



Bounce regime of droplet collisions: A molecular dynamics study



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ABSTRACT

Droplet collisions have complex dynamics, which can lead to many different regimes of outcomes. The head-on collision and bounce back regime has been observed in previous experiments but numerical simulations using macro- or mesoscale approaches have difficulties reproducing the phenomena, because the interfacial regions are not well resolved. Previous molecular dynamics (MD) simulations have not reproduced the bounce regime either but have reported the coalescence and/or shattering regimes. To scrutinize the dynamics and mechanisms of binary collisions especially the interfacial regions, head-on collision processes of two identical nano-droplets with various impact velocities both in vacuum and in an ambient of nitrogen gas are investigated by MD simulations. With the right combination of the impact velocity and ambient pressure, the head-on collision and bounce back phenomenon is successfully reproduced. The bounce phenomena are mainly attributed to the “cushion effect” of the in-between nitrogen molecules and evaporated water molecules from the two nano-droplets. The analysis has verified and also extended the current gas film theory for the bounce regime through including the effects of evaporated water molecules (vapour). Some similarities and some dissimilarities between nanoscale and macro-/meso-/microscale droplet collisions have been observed. The study provides unprecedented insight into the interfacial regions between two colliding droplets.

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1. Introduction

Droplet collisions are encountered in both natural and industrial processes, such as, in the formation of clouds and rain drops [6], in the operation of nuclear reactors and in the process of spraying [5]. In recent decades, efforts have been made to unveil the fundamental mechanisms associated with coalescence and bounce of two identical droplets. Experimental studies have identified that under different atmospheric conditions most of head-on liquid-gas droplet collisions can be described using three distinct regimes: coalescence, bounce and reflexive separation [1,2,9,30]. Other studies using experimental and numerical methods such as the level set, volume of fluid, immersed boundary method, lattice Boltzmann method have already presented various phenomena of droplet collisions [4,7,14,17–19]. Even so, details of the collision process are difficult to obtain through experiments and continuum simulation methods, especially when the approaching droplets are

within a distance comparable to the molecular mean free path. It should be noted too that the lattice Boltzmann method has been successful in reproducing all the collisions regimes except the head-on collision and bouncing regime [18]. Thus, computer simulations considering atomic effects become the only method to understand droplet dynamics when the separation distance comes within nanoscale. Yet up to the present time, the published simulations have only reproduced coalescence and shattering regimes [8,11,12,16,22,26,31] but not the bounce regime. Such an absence is intriguing as it suggests the possibility that the bounce regime may not exist in nano-droplet collisions while it was observed in micro- and macro-droplet collisions. Our study has, however, successfully observed the bounce behaviours with two nanoscale water droplets, thereby completing the regime map of the nano-droplet collision phenomena.

In this research, molecular dynamics (MD) simulations of droplet collisions in vacuum and in ambient gas have been conducted to reproduce the bounce behaviours of nano-droplets. Our research will demonstrate that bounce frequently occurs in nanoscale droplet collisions. Such occurrences are influenced by parameters including pressure and impact velocity. Moreover, a “cushion effect” will be proposed to reveal the impact of the ambi-

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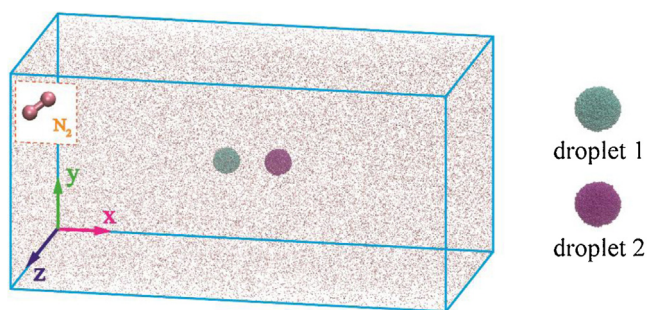


Fig. 1. The initial setup of the simulation system. Binary nano-droplets of 10 nanometers in diameter are submerged in nitrogen gas molecules and approach each other at equal speed along the x direction.

Table 1
Values of potential parameters.

atom	σ (Å)	ε (kcal/mol)
O–O	3.188	0.102
H–H	0.000	0.000
N–N	0.072	3.320

ent gas and vaporized water molecules on droplet behaviours during the bounce process.

2. Molecular dynamics simulations

Fig. 1 illustrates the initial setup of the simulation system with two nano-droplets submerged in the nitrogen gas.

The dimension of the simulation box is $800 \text{ \AA} \times 400 \text{ \AA} \times 400 \text{ \AA}$, and the origin of the coordinates was set at the left bottom back corner. Two identical droplets with diameters of 10 nm were placed along the x direction at the central part of the box with x coordinates being 500 \AA and 1500 \AA , respectively. The TIP3P water model [10,15] was chosen for water molecules because it offers a sufficient description of intermolecular forces in water in MD simulations. Nitrogen molecules were treated as Lennard-Jones particles. Intermolecular interactions between water and nitrogen molecules included both Coulombic and Lennard-Jones (L-J) 12–6 potentials [3,24,27], as shown in Eq. (1).

$$U_{ij} = \frac{q_i q_j}{r_{ij}} + 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad (1)$$

where q represents the charge of particle, and r is the distance between any two atoms, and σ and ε represent the zero energy separation distance and the minimum energy, respectively. The subscripts i and j are the atom indexes. The Lorentz-Bertthelot mixing rule was employed for calculating the potential parameters between water and nitrogen molecules. L-J parameters used in this research are summarized in Table 1. A cut-off distance of 16 \AA was adopted. Periodic boundary conditions were applied to all three directions. All the simulations were carried out using the LAMMPS platform [21].

Equilibrium simulations of droplets and ambient gases were conducted before the collision simulations. For droplets, the equilibrium was undertaken in vacuum at the temperature of 300 K, and the canonical ensemble (NVT) was employed. After equilibrium of 2 ns, a single droplet can be generated by removing all the vaporized molecules around. The second droplet was obtained by duplicating the first one. Meanwhile, ambient nitrogen molecules were also equilibrated at 300 K in a parallel equilibrium simulation.

After equilibrium, the two droplets were first placed in the required positions, and then equilibrated ambient gas molecules

were added to fill the remaining space of the box. A further simulation was conducted for 2 ns to equilibrate the final system consisting of both droplets in ambient gas molecules. In the formal collision simulations, each droplet was assigned the same impact velocity along the x direction.

3. Results and discussion

3.1. Reproduction of bounce regime by MD simulations

Droplet collisions were first simulated in vacuum with impact velocities varying in a broad range from 5 to 500 m/s. Results have shown that the binary droplet collisions in vacuum follow either coalescence regime or shattering regime regardless of how the impact velocities vary, which is consistent with previous studies [13,20]. However, a bounce regime could never be found under the vacuum condition.

Binary collisions were then simulated with the existence of the ambient gas. With the impact velocity 8 m/s ($v=8 \text{ m/s}$) and the ambient pressure 2.7 atm ($p=2.7 \text{ atm}$), we found that the binary collision fell within the bounce regime (Fig. 2b and c). The whole process consists of three key stages. At the very beginning ($t=0-2.8 \text{ ns}$), the two droplets approach each other with very small deformation, whilst a small number of water molecules escape from the two droplets. The second stage ($t=2.8-4.2 \text{ ns}$) is reached when the distance between the two droplets reaches the minimum, where the droplets appear to be stationary. At this stage, the inter-droplet distance remains almost constant, whilst water molecules continue to escape from both droplets. Moreover, some of the water molecules escaping from one droplet are absorbed by the other droplet. The last stage ($t=4.2-5.6 \text{ ns}$) – the bouncing stage – occurs when an increase in the inter-droplet distance is clearly observed. Interestingly, the droplets are found to separate from each other along routes that deviate from the trajectories of the approaching droplets. Moreover, the separation velocity of the two droplets is detected to be smaller than the impact speed ($v=8 \text{ m/s}$). The deviating routes are attributed to the interactions between the water and nitrogen molecules, which are not entirely deterministic. The smaller separation velocity (as compared with the impact velocity) is due to the momentum loss through the escaping molecules as well as interactions with the ambient gas molecules.

3.2. Explanation for bounce regime

As for the cause for bouncing only in the presence of ambient gases, the theory of “gas film” is a popular explanation for droplet dynamics at microscale. Qian and Law [25] stated that the ambient gases form a gas film between the two droplets as the inter-droplet distance becomes tiny in the approaching stage. As the gap between the droplets decreases, the gas film pressure increases dramatically, leading the droplets to bounce back. Our results appear to support this physical picture, but at nanoscale. Furthermore, we have extended the “gas film” theory, which will be shown in detail in the following discussion.

The first step is to scrutinize the composition of the gas film. To distinguish whether a water molecule belongs to the parent droplet or has evaporated, the surface of the droplet should be defined. However, at the molecular scale, a nano-scale droplet has no well-defined surface as its macro-scale counterpart usually does. Thus, a criterion has been proposed to definite the surface. For two random molecules in the simulation box, if their distance (r_{ij}) is smaller than a critical value (R_{cl}), the two molecules are regarded in the same droplet. The droplet is defined as a set of molecules, each of which is within the R_{cl} from one or more molecules in the droplet Powles [23] had applied this method and suggested $R_{cl} = 1.9\sigma$. Any water

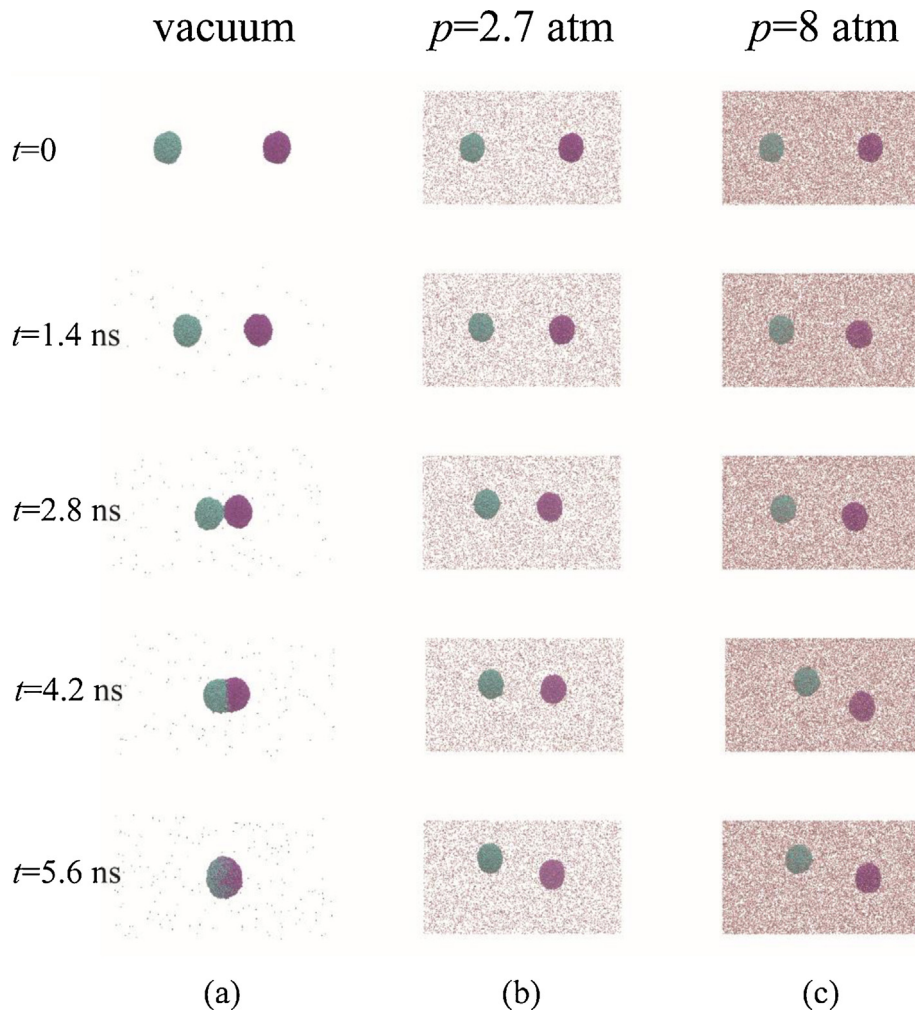


Fig. 2. Different collision regime for three different ambient gas pressure when $v=8$ m/s.

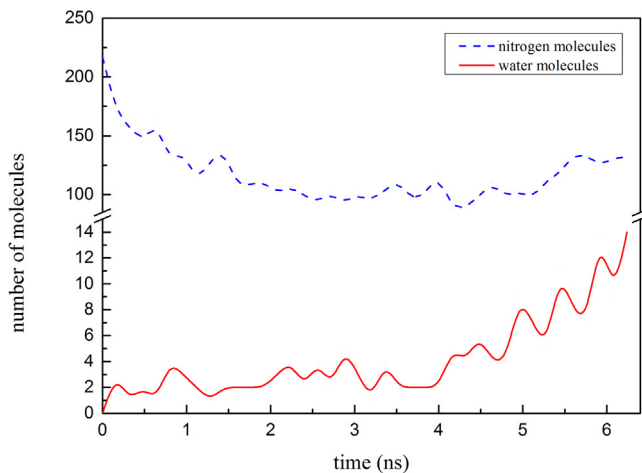


Fig. 3. The evolution of numbers of nitrogen and evaporated water molecules between the two droplets when $v=8$ m/s and $p=2.7$ atm.

molecule can be regarded exactly as an evaporated molecule or an intra-molecule of the droplet with this method.

Using the artificial surface method, the instantaneous numbers of nitrogen and evaporated water molecules in the gas film between the two droplets have been counted and shown in Fig. 3. The gap which is the rectangular region between the two droplets

can be defined by the position of molecules in the surface in all the directions. For example, at time=0 ns, the two droplets with diameters of 10 nm were placed along the x direction at the central part of the box with x coordinates being 200 Å and 600 Å. The 300 Å × 100 Å × 100 Å rectangular region between the two droplets is where the 225 nitrogen molecules in. In Fig. 3, when the two droplets are approaching each other ($t=0$ –2.8 ns), the number of nitrogen molecules between the two droplets decreases, which means that the nitrogen molecules are squeezed out of the space between the droplets. Meanwhile, an increasing number of evaporated water molecules occupies the in-between space. Interjacent molecules between the droplets therefore constitute both the nitrogen molecules and the evaporated water molecules. In the second stage (from 2.8 ns onwards), the two droplets have slowed down significantly, and the number of interjacent nitrogen molecules stops decreasing, but more water molecules continue to evaporate to fill the in-between space. As evaporating water molecules further reduce the momentum of the droplets, the droplets are not able to overcome the gas film and consequently come to an almost standstill ($t=2.8$ –4.2 ns). The process resembles droplets hitting a cushion, which can be called the “cushion effect” of the interjacent molecules. Afterwards, momentum exchange between the two droplets through the interjacent gases leads to the bounce back of the two droplets, which is aided by the continuing evaporation of water molecules from the droplet surfaces.

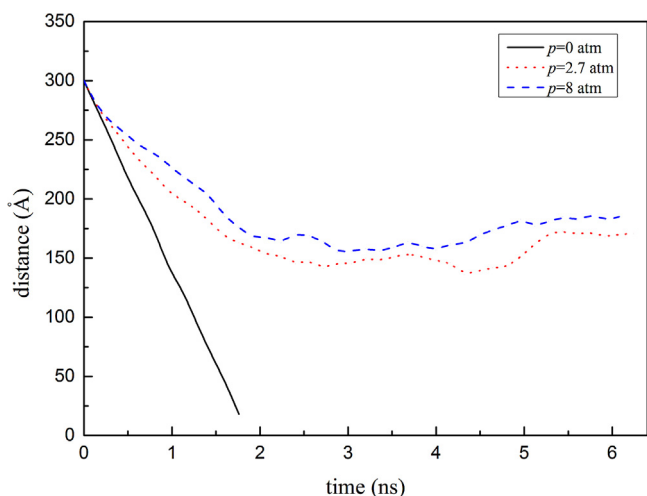


Fig. 4. Evolutions of two droplet frontier distances when $v = 8$ m/s and $p = 0, 2.7$ atm and 8 atm.

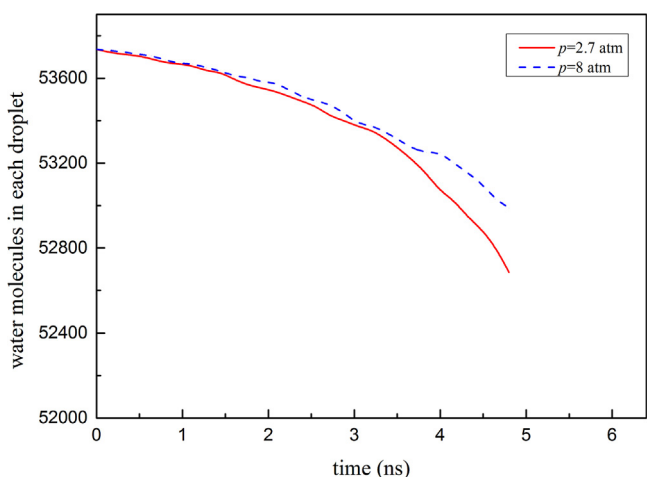


Fig. 5. Evolutions of water molecules at $v = 8$ m/s with pressures of 2.7 atm and 8 atm.

3.3. Influencing parameters of bounce regime

In our research, ambient pressure and impact velocity of droplets are two key parameters which may influence the droplet behaviours. To scrutinize their effects on the bounce regime, simulations with different ambient pressure and impact velocity have been conducted.

3.3.1. Ambient pressure

As mentioned previously, coalescence happens (Fig. 2a) when two droplets collide in vacuum which is an extreme case of decreasing ambient pressure.

When the ambient pressure increases to 8 atm, the bounce regime occurs as expected. Compared with the lower pressure case ($p = 2.7$ atm) in which the minimum distance between the two droplet frontiers is 141 Å, the higher pressure causes a larger droplet frontier distance (155 Å), as shown in Fig. 4. The number of water molecules in each droplet at pressures of 2.7 atm and 8 atm are also recorded and shown in Fig. 5. Obviously, a higher pressure inhibits the evaporation of water molecules. In fact, higher pressure contributes to a more compact layout of molecules and shorter inter-molecules distances, and thus stronger atomic or molecular interactions. In the meantime, when pressure is higher, nitrogen molecules are more densely distributed and more nitrogen molecules stay in the in-between space. The gas film would

feel more “stiff” less “elastic”. Consequently, droplets would find it more difficult to approach each other and the minimum distance between the two droplet frontiers increases.

3.3.2. Impact velocity

When the impact velocity increases to 15 m/s, coalescence, instead of bounce, of the two droplets can be observed (Fig. 6a). Analogous to the vacuum low-impact-velocity collision simulation (Fig. 2a) and experimental observation [28,29], the two droplets rapidly approach each other before they finally merge into a large droplet ($t = 1.6$ ns). During the approaching process, the two droplets dramatically decrease the in-between space for accommodating nitrogen molecules and evaporated water molecules. Thus, “cushion effect” of the gas film is not strong enough and the two droplets combine into a large one. These results indicate that the bounce regime occurs as a balance between the competing factors of impact velocity and pressure, leading to different levels of the “cushion effect”.

Meanwhile, another case in which two droplets in an ambient of nitrogen gas are placed at the original positions without impact velocities (that is, $v = 0$) has been simulated (Fig. 6b). Several cases have been considered for ambient pressures $p = 0, 1$ atm, 2.7 atm and 8 atm, respectively (with the corresponding nitrogen densities of 0, 1.138 kg/m³, 3.074 kg/m³, and 9.116 kg/m³). The two droplets oscillate in all three directions with a maximum offset of 12 Å. At this separation distance, the van der Waals attractive forces are not effective while there are no bulk velocities to move the droplets in any specific directions. Instead, the oscillating positions of the nano-droplets reflect the random interactions between the in-between nitrogen molecules and the water vapour. These results have unveiled different behaviours of nano droplets from their macro or micro counterparts which tend to remain stationary without an impact velocity.

Both the higher ambient pressure and the lower impact velocity have been seen to promote bounce back, which can be attributed to the stronger interactions between interjacent molecules and two moving droplets. In vacuum, interjacent molecules only comprise water molecules evaporated from the droplets. The number of evaporated water molecules is too limited to push the droplets back, which allows further approaching, contacting and coalescence of the droplets. This kind of coalescence in vacuum at low impact velocities has been corroborated by previous studies [28,29]. When nitrogen molecules are introduced to provide an ambient pressure, interjacent molecules include both nitrogen and water molecules. The interactions between interjacent molecules and moving or stationary droplets become large enough to prevent coalescence, thereby enabling bounce to occur. When the impact velocity exceeds a certain threshold, however, the large momentum of the two moving droplets would overcome the “cushion effect” of the interjacent molecules, get into contact and coalesce.

3.4. Nano-scale collision regimes

The above zero impact velocity simulation indicates that nanoscale collisions have different behaviours from their macro- or micro-counterparts. The macroscale collision regimes successively contain stationary ($v = 0$), coalescence, bounce, coalescence and separation as the impact velocity increases [27]. The nanoscale collision regimes include approaching ($v = 0$), bounce, coalescence, shattering (in our follow-on paper) and possibly other regimes as the impact velocity increases. More detailed analysis of these issues are beyond the present paper and will be examined in future studies.

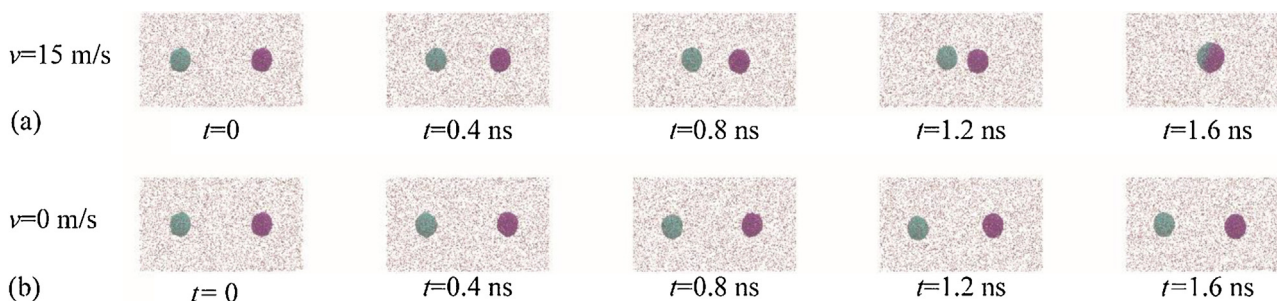


Fig. 6. Droplet behaviours at $v = 15$ m/s and $v = 0$ with $p = 2.7$ atm.

4. Conclusions

MD simulations of droplet collisions in vacuum and in ambient gas have been conducted to scrutinize the dynamics and mechanisms of binary collisions at molecular scale. The head-on collision and bounce phenomenon is successfully reproduced for the first time. The bounce phenomena are mainly attributed to the “cushion effect” of the in-between nitrogen molecules and evaporating water molecules from the two nano-droplets. The study has verified and extended the current gas film theory for the bounce regime by including the additional effects of evaporating water droplets. Moreover, the MD results show that low impact velocity and high ambient pressure promote bouncing. The behaviours of nanoscale droplet collisions have both similarities and dissimilarities to macro-/micro-droplet collisions. Finally, a set of regimes for nano-scale droplet collisions has been identified, but further details such as regime boundaries require extensive further investigations, which will be pursued in our future studies.

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