Chapter 4 Conclusions

Molecular dynamics simulation utilized visualizatioin program “pvwin” has showed the realistic behavior of droplet pictures, whose details should be compared to experiments. There are some conclusions with the different effects are described as follows:

The different velocity effects the development of splashing. For the large value of velocity of the droplet, the kinetic energy of the droplet is able to overcome the surface tension of the liquid and splash takes place. For low values of velocity of the droplet, the droplet tends keep its spherical shape on the surface and spread takes place. However, the film thickness is influential for the latter stages of flow development.

The range of non-dimensional film thickness H_f in the system is between 0.27~ 2.28. The main phenomenon is the crown wall break-up, which commonly starts from the lower part of the crown wall. Subsequently, the very thin crown wall broke up totally into many tiny droplets shortly after impact. The second phenomenon is that not only the upper rim of the crown but the whole crown wall significantly expands outwards as the shape of a bowl.

At the same impact velocity and the film thickness, the splashing radius and height as a function of time. The large droplet spreads faster on the surface. However, the splashing height increased with time, and it is hard to obtain a smooth coating surface. Therefore, it is advantageous to try to minimize the droplet size in order to obtain a smooth coating surface.

The molecular dynamics method is expected to be useful, for getting insight of physico-chemical problems at the molecular level. Further problems, such as surface adhesive properties and polymer blend fractures could be tackled by molecular dynamics simulation.