Chapter 1 Introduction

1.1 Motivation

1.1.1 Droplet collision dynamics

The droplet dynamics plays an important role in industrial applications such as a raindrop splashing on the ground, the impact of a fuel droplet on the walls of a combustion chamber, pesticide sprays, ink-jet printing, even more a comet impacts a planet, etc. The collision dynamics can be divided into two categories, including the droplet collision and the droplet collision on a liquid or solid surface. In the collision process, it is found that qualitatively different behaviors and phenomena can occur under different condition: the drop coalescence with the liquid surface, splashing by creating a crown, a so-called Worthington jet or a vortex, droplet rebound, etc.

1.1.2 Continuum scale

The normal impact of a single drop onto a liquid film is a complicated fluid mechanics phenomenon. The major physical processes include mass, momentum and energy conservation due to spray drop impingement, splashing effects, various shear forces, piston acceleration, dynamic pressure effects, gravity driven flow, conduction, and convective heat and mass transfer. In process of collisions, the droplet will lose kinetic energy as the droplet strains and deforms. The strains will lead to viscous dissipation, accounting for some conversion of mechanical energy to heat. To continue, the droplet surface increases and surface energy increases as well. The surface energy can be regarded as a potential energy and conservation of kinetic energy to surface energy can be regarded as a conservative process. The increase of surface energy during the early part of a collision will result in recoiling and rebounding later through the conversion of surface energy back to kinetic energy. The momentum balance occurs through a force imposed on the droplet by the wall in a collision as the droplet loses velocity.

1.1.3 Atomic scale

Due to the development of atomic-scale technology, nowadays it is unable to utilize the macro-vision of continuum model to explain the atomic-scale phenomenon. In order to understand the atomic-scale physical mechanism, molecular dynamics (MD) simulation is the most widespread and useful method to solve the atomic scale problem. To discuss the behaviors of droplet impacting on a liquid film, the MD method can be applied to all phases of gas, liquid and solid and to interfaces of these three phases.

1.2 Background

1.2.1 Droplet-solid collision

Recently, the droplet collision near solid surface can sort some states; one of them is the droplet impacting on solid surface directly, droplet impacting on the fixed hemispherical surface or droplet impacting onto the solid wall with thin film. The focus of this study is to investigate the phenomena of a droplet impinging onto the solid wall with thin film. (Fig.1.1).

1.2.1.1Droplet stick

The droplet stick occurs when the kinetic energy of collision is a “perfect” value for stable or the droplet material is very different and non-mixed with the material of film. It is a very typical behavior of droplet-film collision dynamic.

1.2.1.2 Droplet bounce

Droplet bounce of droplet-film collision is the some in the droplet pair collision, which is occurred by the kinetic energy of collision, is insufficient to expel the intervening layer of gas.

1.2.1.3 Droplet spread (absorption)

Droplet spread of droplet-film collision as the droplet coalescence of droplet-droplet collision. The droplet spread a post-collision droplet is formed whose mass is equal to the sum of the mass of the pre-collision droplets, follows droplet contact. The film will absorbed the colliding droplet when the air film thickness is a critical value

1.2.1.4 Droplet splash

Droplet splash is like the fragmentation in droplet pair collision, but the mass of film is usually huge than the droplet since a part of droplet mass will be absorbed by film, the others will be splashed into the air and break-up into numerous small droplets. The behavior usually follows with the "jet" or the "crown" phenomenon of liquid film.

1.2.2 Governing parameters

A droplet impinging normally onto the film creates a lamella and a crown whose dimensions vary in time. The main parameters of the impinging process is governed by non-dimensional parameters including the droplet Weber number(We), the Ohnesorge number(Oh), Reynolds number(Re), the non-dimensional wall film thickness $H_f = h/D$, and the impact velocity U_0 of the single droplet are introduced.

1.2.2.1 Weber number (We)

The Weber number is the ratio of the inertial force to the surface force and is defined as:

$$We = \rho U^2 D_s / \sigma \tag{1.1}$$

Where ρ is the droplet density, D_s is the diameter of the smaller droplet and σ is the surface tension of the droplet fluid

1.2.2.2 Non-dimensional film thickness (H_f)

The non-dimensional film thickness is dimensionless film thickness normalized by drop diameter:

$$H_f = h / D$$

Where h is the film thickness, D is the droplet diameter,

1.3 Literature review

The characteristics of the droplet/surface interactions depend upon the properties of the droplet, the impacted surface, impact velocity, impact angle, geometry, and the medium through which the droplet traverses prior to impact. The fluid flow associated with it is rather complicated and not understood in detail despite many investigations since more than one hundred years ago [1]. Rein reviewed it some years ago [2]. An important distinction made for liquid droplet/surface interaction is the type of impacted surface. The target surface can be either a solid or a liquid surface. Depending on the type, the dynamics process of the impacting can be vastly different. The fluid mechanics of droplet collision with a solid surface has been studied in great detail by the experimental [3-8] and numerical simulation method [9-13]. The research on the impact of a liquid droplet with a liquid surface is comparably rare. In several cases, one or more bubbles can be entrained by the drop impact. The entrained bubbles are thought as the reason of the rejected jet [14, 15]. This phenomenon does not occur in the cases of shallow liquid surface [16]. Hobbs and Osheroff [17] studied the splashing of a drop after impacting on the liquid pool with different depths using the photographs taken by a high-speed camera. They found that the phenomena had close relation to the depth of the target liquid pool. In their experiment, it was found that no jet drops were produced for the pool depth less than 3 mm. Clearer photos were gotten by Macklin and Hobbs [18] by high-speed movies. They also explained the phenomena by the interaction of the subsurface cavity with the solid surface beneath the liquid. Wang and Chen [19] experimentally studied the drop impingement onto liquid films with thickness of the order of 1 mm using the glycerol－water solution. The thickness of liquid film is varied to study the effect of it. The effect of viscosity is also studied by changing the proportion of glycerol to water. In Manzello and Yang's paper [20], the depth of the impacted liquid pool was varied from 2 to 25 mm to show the role of the depth of impacted liquid surface. Weiss and Yarin [16] used a boundary-integral method to numerically simulate the single drop impact onto liquid film. In their paper, the potential flow is assumed to build the model. To simulate large deformation of free surface like the drop impact, particle method has natural advantage because in this method it is not necessary to use artificial method to track the free surface and the interfaces are always clear. The numerical diffusion can also be avoided because the motion of particles calculated the convection directly. Nikolopoulos et al [21] investigated the impingement process of a droplet normally onto a wall film. The numerical method is based on the finite volume solution of the Navier-Stokes equations, in their axisymmetric formulation, expressing the flow field of the two phases, liquid and gas, coupled by the volume of fluid method (VOF).Christophe and Ste´phane [22] also use VOF methods to study the viscosity and surface tension and solved the Navier-Stokes equations with sharp interfaces between a liquid and a gas phase. Momentum balance was solved on a very fine square grid.

1.4 Objectives

In the past, it is rare to utilize molecular dynamics method to discuss the behavior of the liquid droplet impacting on the liquid film laid on the solid surface. In this work, we use molecular dynamics simulations to study the dynamics spreading behavior of a argon droplet on a liquid argon film laid on a solid surface at atomic length scales. We use neighbor-list combine with link-cell methods to calculate force, and choose Lennard-Jones (L.J.) potential to deal with interactions between argon droplet and argon substrate. And, we apply the completed parallel MD code to investigate the phenomena of the droplet spreading.