Chapter 3 Results and discussion

3.1 Simulation model

In this study, we used molecular dynamics simulations to investigate the dynamic behavior of single droplet on a liquid film laid a solid surface. The dimension of the substrate and the droplet are described in detail as follows:

3.1.1 The substrate

The substrate was composed of the liquid film layer and the solid layer. The liquid film and solid layer were arranged in face-centered cubic (FCC) lattice (001) surface. The dimension of the solid layer was $50\sigma\times50\sigma\times3\sigma$, where σ was the lattice constant. We used the different species, which were helium, argon and xenon in the same case. The dimension of the liquid film was $50\sigma\times50\sigma\times4\sigma$, $50\sigma\times50\sigma\times8\sigma$ and $50\sigma\times50\sigma\times16\sigma$, respectively. The total atoms of substrate were 54336,78672 and 127344, respectively. The number density of liquid film was $0.0127\,\mathring{A}^{-3}$ regarded as a liquid phase and the number density of solid layer was $0.0253\,\mathring{A}^{-3}$ regarded as solid phase. Before collision the substrate were equilibrated at 84K for 100000 time steps and the periodic boundary conditions were applied to the system.

3.1.2 The droplet

We used the three different radiuses to deal with the droplet, which were 7σ, 11σ and14.5σ, respectively. The total numbers of droplet were 1227,4759 and 9835. The droplet was also arranged in FCC lattice. The number density of droplet and liquid film were the same and equilibrated at 84K for 100000 time steps. The periodic boundary conditions were applied to the system. The Lennard-Jones potential supplied for both of the substrate and the droplet. The length scale σ and energy scale ε were show in Table 2.2.

3.2 The effect factors

When a droplet impacts vertically on a liquid film, it may eject a thin horizontal sheet (crown) or spread out the film surface. These behaviors depend on impinging drop size, impact velocity, liquid characteristics, and film thickness. We discussed the different effect and deformation of the droplet in detail as follows:

3.2.1 Impact velocity

There were three impact velocities to deal with the droplet, which were 500m/s, 1000m/s and 2000m/s. The sequences of phenomenon from 1 to 15 time steps utilizing visualization program “pvwin” were shown in Fig. 3.1~Fig. 3.81.

Fig. 3.82 showed the comparison of non-dimensional deformation radius and height of droplet with different impact velocity, 500m/s, 1000m/s and 2000m/s for droplet size = 11 σ_{Ar} and film thickness =8 σ_{Ar} .

3.2.1.2 Results

The phenomena of spread or splash were observed. However, the state of helium seemed to be a vapor phase and the argon seemed to be a solid phase. Therefore, these conditions were not to fit in with our expectation. So, we only centered on the condition for argon case. The results revealed that for the large impact velocity of the droplet (Weber umber is large), the inertia force of the droplet may overcome the surface tension of the liquid and splash takes place and for low impact velocity of the droplet, the droplet tends keep its spherical shape on the surface and it was like the spread behavior.

3.2.2 The film thickness

There were three-film thickness of the substrate that was 4σ, 8σ and 16σ to investigate the splash or spread phenomenon. The sequences of phenomenon from 1 to 15 time steps utilizing visualization program “pvwin” were shown in Fig. 3.1~Fig. 3.81.

Fig. 3.83 showed the comparison of non-dimensional deformation radius and height of droplet with different film thickness, $4\sigma_{Ar}$, $8\sigma_{Ar}$ and $16\sigma_{Ar}$ for droplet size=$11\sigma_{Ar}$ and impact velocity=1000m/s.

3.2.2.2 Results

The non-dimensional film thickness was between 0.135 ~ 1.14. The results revealed that the deformation of droplet with time. For the low H_f, the main phenomenon of droplet is like the crown breaking up into many tiny droplets shortly after impact. The whole crown expands outwards as the shape of a bowl. It occurred might the momentum transition from the film to the droplet in the system. The mechanism may the system In contrast, the droplet developed approximately cylinder-like crown normal to the surface for the large H_f.

3.2.3 The droplet size

There were three droplet size: the radius of droplet were 7σ, 11σ and 14.5σ, respectively. The sequences of phenomenon from 1 to 15 time steps utilizing visualization program “pvwin” were shown in Fig. 3.1~Fig. 3.81.

Fig. 3.84 showed the comparison of non-dimensional deformation radius and height of droplet with different droplet size, $7\sigma_{Ar}$, $11\sigma_{Ar}$ and $14.5\sigma_{Ar}$ for film thickness=$8\sigma_{Ar}$ and impact velocity=1000m/s.

3.2.3.2 Results

The similar behavior of non-dimensional film thickness related to the droplet was observed. But, when the droplet size was large, the droplet spread took place and easily spread over the surface. However, the deformation height is higher and it was hard to obtain the smooth surface. In contrary, the droplet size is small, the deformation height of droplet is small and it tends to spread slowly. It might be able to obtain the smooth surface.

3.2.4 The atom species

There were three species, helium, argon and xenon to deal with all atoms in molecular dynamics simulation. The sequences of phenomenon from 1 to 15 time steps utilizing visualization program "pvwin" were shown in Fig. 3.1~Fig. 3.81.

3.2.4.2 Results

In the simulation system, we assumed that number density and the real temperature were the same for all species. However, the results revealed that the phase of atom was not the state we anticipated for helium and xenon. The helium atoms seemed to be vapor and the xenon atoms seemed to be solid. So, we discussed mainly the argon system in the next chapter.