai and W. Choi. Unidirectional Wetting in the Hydrophobic Wenzel Regime, *Advanced Materials Interfaces*, Vol. 2(2015) , No. 4, p1400444.
- [8] Y. Gerbig, A. Phani and H. Haefke. Influence of nanoscale topography on the hydrophobicity of fluoro-based polymer thin films, *Applied Surface Science*, Vol. 242(2005), No. 3, p. 251-255.
- [9] S. Cui, S. Lu, W. Xu, B, et al. Fabrication of robust gold superhydrophobic surface on iron substrate with properties of corrosion resistance, self-cleaning and mechanical durability, *Journal of Alloys and Compounds*, Vol. 728(2017), p. 271-281.