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Self-Propelled Jump Regime in Nanoscale Droplet Collisions: A Molecular Dynamics Study

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Abstract. Self-propelled jump of droplets is among the most striking phenomena in droplet collisions on substrates. Self-propelled jump phenomena of droplets have been observed in experiments, which have also been reproduced in macro- or mesoscale numerical simulations. However, there have been few previous studies on the phenomena at nanoscales. To unravel the dynamics and mechanisms of nanoscale binary droplet collisions on substrates, head-on collision processes of two identical water droplets with diameters of 10nm on graphite substrates are investigated by molecular dynamics (MD) simulations. By varying the impact Reynolds number of binary droplet collisions on hydrophilic or hydrophobic substrates, we successfully reproduce self-propelled jump of droplets on a super-hydrophobic surface with a contact angle of 143° and a relatively high impact Reynolds number of 17.5. Parametric studies indicate that both high impact Reynolds numbers and high hydrophobicity promote self-propelled jump. Moreover, the criterion based on the Ohnesorge number derived from the mesoscopic self-propelled jump regime is insufficient to precisely predict a nanoscale self-propelled jump phenomenon. For this reason, our study includes the impact Reynolds number and the substrate properties like contact angle as additional criteria to refine and extend the current theory for the self-propelled jump behaviours to nanoscales. The study provides insight into the mechanism of self-propelled jump phenomenon at nanoscales.

AMS subject classifications: 76T99

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1 Introduction

Self-propelled jump of droplet phenomena, depicting that a large droplet formed by binary droplet collisions on a super-hydrophobic surface propels itself to jump away from the surface [1], are frequently encountered in both natural and industrial processes like water-repellent surfaces [2, 3]. These interesting phenomena have been applied to developing functional surfaces which are effective in anti-dew [4], anti-icing [5] or self-cleaning [6]. Despite some successful applications of the phenomena, understanding of the mechanisms associated with the self-propelled jump regime is still preliminary [7, 8]. Experimental and numerical studies using, for example, lattice Boltzmann method (LBM) have already reported self-propelled jump regime in macro- and mesoscales, and their analyses are mostly from the perspectives of energy, without any detailed account of flow dynamics [9, 10]. Details of the nanoscale collision process are difficult to obtain through experiments or continuum simulation methods, especially when the substrate-droplets distance is within a distance comparable to the molecular mean free path. Thus, computer simulations considering atomic effects are currently the only way to reveal droplet dynamics when the substrate-droplet distance comes within nanoscale [11]. Yet up to the present time, the published simulations have not considered the atomic effects. Such an absence is intriguing as it suggests the possibility that the self-propelled jump phenomenon may not exist in nano-droplet collisions on a substrate while it was observed in micro- and macro-droplet collisions.

In this research, molecular dynamics (MD) simulations of water nano-droplet collisions on hydrophobic and hydrophilic substrates will be conducted. By varying the impact Reynolds number and substrate properties like contact angles, we successfully reproduce the self-propelled uprising behaviours under a proper combination of impact Reynolds number and contact angles. Meanwhile, a series of MD simulations will be undertaken to explore the different facets of the self-propelled jump phenomenon.

2 System construction and simulation details

2.1 System construction

To study the distinctive behaviours among hydrophilic and hydrophobic droplets on graphite substrates, three simulation systems were constructed. Each setup comprises two nano-droplets and a double-layer graphite surface, as shown in Fig. 1. The first system is an equilibrium system, and the other two systems aim to study the effects of hydrophobicity on droplet collision behaviours. Therefore, two contact angles between droplets and graphite substrates have been selected to represent different hydrophobicity. The contact angle, θ, of each simulation is 143 and 108 degrees, respectively.

The graphite substrate consists of two square staggered sheets with an interlayer distance of 3.4Å. The side length of each square graphite layer is 500Å. All the carbon atoms are individually fixed at their initial positions to represent an inert substrate. The origin