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Analysis of impact phenomenon on superhydrophobic surfaces based on molecular dynamics simulation

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ABSTRACT

The dynamic behavior of hydrophobic material directly effects its application. The impact phenomenon of droplets on hydrophobic materials is an important indicator to characterize the dynamic properties of hydrophobic materials. At present, the study on impact phenomenon mainly focuses on macroscopic experiments and theoretical analysis. This paper adopts molecular dynamics simulation to systematically investigate the impact phenomenon of a nano-sized water droplets on pillared graphite surface on the nano-scale. The effects of impact speed and angles of nanodroplets on impact phenomenon of droplets was quantitatively analyzed by a variety of impact simulations. Results showed that the droplets experience Cassie, Cassie-Jumping, Wenzel-Jumping, Wenzel-Cassie and Wenzel state successively with the increase of the collision angle and velocity. A rebounce occurs easily at an intermediate collision angle and bigger velocity. By changing the gap, height and area of the pillars on substrate, the influence of the hydrophobic property on impact phenomenon is analyzed. Studies illustrates that the dimensions of the gaps and height of pillars on graphite substrate have a more significant effect on the impact phenomenon when compared with the area of pillars. This research can provide a theoretical reference for the study of dynamic wetting behavior of hydrophobic material.

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1. Introduction

Hydrophobic materials have great potential in engineering applications such as pipeline transportation, filtration and drag reduction on water surface etc. due to the superior water repellency properties [1–3]. Hydrophobic property of material includes two parts: the static property and the dynamic property. The static property mainly characters the water repellency of the material, and the dynamic property considers the robustness the water-repellent state and the stability of the hydrophobic material.

Physical conditions, such as impinging, increasing of the droplet's mass, hydraulic pressure etc. can cause the failure of hydrophobicity [4]. Wherein, there exist a variety of phenomenon when droplets impinging a superhydrophobic surface, including expansion along the surface, splashing and bouncing etc. [5–8]. By studying the impact phenomenon of the droplets, the wettability of hydrophobic material, especially the dynamic hydrophobic properties can be deeply understood.

Hydrophobicity of the solid surface is governed by its surface chemical property and geometrical microstructure. It can be improved by reducing the surface free energy of the surface and designing the micro/nano structures of projections [9–13].

Researchers has carried out extensive research on the influence of micro/nano structure on hydrophobicity. Goodwyn et al. [14] demonstrated for the first time the mechanism of the superhydrophobicity of the cuticle of water striders and pointed out that the topography of the surface plays a dominant role in superhydrophobicity. Lundgren et al. [15] studied the behavior of nanoscale water droplets at solid surfaces and pointed out the importance of detailed topography and composition of the solid surface. Jin et al. [16] prepared superhydrophobic aligned polystyrene nanotube via a simple template wetting method, and the CA achieved was 162°. Rafiee et al. [17] studied the influence of graphene coatings on wetting properties of materials and confirmed through molecular dynamics simulation (MDS) that graphene's wetting transparency is related to its extreme thinness. Ambrosia et al. [11] researched the effect of pillar surface fraction and pillar height on CAs by MDS and found that the smaller the pillar surface fraction, the larger the change in the CA as the pillar height increased. Yong et al. [18] researched the correlations between the contact angle, roughness factor and surface fraction on groove-patterned surfaces. Niu et al. [19] evaluated the dynamic behavior of the water droplets on pillared solid surfaces by applying a vibration to the surface.

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For the dynamic hydrophobicity, Reyssat et al. [20] researched the factors influencing the bouncing of droplets by changing the dimension of microstructure on hydrophobic surfaces. The research found that the increase of the height of pillars make the threshold velocity increase. Bartolo et al. [21] found that the bouncing only occurred within a certain range of velocity. The simulation of a bouncing droplet on nano scale is deficient. Koishi et al. [22] studied the free-energy barrier of graphite substrates with different height of nanopillars by a series of kinetic rainning simulations. Hirvi et al. [23] investigated the rebouncing of nanodroplets on most hydrophobic PE and less hydrophobic PVC and illustrated that bounce occurred on most hydrophobic PE surface with a medium speed.

At present, the research on hydrophobic property, including experiments and simulations, is mainly focused on the static aspect. For the dynamic hydrophobic prosperity, Researchers has studied the impact phenomenon by a series of experiments, due to size restriction, experiments can't observe and study the microscopic interaction between the hydrophobic surface and water intuitively. In recent years, with the development of computer speeds and simulation software, The MDS method has been used to research the dynamic hydrophobicity and many studies have proved good agreement between macro-scale experimental data and nano-scale MD simulations. MDS method can break through the limitation of scale, explore the influences of microscopic nature on the macroscopic phenomena and expand the research on the experiments that are difficult to be realized on a macro level. [22,23] provides a new thinking for impact phenomenon of water droplets on hydrophobic surface. But [22] is mainly focused on the influence of a vertical impact droplet on free-energy barrier, [23] only researched the rebounce phenomenon and critical rebounce velocity of a vertical impact droplet on two different hydrophobic surfaces. The simulation on impact phenomenon is still incomplete.

In this paper, MDS were used to systematically investigate the impact phenomenon of droplets on hydrophobic graphite surface with quadrangle pillars. The goal of this research is to understand the impact phenomenon on the nano-scale and clarify how the dimensions of the quadrangle pillars affects the impact phenomenon. To reach this goal, MDS model was prepared for a water droplet of 4096 molecules to impact the pillared graphite with a ranges of impact velocities and collision angles. The effect of dimensions of the pillars on the substrate was also investigated by changing the areas, gaps and height of the pillars.

2. MDS model and simulation method

2.1. Cassie and Wenzel model

The wettability of hydrophobic material is mainly characterized by Wenzel state and Cassie-Baxter state. Wenzel theory predicts the contact angle of a wetted contact as a result of the surface roughness (r) on a rough surface, as shown in Eq. (1) [24].

$$\cos\theta = r\cos\theta_0 \tag{1}$$

While Cassie and Baxter derived another equation to approximate the contact angle as

$$\cos\theta = f(\cos\theta_0 + 1) - 1$$

where θ is the contact angle on the rough surface, θ_0 is the contact angle on a perfectly flat surface, r is surface roughness factor which is defined as the ratio of the actual area of the rough surface to the geometric projected area. f is the ratio of the actual solid/liquid interface to the geometric projected area.

2.2. MDS model

2.2.1. Configuration of substrates

This paper chose graphite as a base material, since its hydrophobic properties could be easily adjusted. Referred to [22], the configuration of the pillars, including the lateral size of quadrangular pillars $P_x \times P_y$, the spacing between two adjacent columns $G_x \times G_y$ and the height of the pillars, is illustrated in Table 1 (see Fig. 1).

2.2.2. Simulation model

Fig. 2 illustrates the simulation model. A 16 × 16 × 16 (4096) water molecules cube with a side length of 49.6 Å was built 85 Å from the top of the substrate, so the density of the water cube is about 0.997 g/cm^3 at 298 K. The dimensions of the substrate were 200 Å × 200 Å. In this case, the lateral size of the solid surface was about 4 times the length of the water cube, there were no significant interactions beyond the boundary. Atoms of the solid surface were fixed. All simulations were performed based on the LAMMPS package. Non-polarized rigid-body SPC/E water molecules were used. The hydrogen bond length and bond angle of water molecules were constrained by SHAKE method during the simulation. The forces of the SPC/E model included 2 terms, the Coulomb force and LJ potential. The Coulomb force was calculated as the interaction force of a hydrogen atom with another hydrogen or oxygen atom. The LJ potential was considered only between O and O atoms in order to simplify the calculation. The simulations were performed with a constant number of molecules, volume and temperature (NVT ensemble). The temperature of the system was controlled at 300 K by Nose/Hoover thermostat. Periodic boundaries were defined in the X and Y direction to reduce the number of atoms required for the simulation. The water cube was equilibrated in the initial position for 500 ps. Then the droplet was imposed a certain velocity and angle to impact the pillared surface without an effect of temperature coupling to the velocities, so that the velocity maintained unchanged before interacting with the graphite. The total system was equilibrated for 1 ns with a time interval of 2 fs.

2.2.3. Wetting state

The impacting process when a droplet impacts the pillared surface can be divided into four stages, as shown in Fig. 3. The initial stage is the stage the droplets begin to impact and touch the pillared surface. Then the droplet will expand rapidly, the height of the center of mass (CM) will decrease continuously until the vertical velocity component reduces to 0, which is called impact stage. Subsequently, the droplet will react due to the deformation of the droplets and hydrophobicity of the surface, resulting in the raising of the droplet, which is called recovery stage. After the recovery stage, the droplet can either bounce off the surface or stay on the substrate in Cassie or Wenzel state, which is called the equilibrium stage. It can be founded by a large number of simulations that there exist a variety of phenomena when a droplet impact the pillared surface with different angles and velocities. The wetting state

Table 1
Lateral pillar and gap dimensions.

Type	$P_x \times P_y$	$G_x \times G_y$	H
$P_1G_3H_2$	7.5 Å × 7.5 Å	12.5 Å × 12.5 Å	13.6 Å
$P_2G_3H_2$	10.0 Å × 10.0 Å	12.5 Å × 12.5 Å	13.6 Å
$P_3G_3H_2$	12.5 Å × 12.5 Å	12.5 Å × 12.5 Å	13.6 Å
$P_3G_1H_2$	12.5 Å × 12.5 Å	7.5 Å × 7.5 Å	13.6 Å
$P_3G_2H_2$	12.5 Å × 12.5 Å	10.0 Å × 10.0 Å	13.6 Å
$P_3G_3H_1$	12.5 Å × 12.5 Å	12.5 Å × 12.5 Å	6.8 Å
$P_3G_3H_3$	12.5 Å × 12.5 Å	12.5 Å × 12.5 Å	20.4 Å

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