Tables

Fundamental Quantities

Mass	m = mass of one atom
Length	σ
Energy	ε
Time	$\sigma\sqrt{m/\varepsilon}$

Derived Quantities

Adiabatic compressibility	$\kappa_s^* = \kappa_s \varepsilon / \sigma^3$
Configurational internal energy	$U_c^* = U_c / N\varepsilon = \langle \mathscr{U}^* \rangle = \langle \mathscr{U} / N\varepsilon \rangle$
Density	$\rho^* = N\sigma^3 / V$
Force	$F^* = F\sigma / \varepsilon$
Heat capacity	$C_v^* = C_v / Nk$
Radial position	$r^* = r / \sigma$
Pressure	$P^* = P\sigma^3 / \varepsilon$
Temperature	$T^* = kT / \varepsilon$
Thermal pressure coefficient	$\gamma_v^* = \gamma_v \sigma^3 / k$
Total energy	$E^* = E / N\varepsilon$
Velocity	$v^* = v\sqrt{m/\varepsilon}$

Table 2.1 System of units used in soft-sphere molecular dynamics programs

Interaction Pair	ε (eV)	σ ($\mathring{A}$)
He	0.88075	2.6
Ar	10.35	3.405
Xe	19.83	4.055

Table 2.2 The physical parameters of helium, argon and xenon in Lennard-Jones potential

Figures

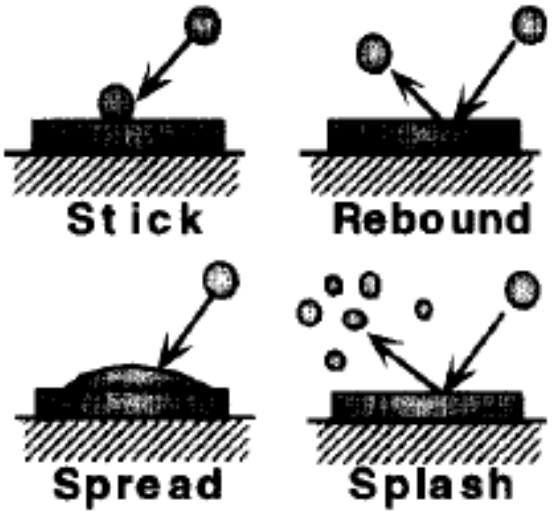

Fig.1.1 The various impingement of regions identified in the spray-film interaction model

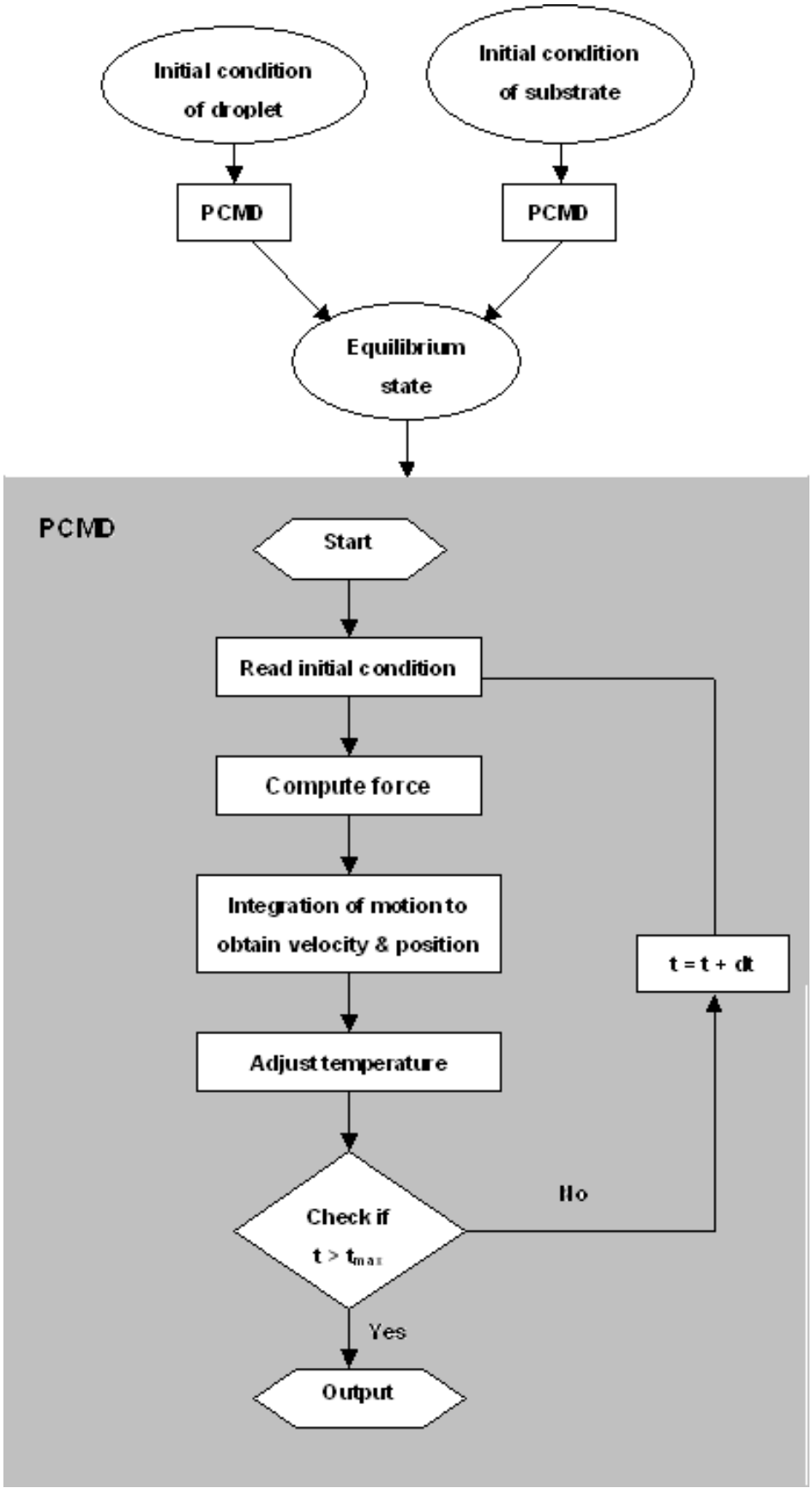

Figure 2.1 Molecular Dynamics flow chart

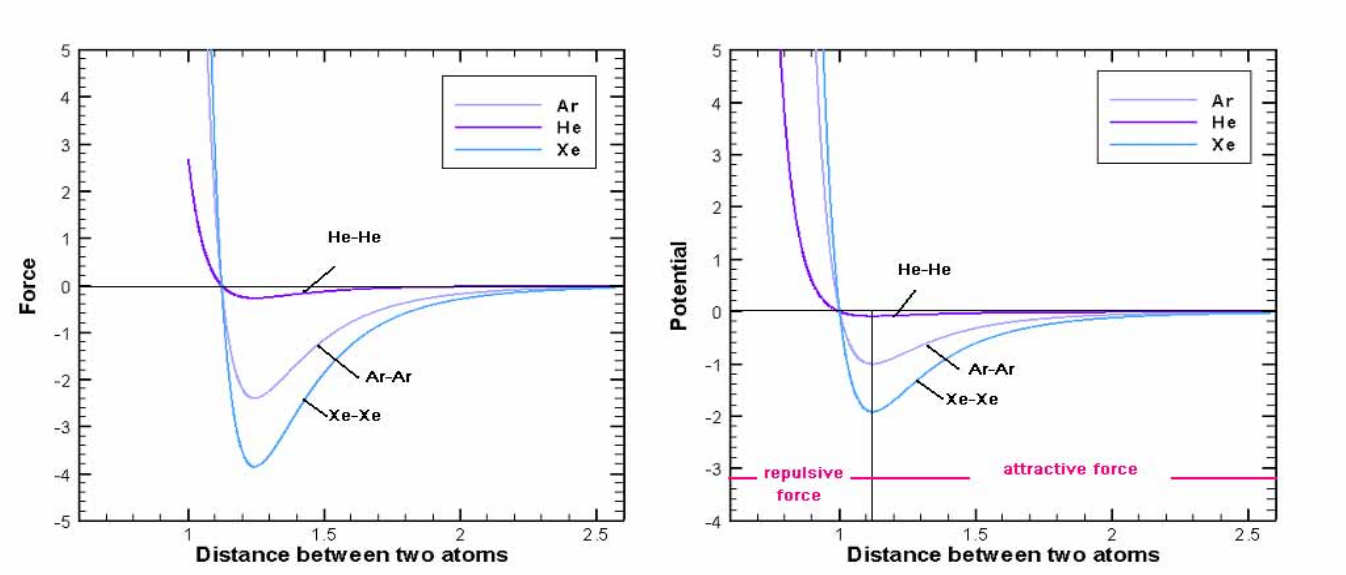

Figure 2.2 The Lennard-Jones pair potential and pair force for argon, helium and xenon.The units here are $r^* = r/\sigma, u^* = u/\varepsilon$, and $F^* = F\sigma/\varepsilon$

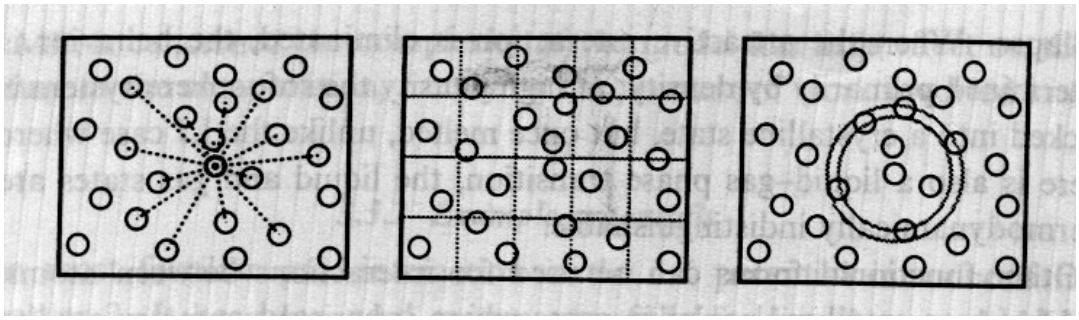

Figure 2.3 The different approaches to computing interactions: all pairs, cell subdivision, and neighbor lists

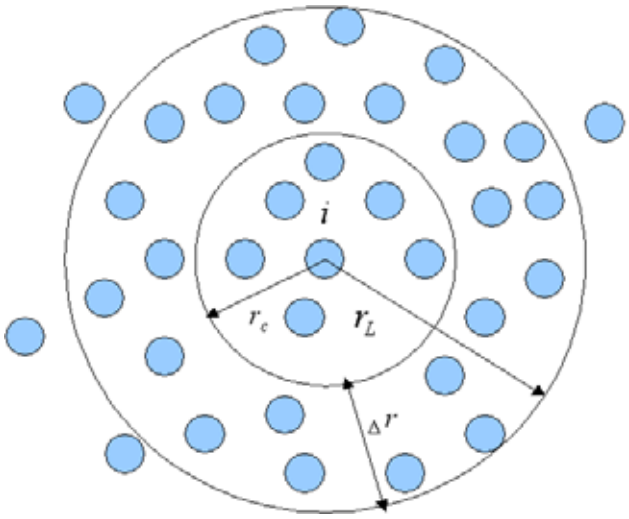

Figure 2.4 The neighbor lists method

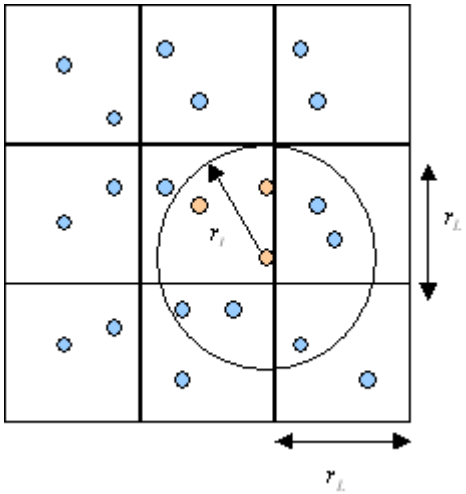

Figure 2.5 The neighbor list + link-cell method

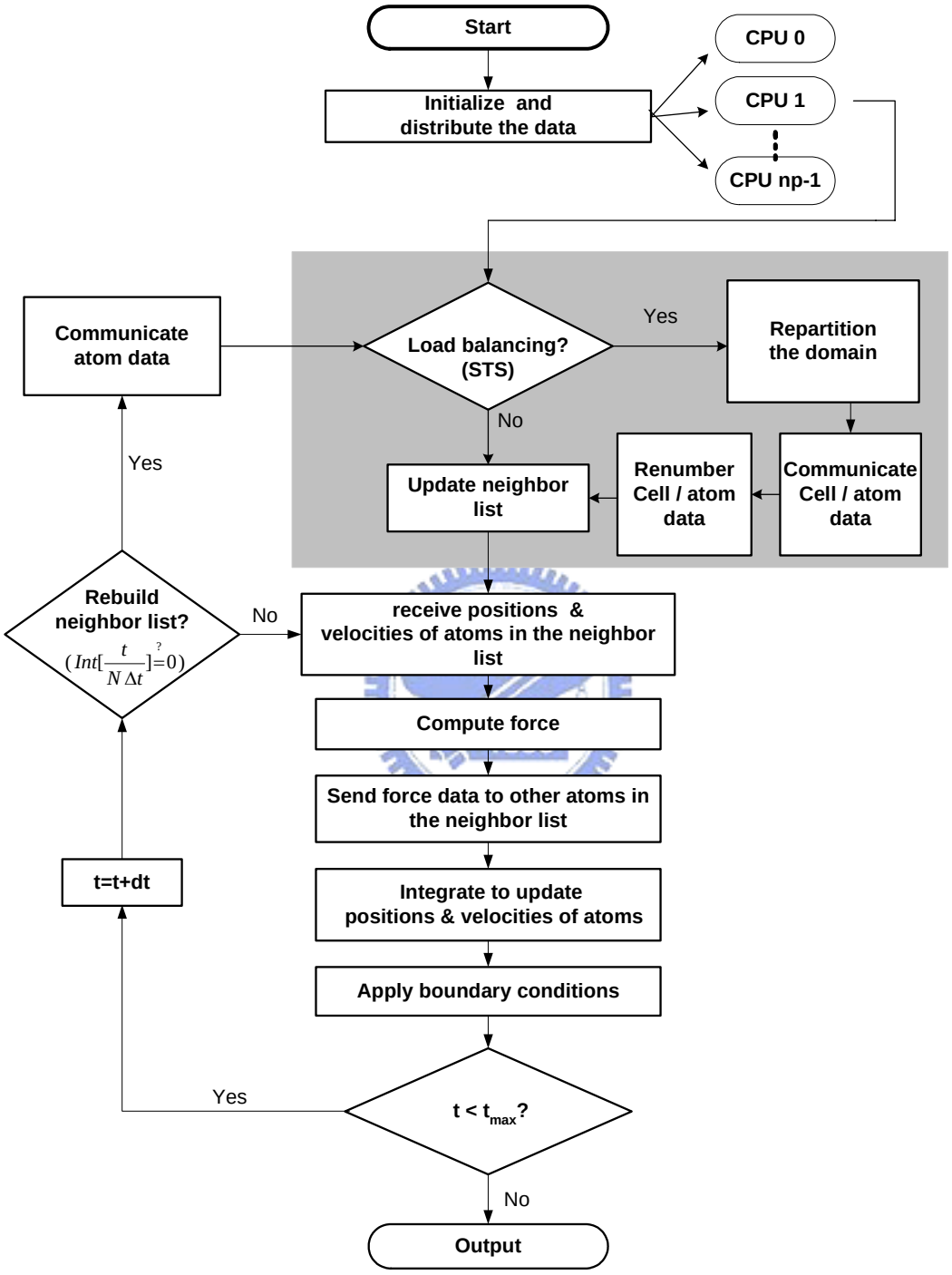

Figure 2.6 The flow chart for parallel molecular dynamics simulation using dynamic domain decomposition.

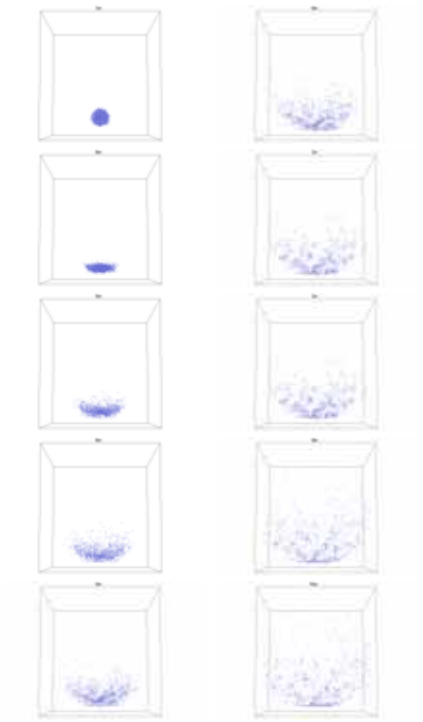

Figure 3.1 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

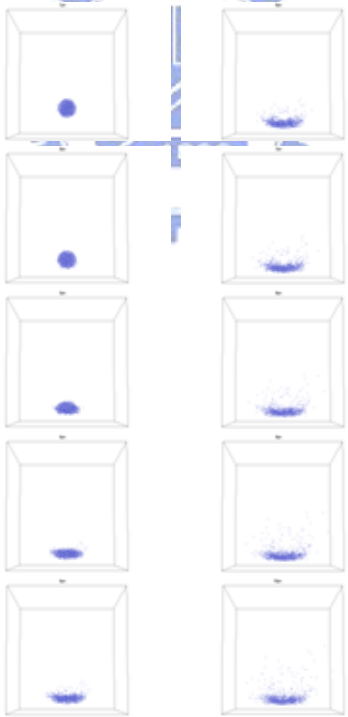

Figure 3.2 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

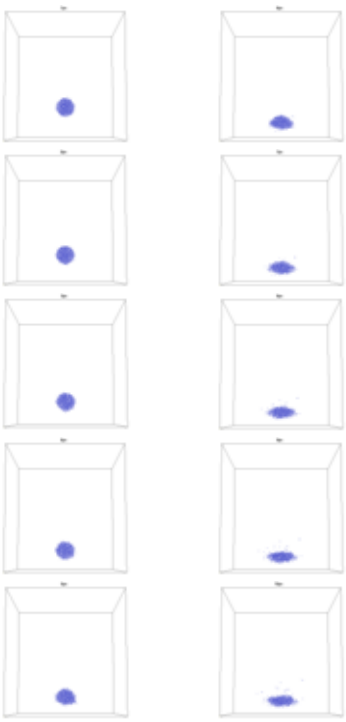

Figure 3.3 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

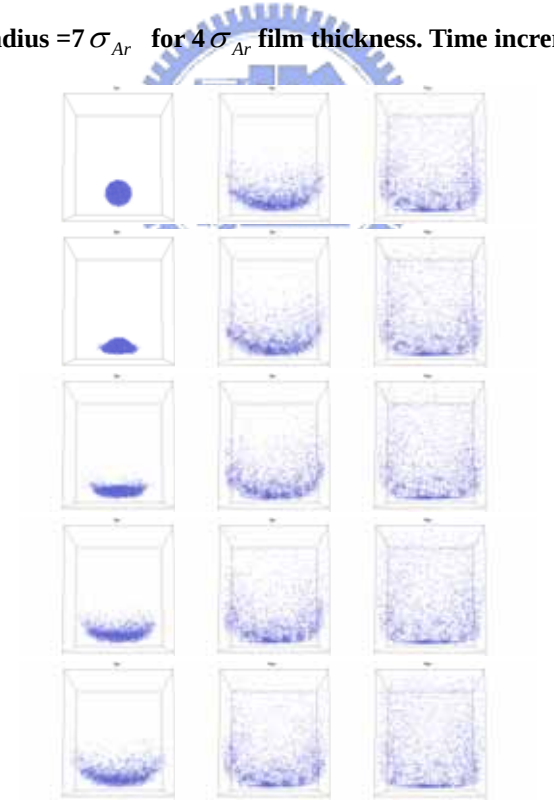

Figure 3.4 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

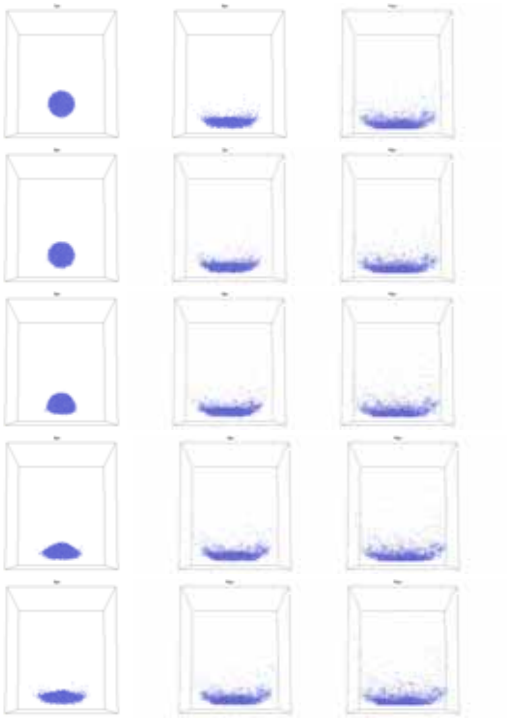

Figure 3.5 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

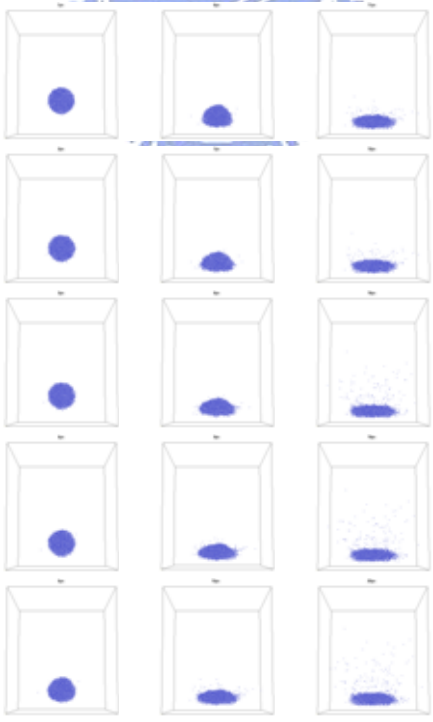

Figure 3.6 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

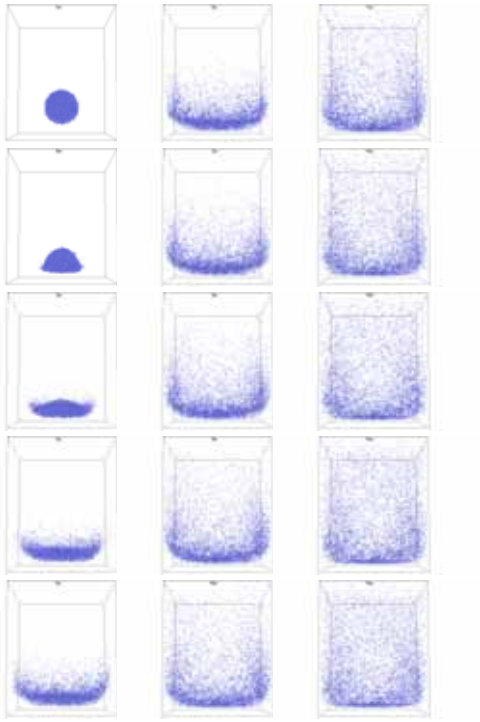

Figure 3.7 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

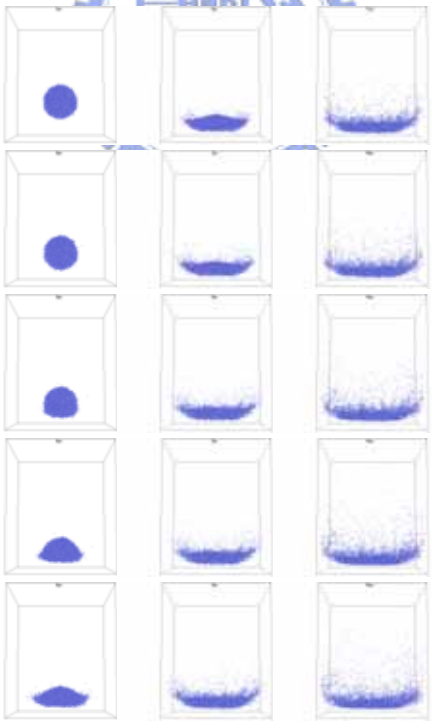

Figure 3.8 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

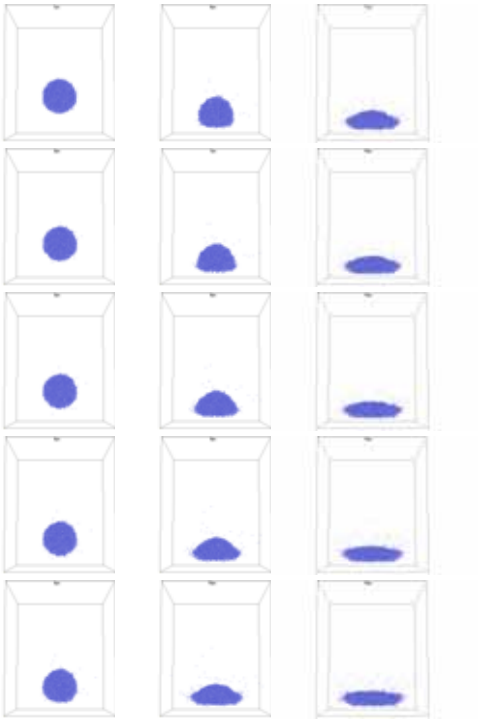

Figure 3.9 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Ar} for 4 σ_{Ar} film thickness. Time increment: 1 time step

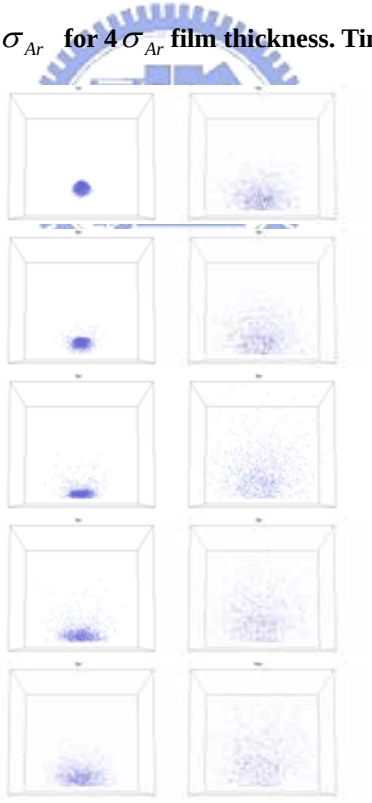

Figure 3.10 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

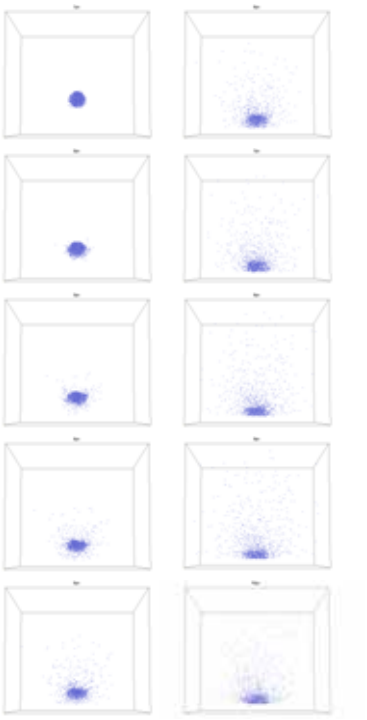

Figure 3.11 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

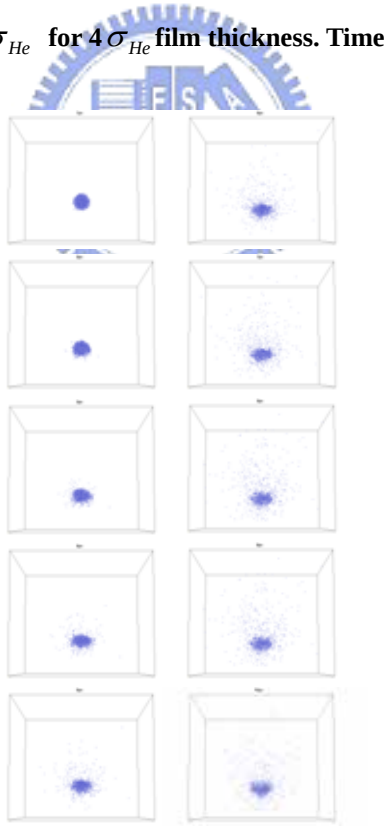

Figure 3.12 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

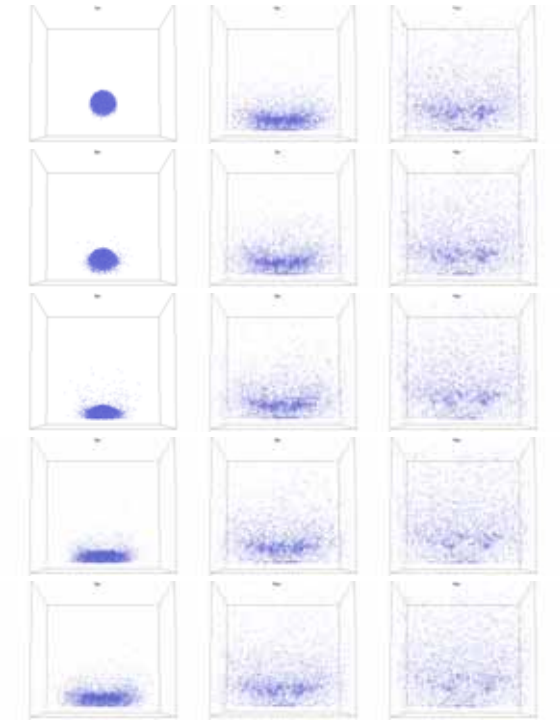

Figure 3.13 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

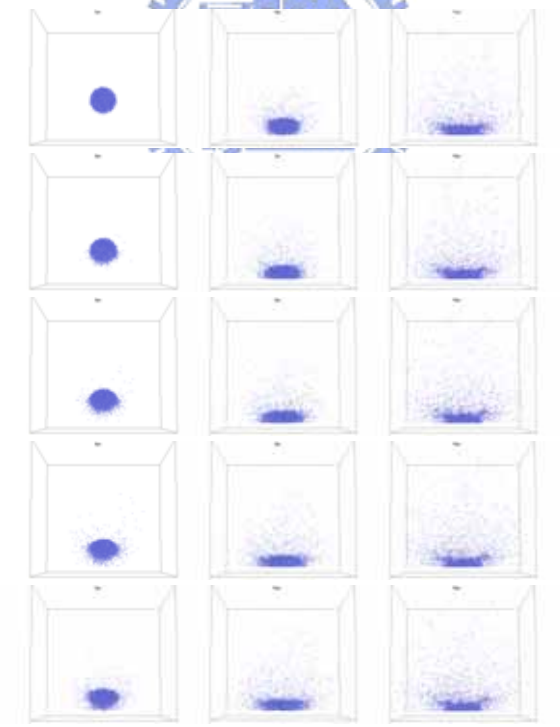

Figure 3.14 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

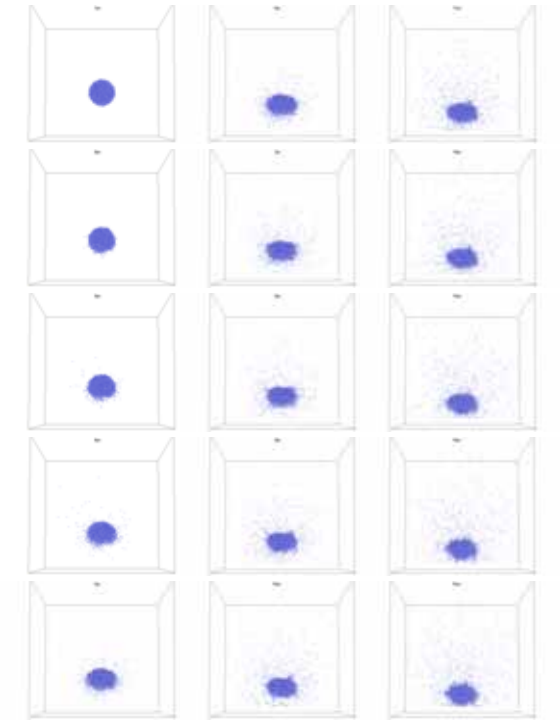

Figure 3.15 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

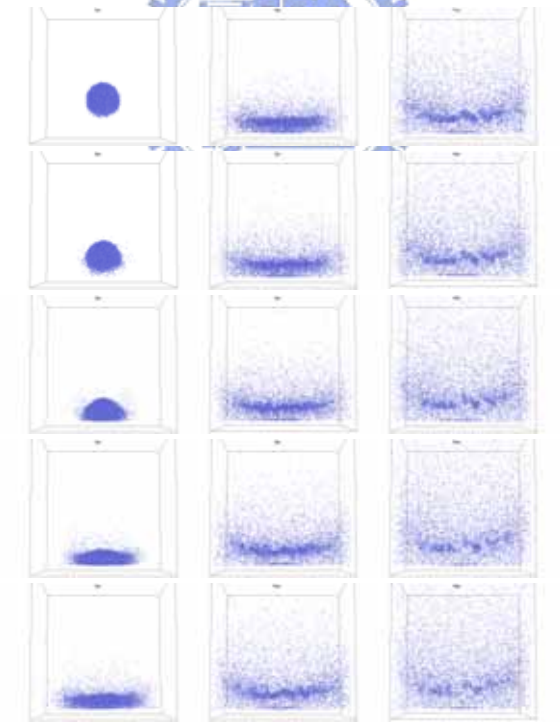

Figure 3.16 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

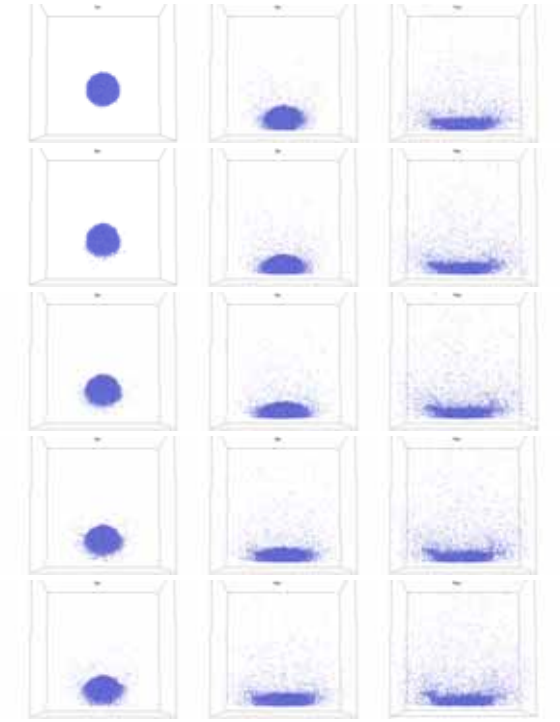

Figure 3.17 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

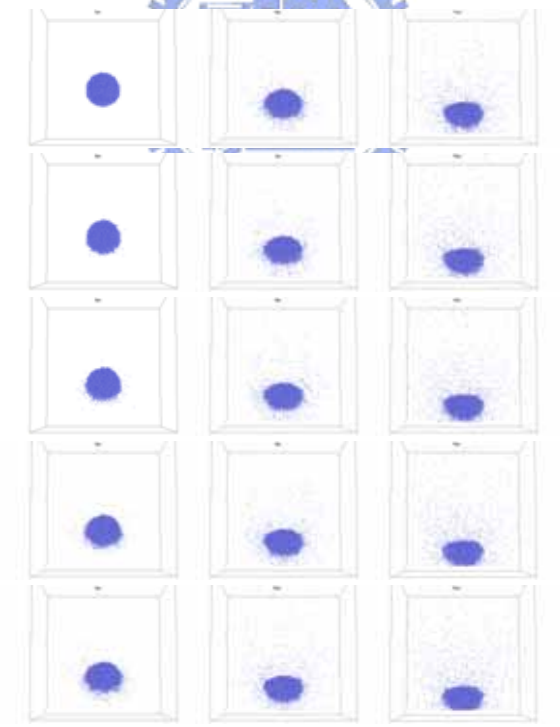

Figure 3.18 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{He} for 4 σ_{He} film thickness. Time increment: 1 time step

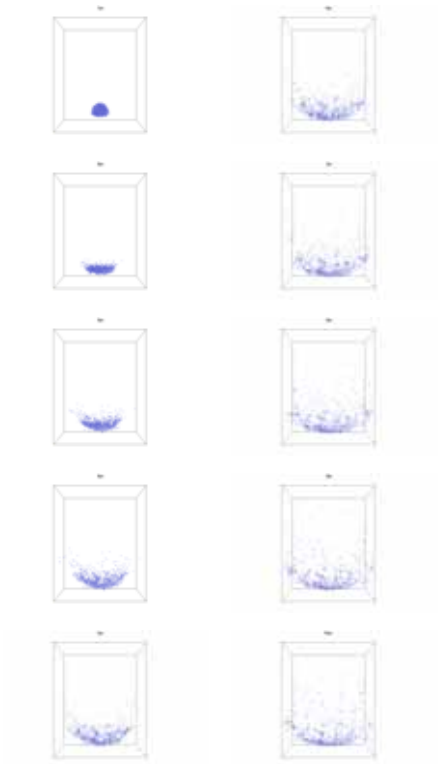

Figure 3.19 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

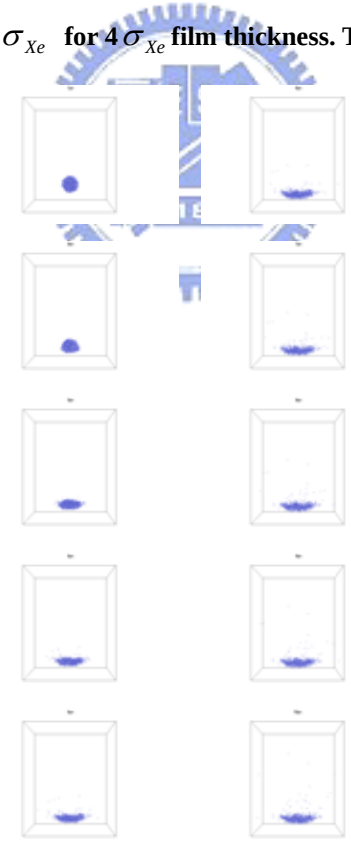

Figure 3.20 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

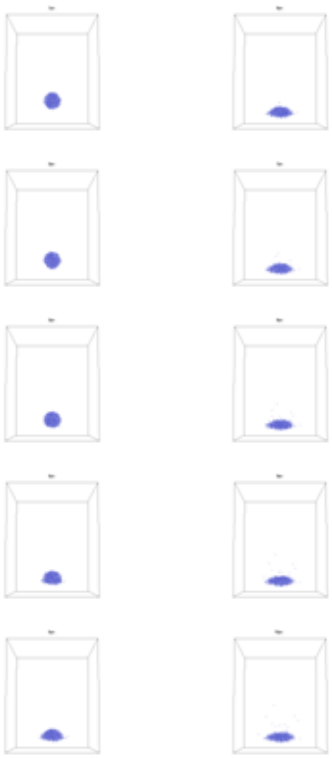

Figure 3.21 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

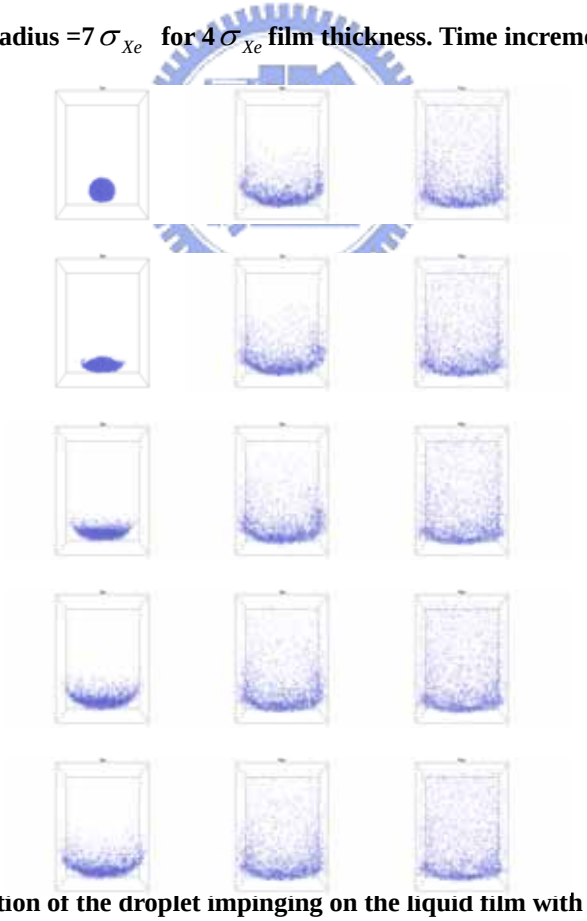

Figure 3.22 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

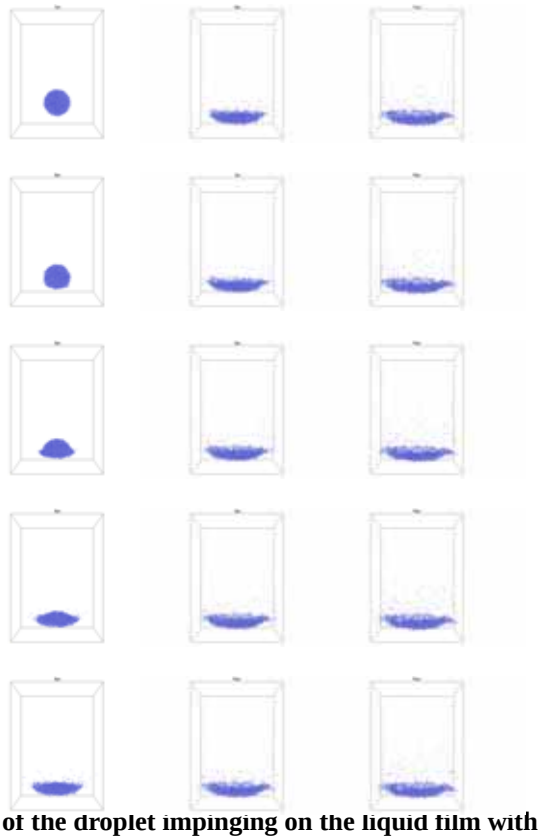

Figure 3.23 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

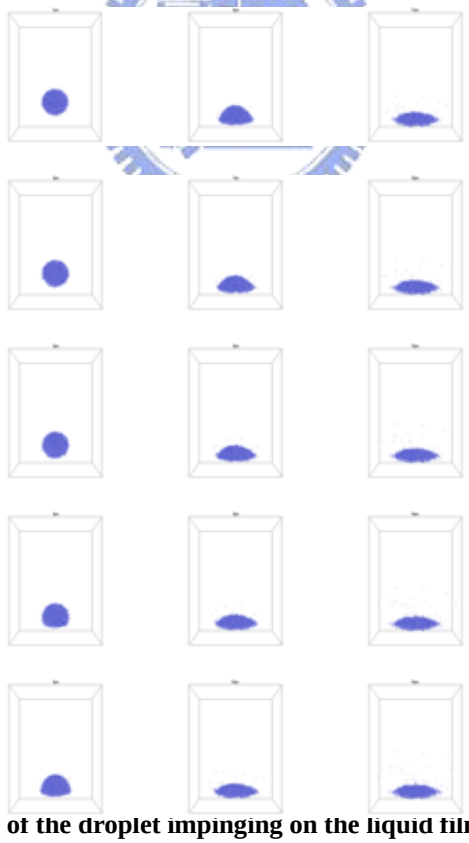

Figure 3.24 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

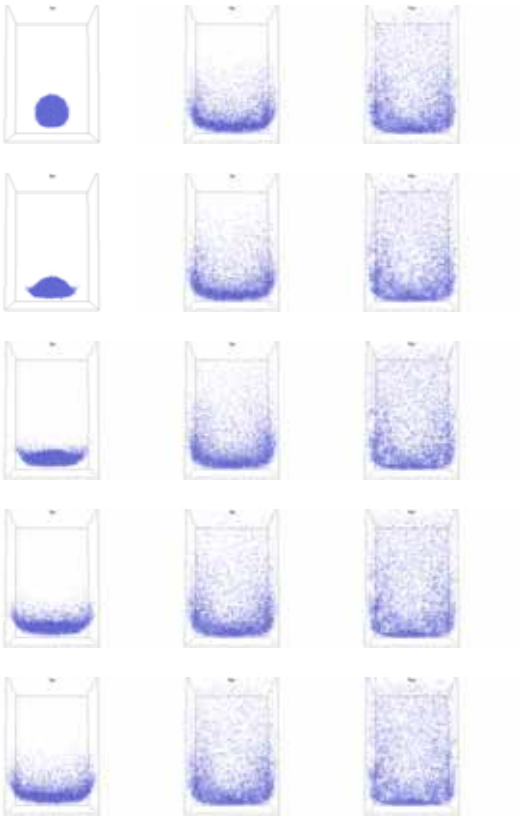

Figure 3.25 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

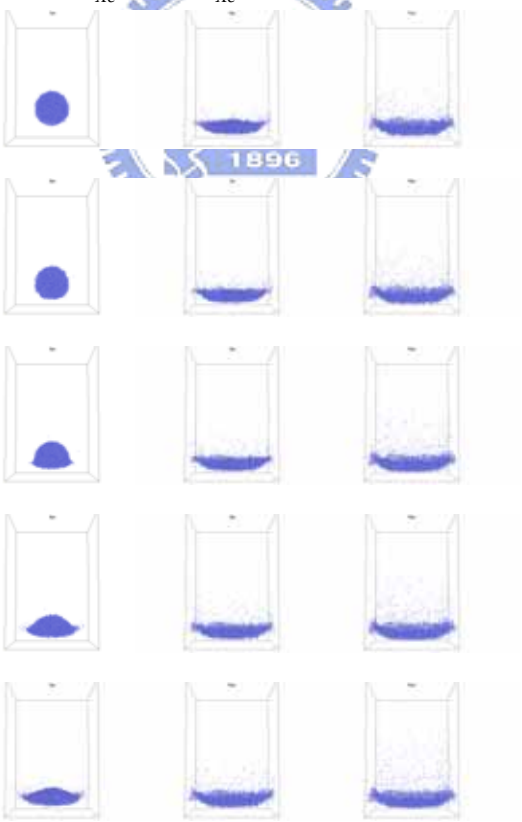

Figure 3.26 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

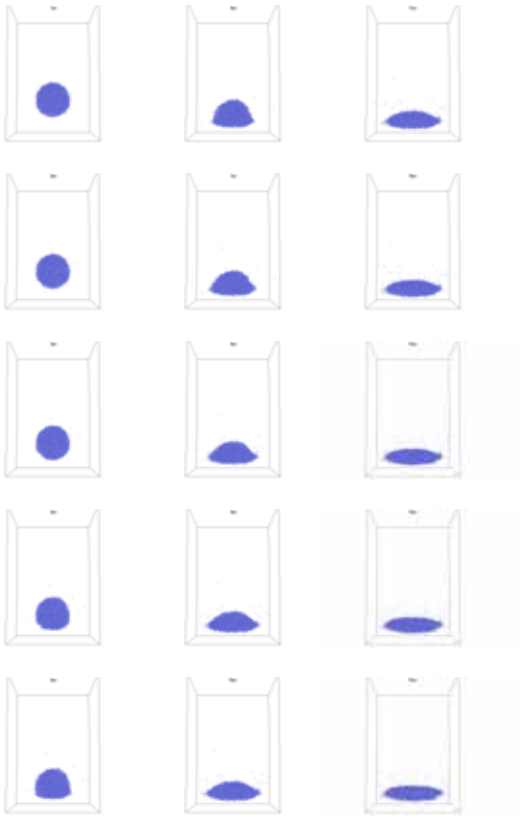

Figure 3.27 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Xe} for 4 σ_{Xe} film thickness. Time increment: 1 time step

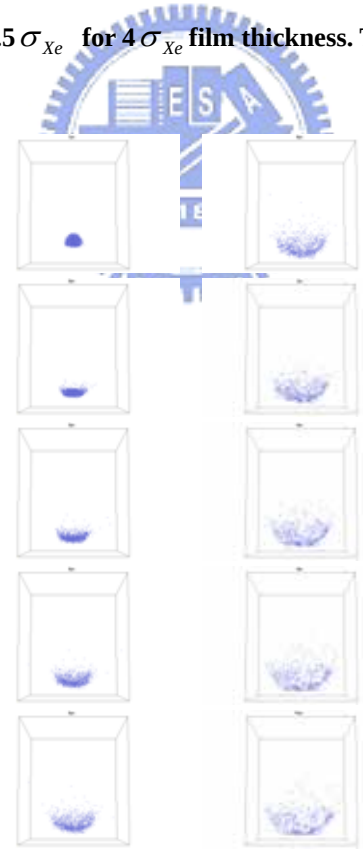

Figure 3.28 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

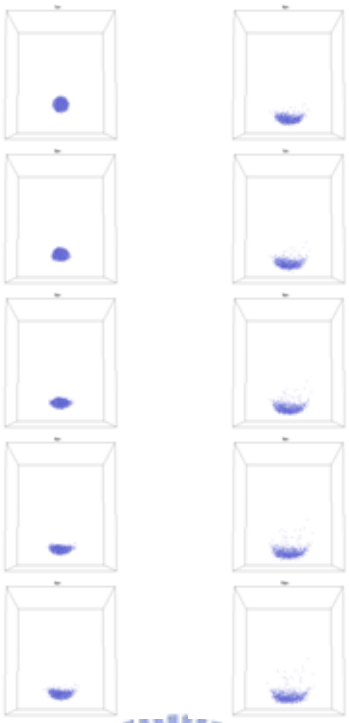

Figure 3.29 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

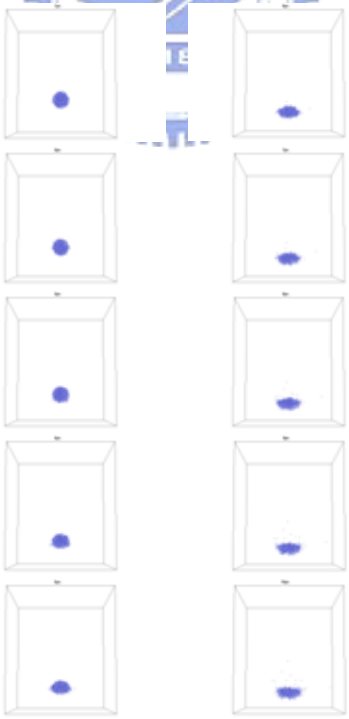

Figure 3.30 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

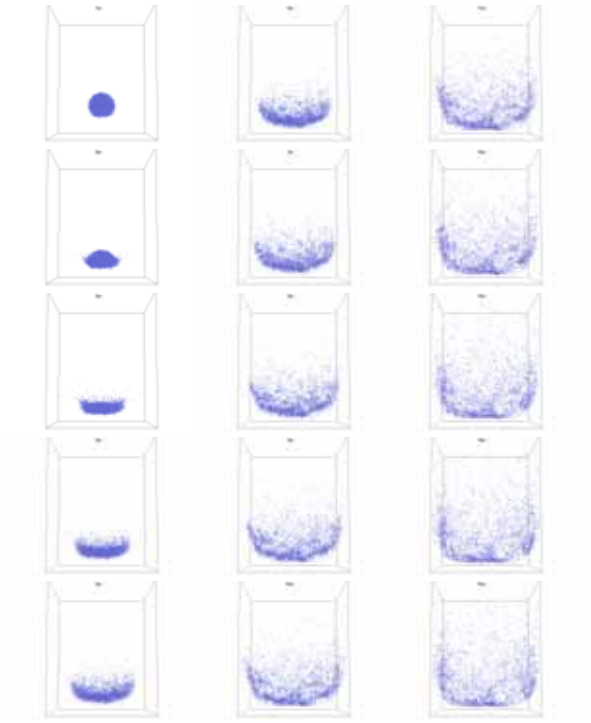

Figure 3.31 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

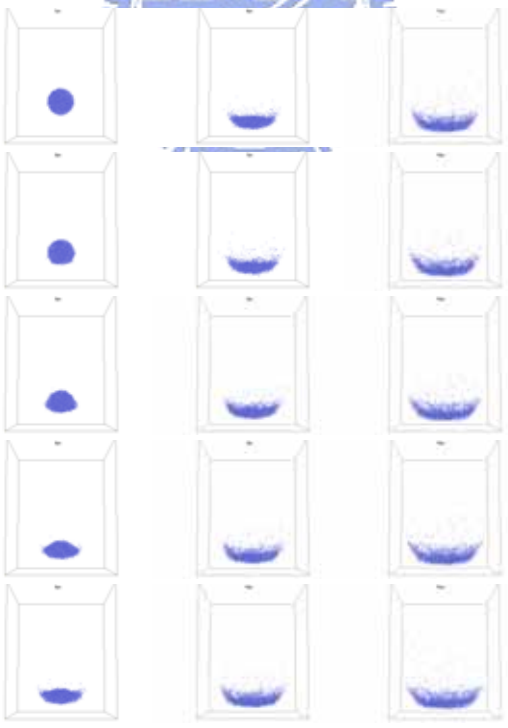

Figure 3.32 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

Figure 3.33 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

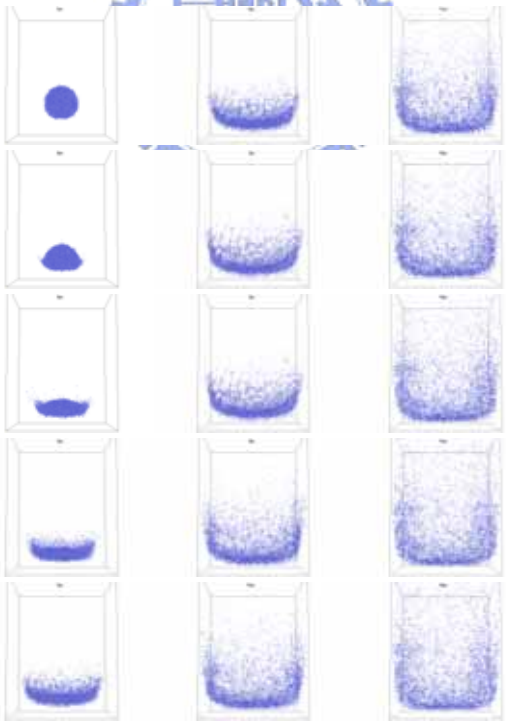

Figure 3.34 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

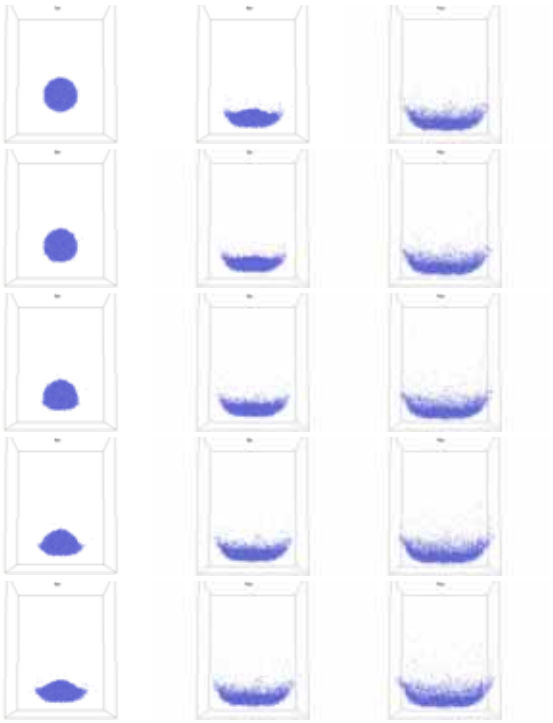

Figure 3.35 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

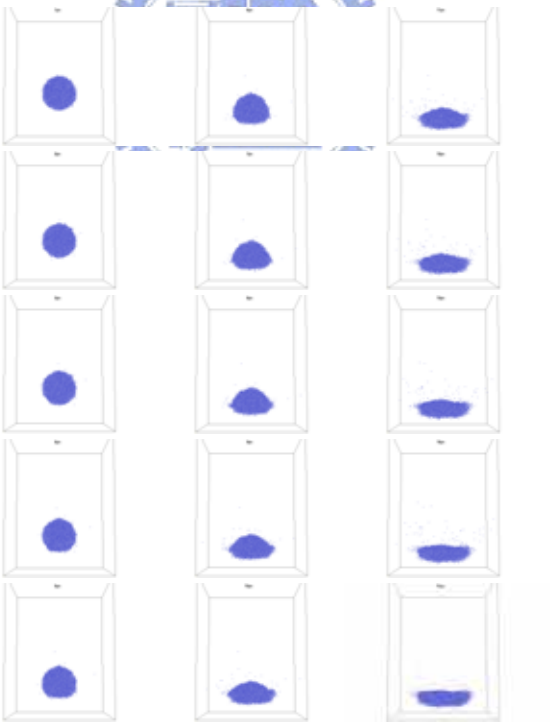

Figure 3.36 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Ar} for 8 σ_{Ar} film thickness. Time increment: 1 time step

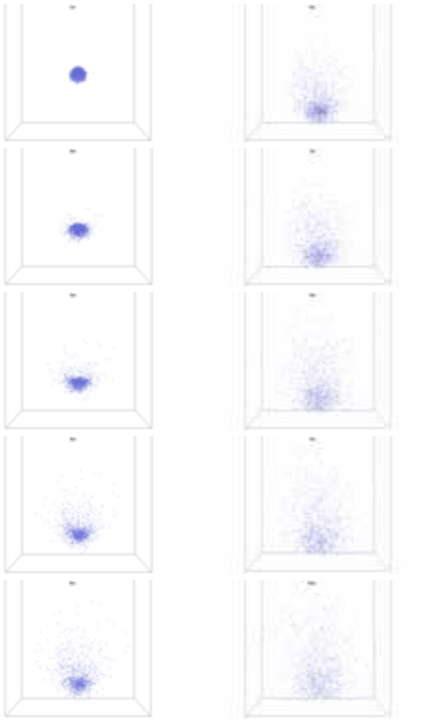

Figure 3.37 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

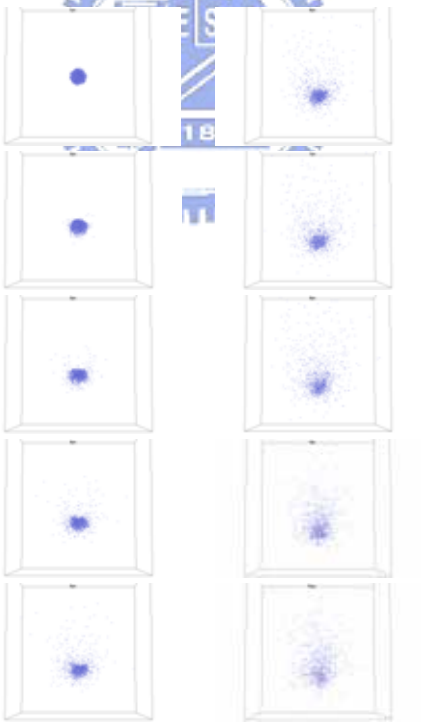

Figure 3.38 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

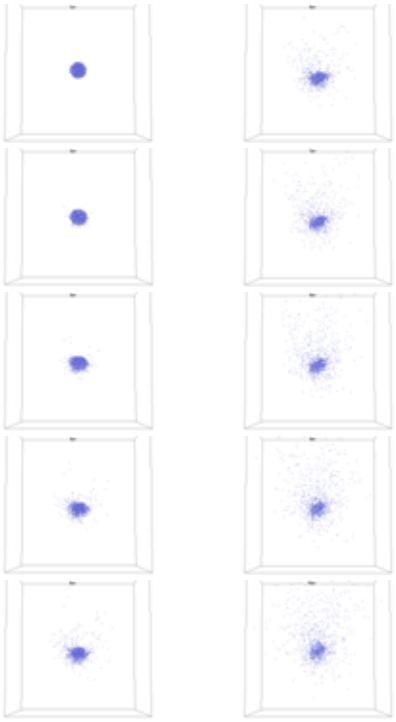

Figure 3.39 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

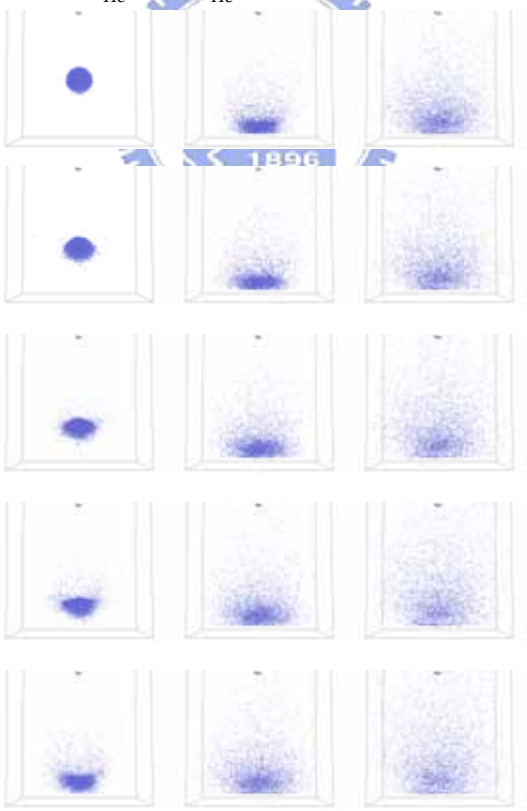

Figure 3.40 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

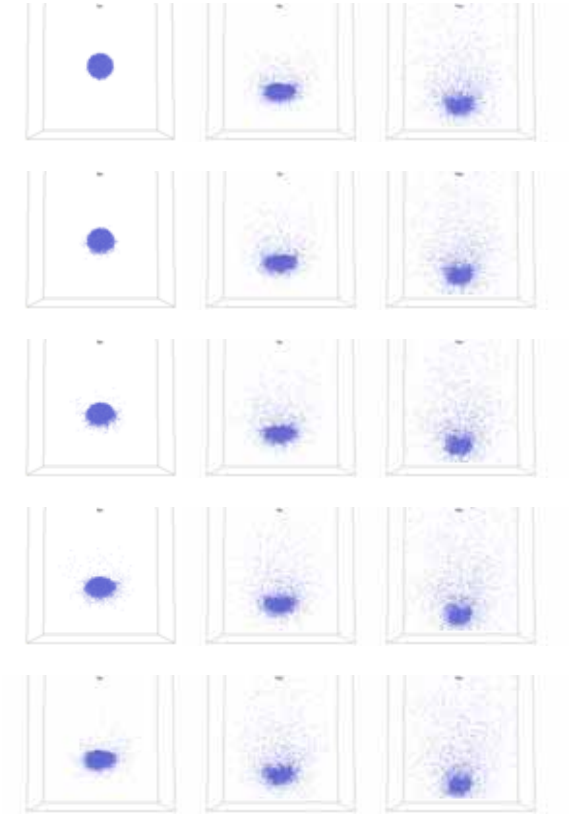

Figure 3.41 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

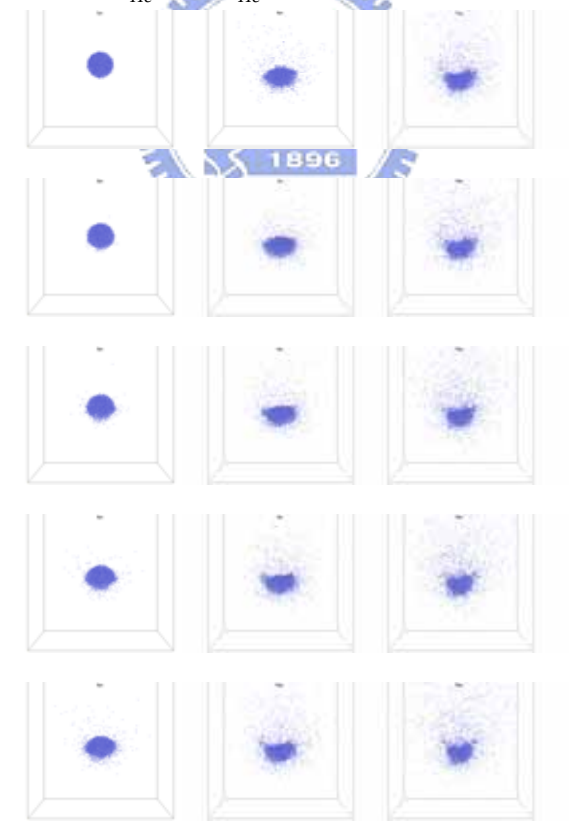

Figure 3.42 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

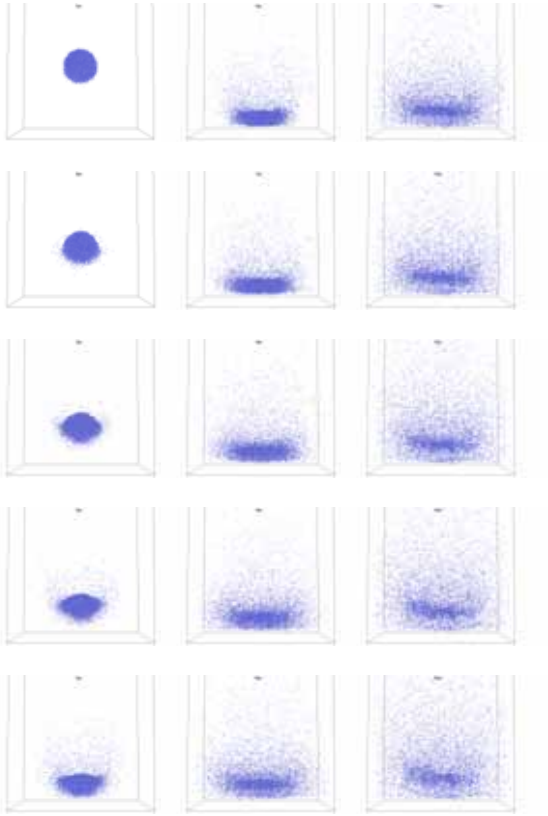

Figure 3.43 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

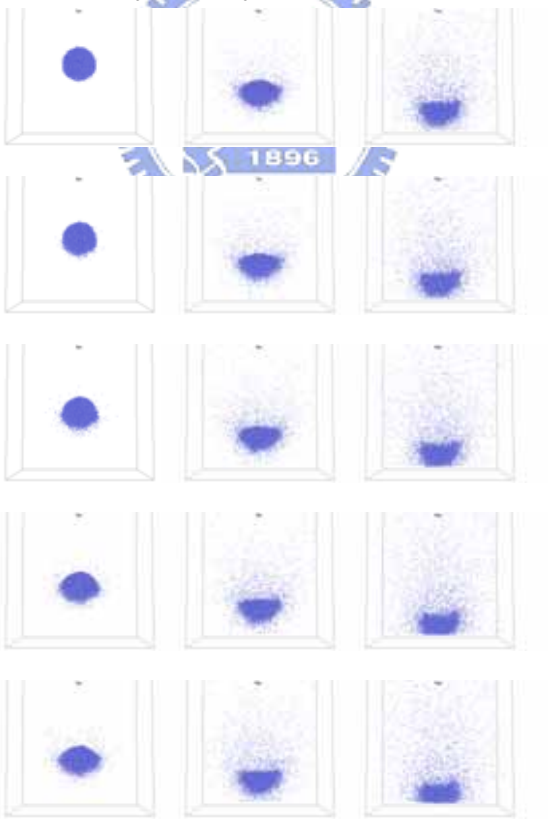

Figure 3.44 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

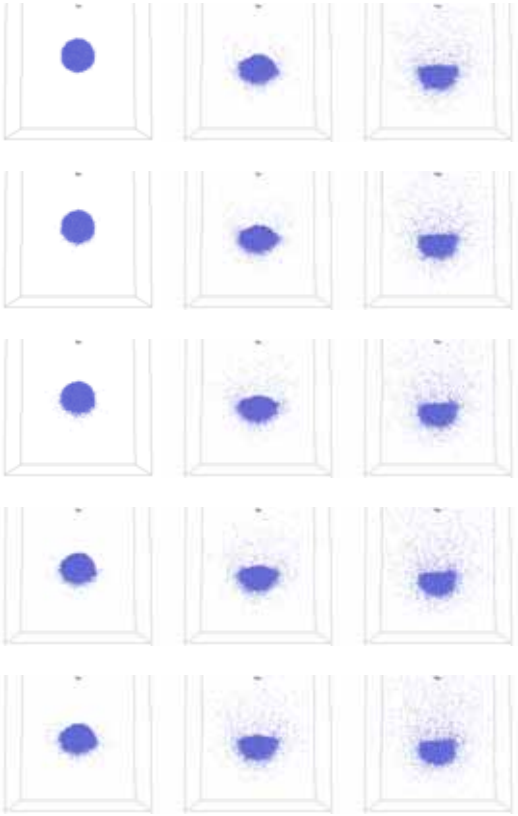

Figure 3.45 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{He} for 8 σ_{He} film thickness. Time increment: 1 time step

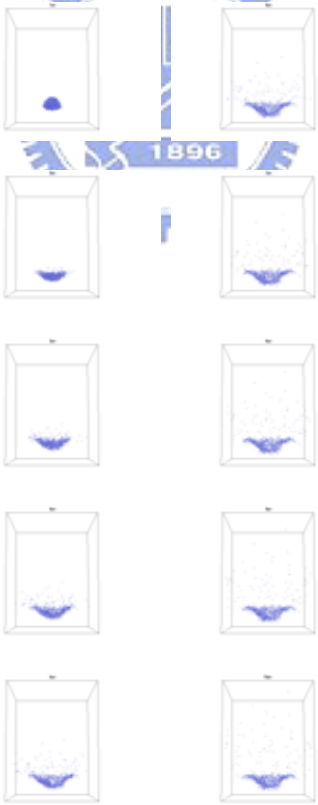

Figure 3.46 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

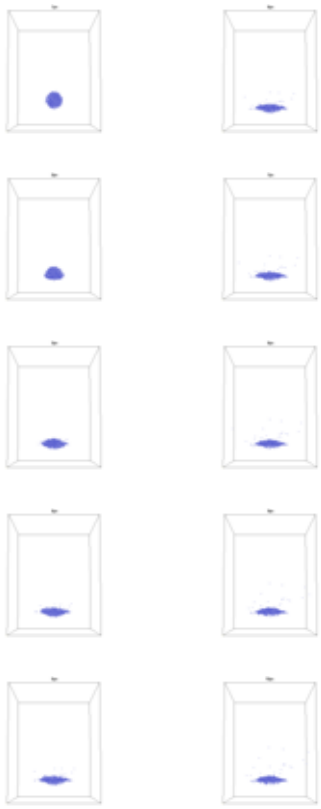

Figure 3.47 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

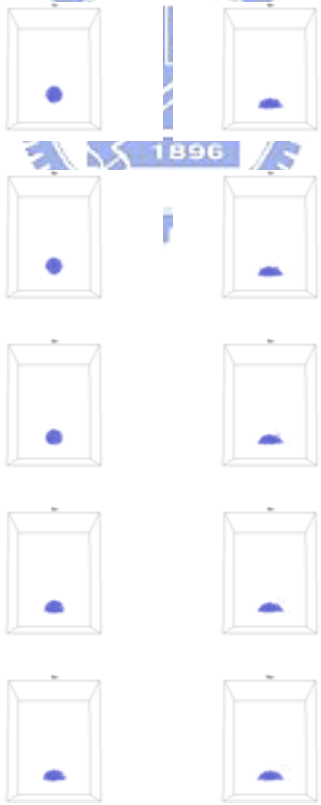

Figure 3.48 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

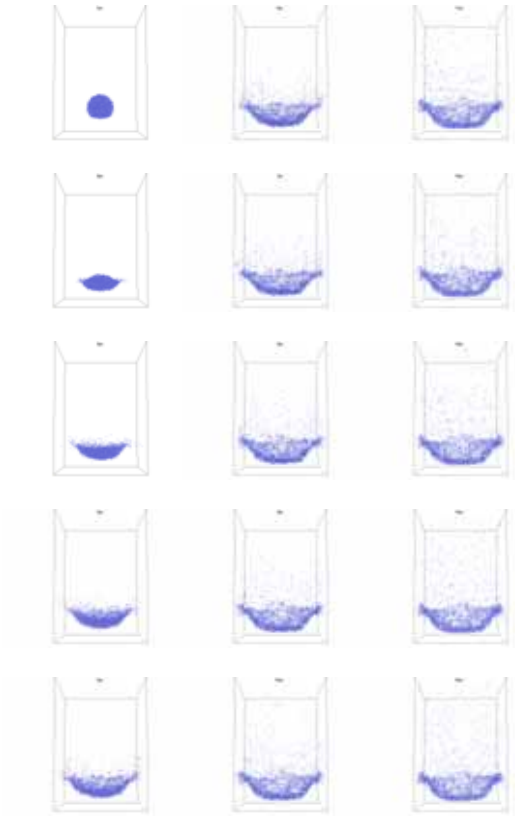

Figure 3.49 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

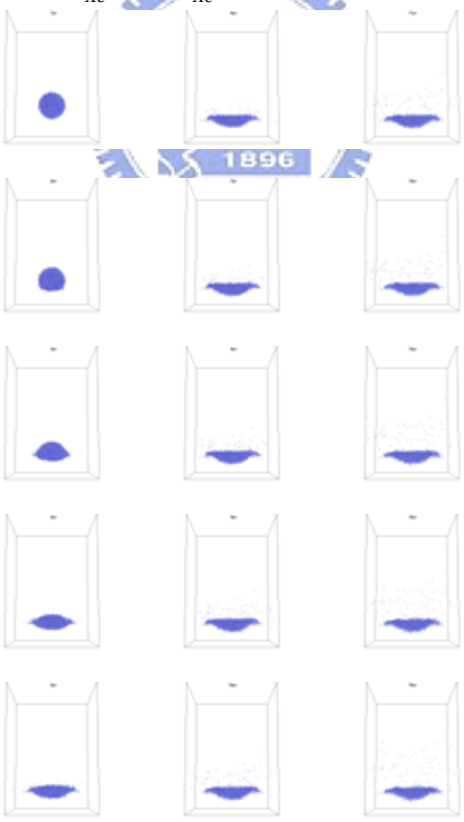

Figure 3.50 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

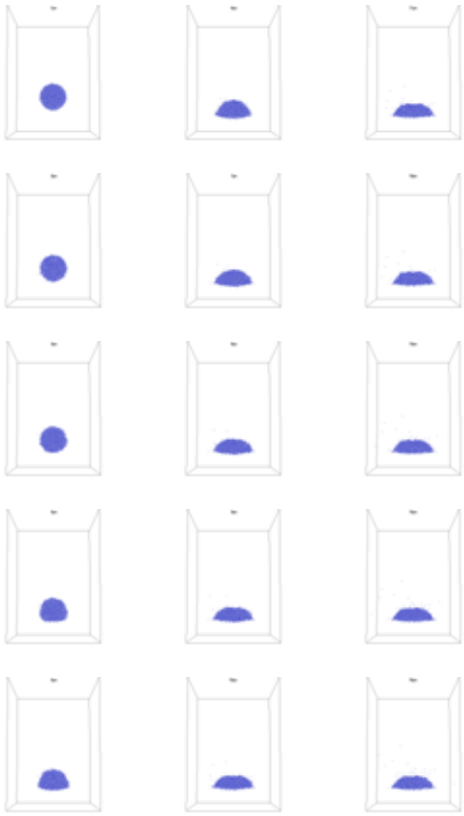

Figure 3.51 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

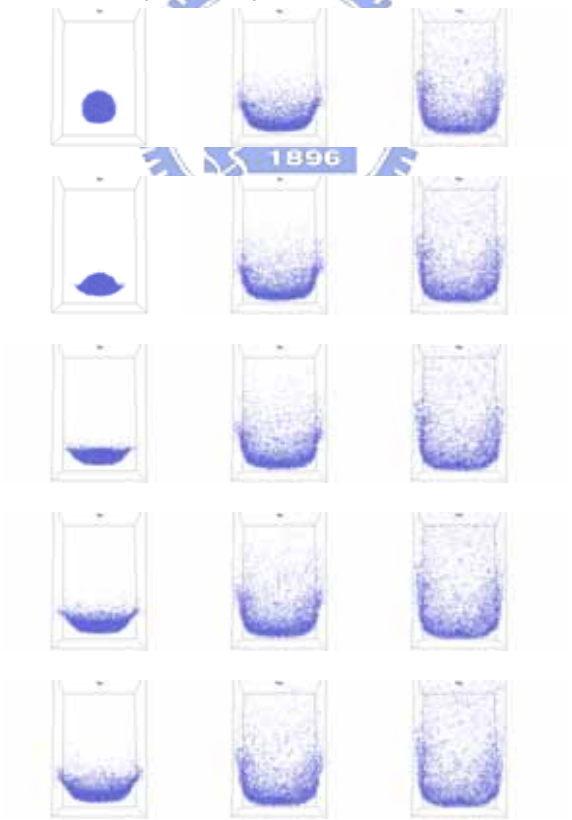

Figure 3.52 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

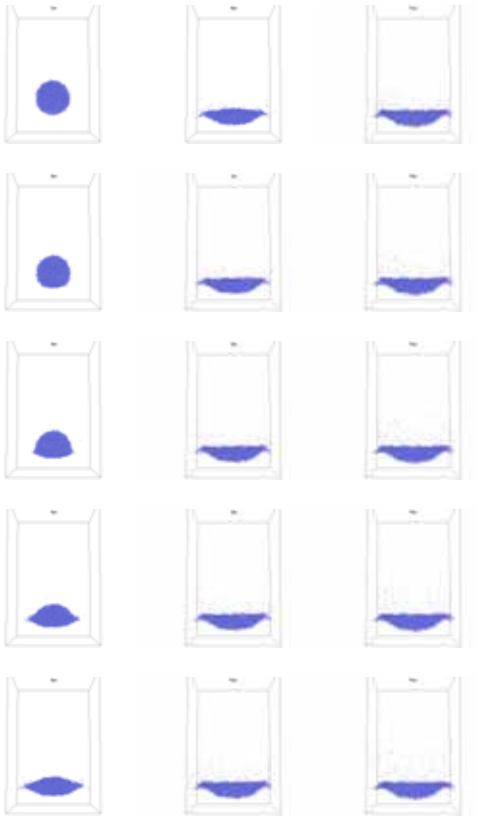

Figure 3.53 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

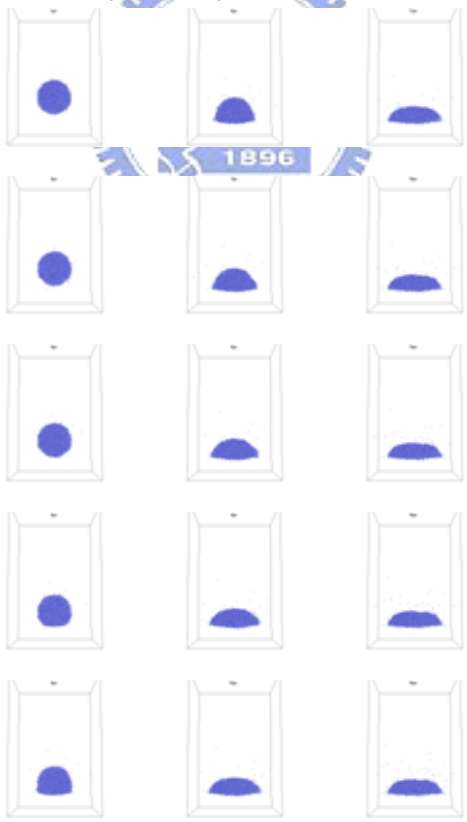

Figure 3.54 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Xe} for 8 σ_{Xe} film thickness. Time increment: 1 time step

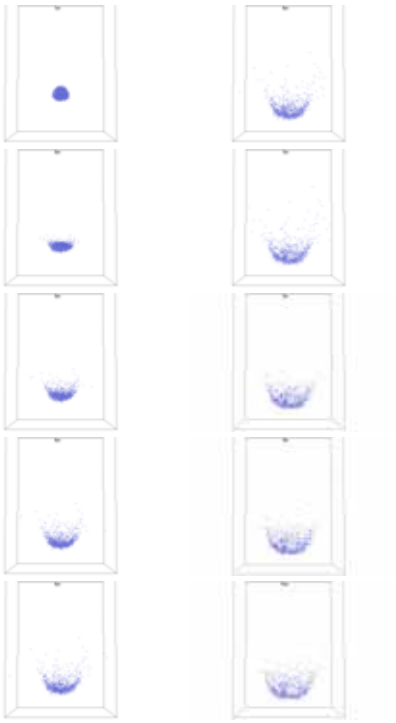

Figure 3.55 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

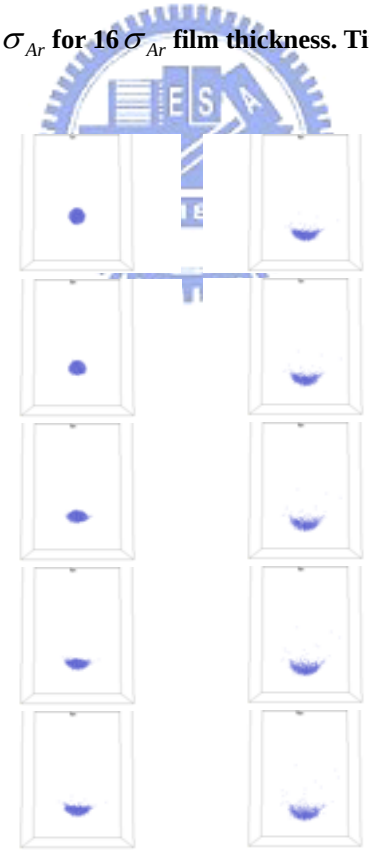

Figure 3.56 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

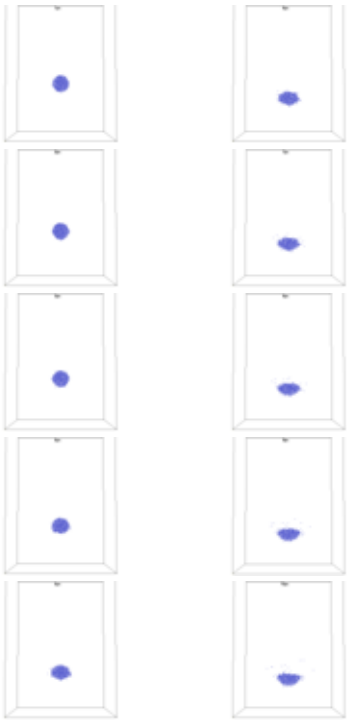

Figure 3.57 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

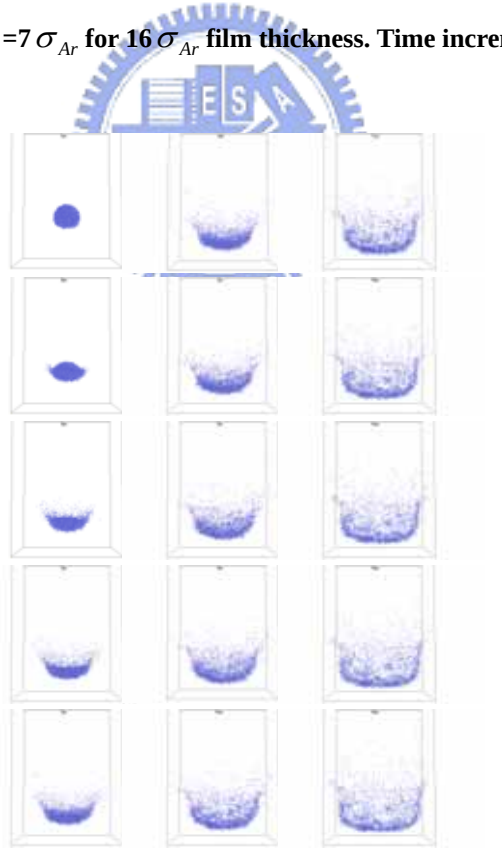

Figure 3.58 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

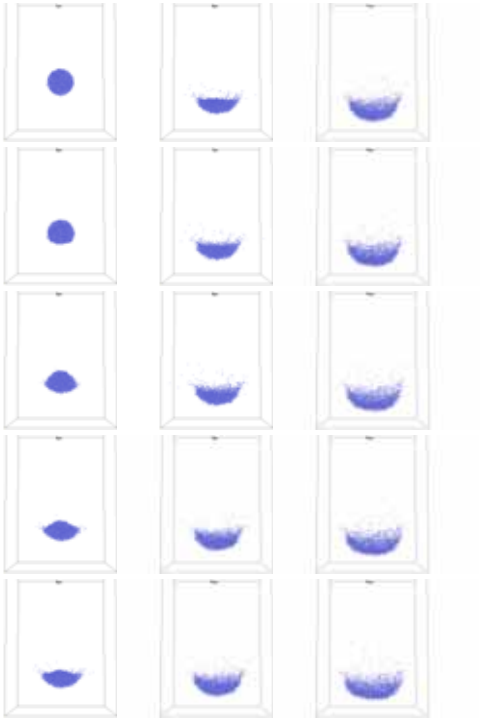

Figure 3.59 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

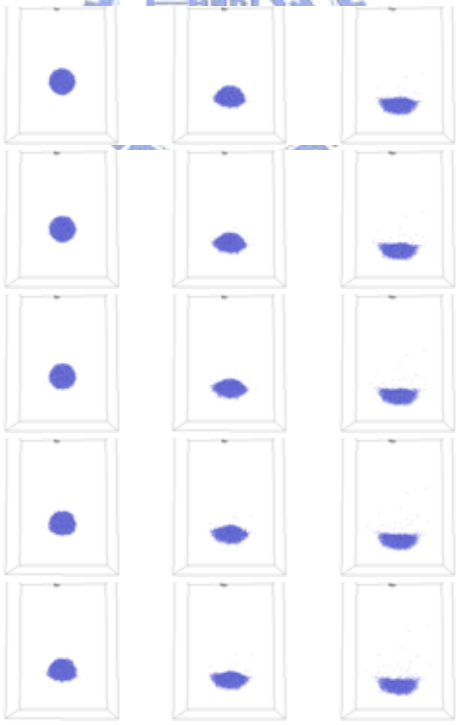

Figure 3.60 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

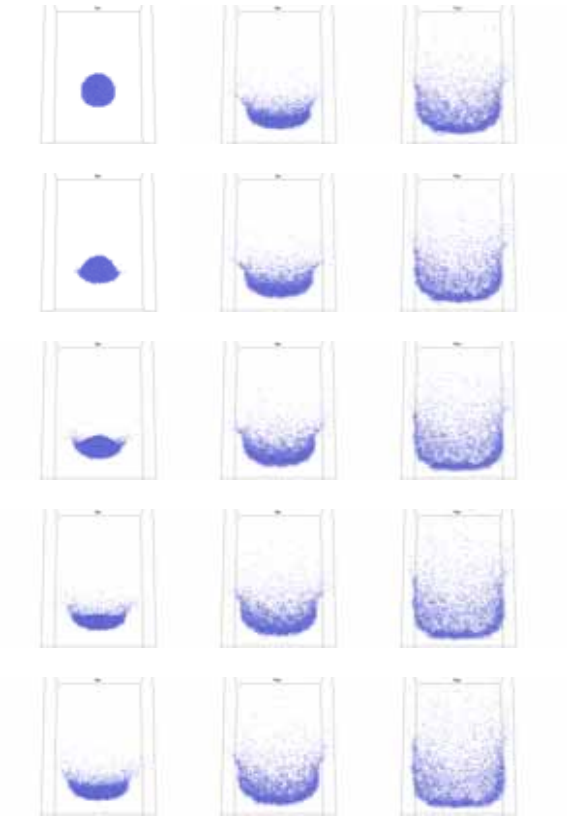

Figure 3.61 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

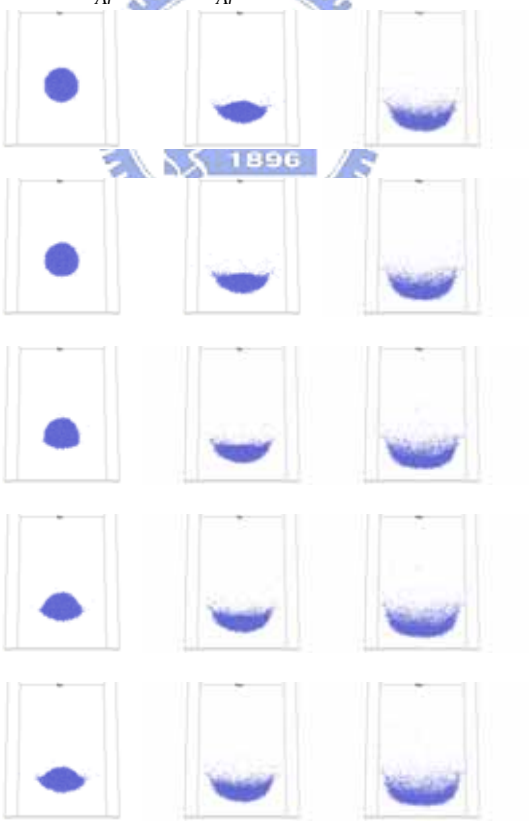

Figure 3.62 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

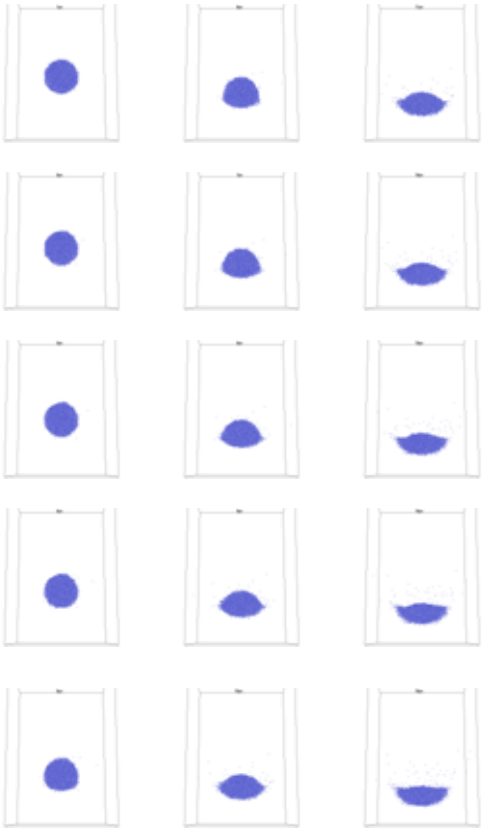

Figure 3.63 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Ar} for 16 σ_{Ar} film thickness. Time increment: 1 time step

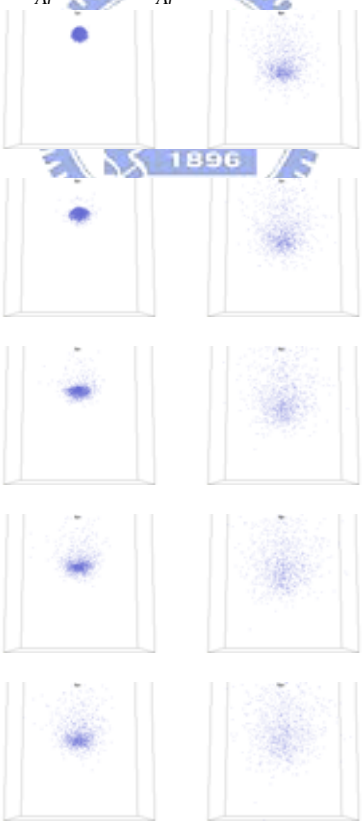

Figure 3.64 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

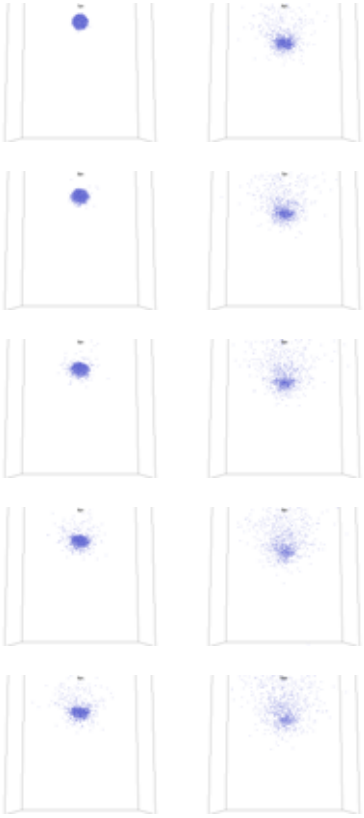

Figure 3.65 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

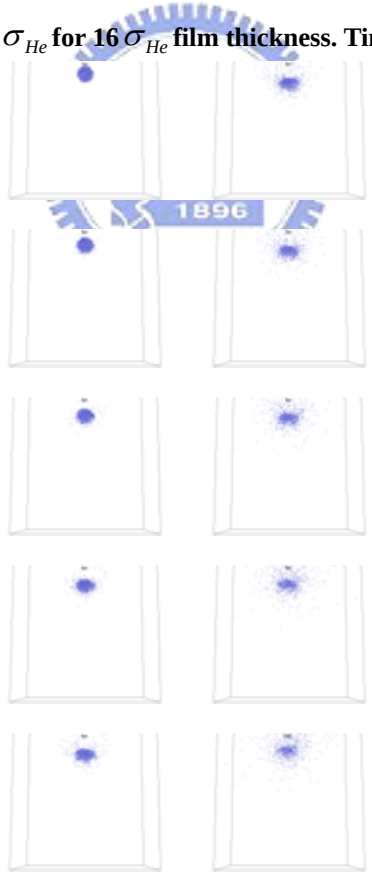

Figure 3.66 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

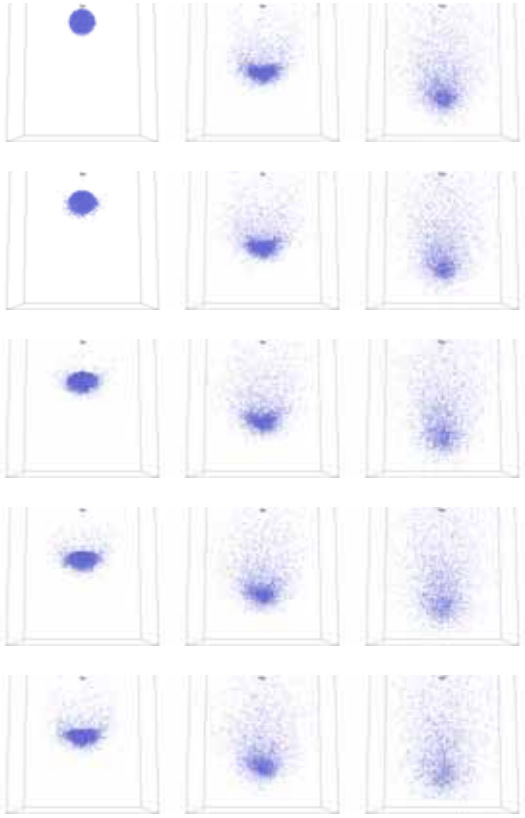

Figure 3.67 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

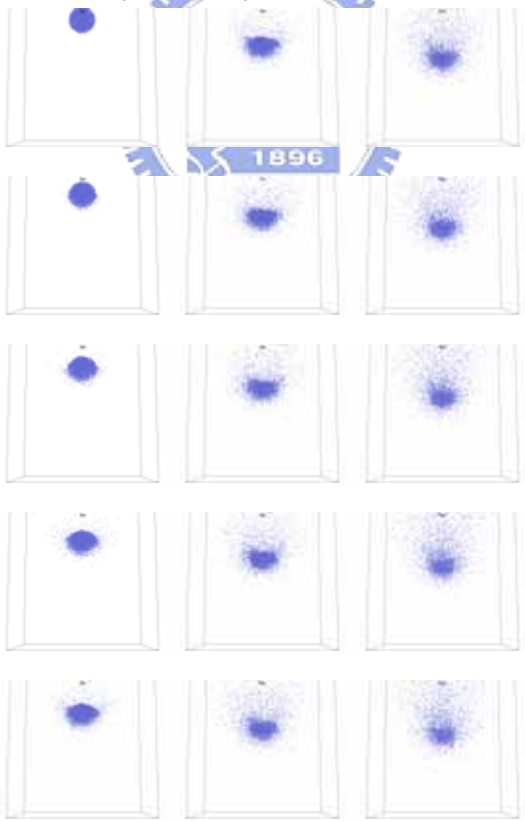

Figure 3.68 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

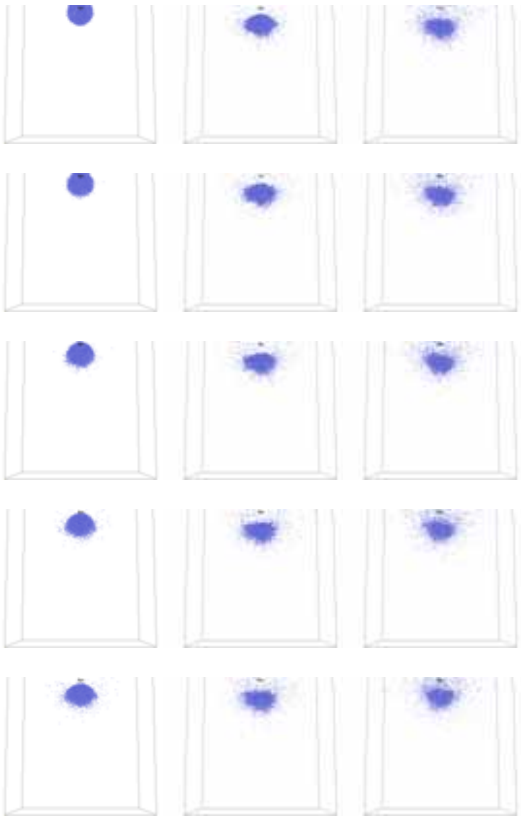

Figure 3.69 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

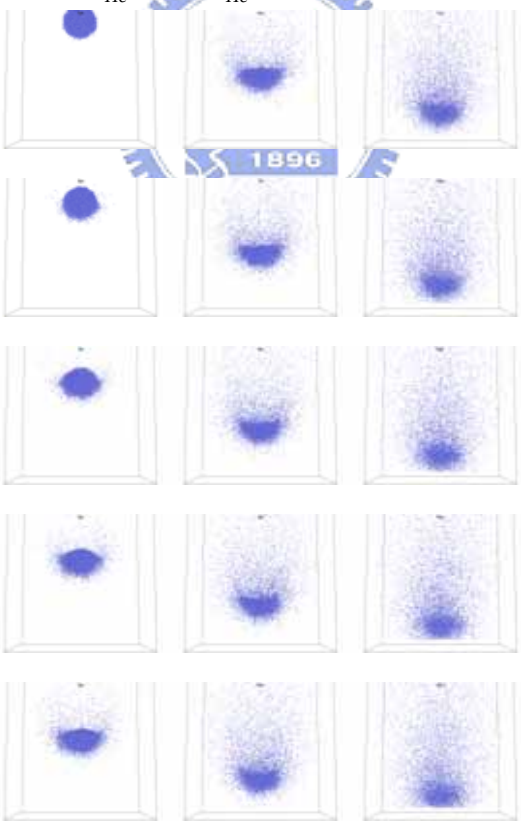

Figure 3.70 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

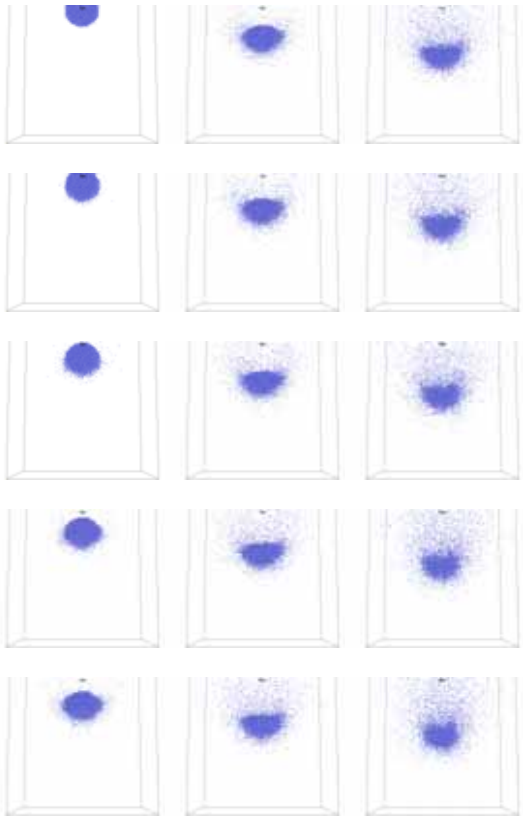

Figure 3.71 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

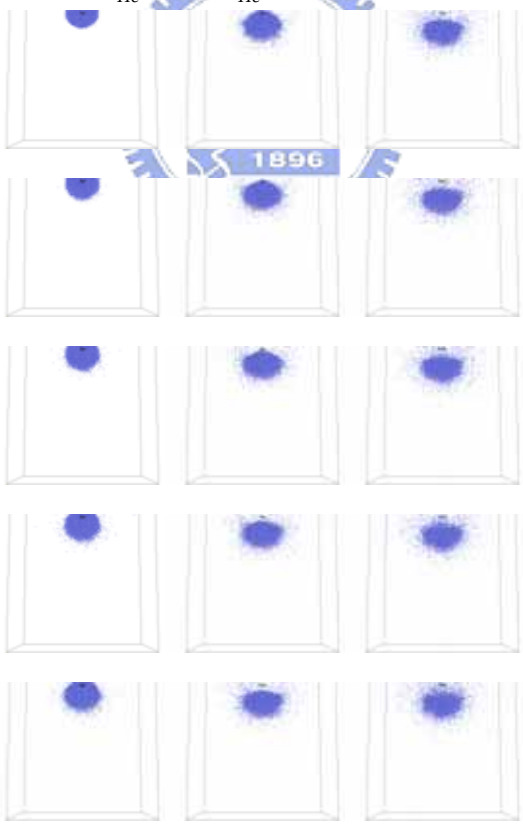

Figure 3.72 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{He} for 16 σ_{He} film thickness. Time increment: 1 time step

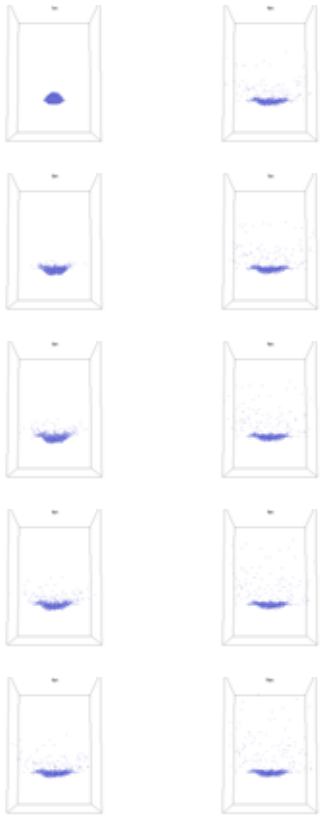

Figure 3.73 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =7 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

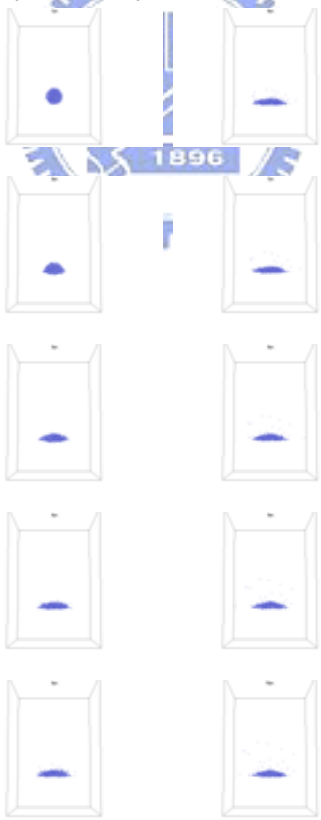

Figure 3.74 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =7 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

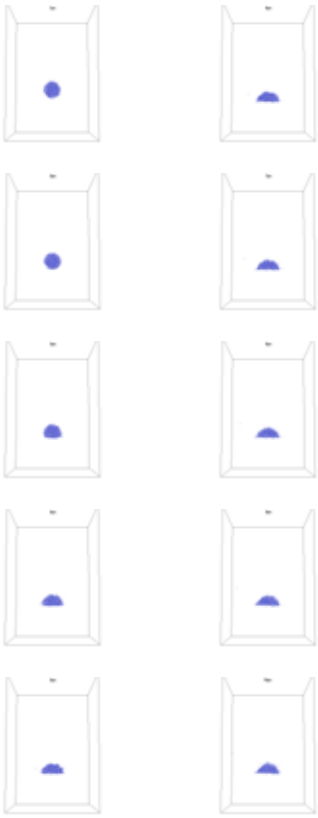

Figure 3.75 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =7 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

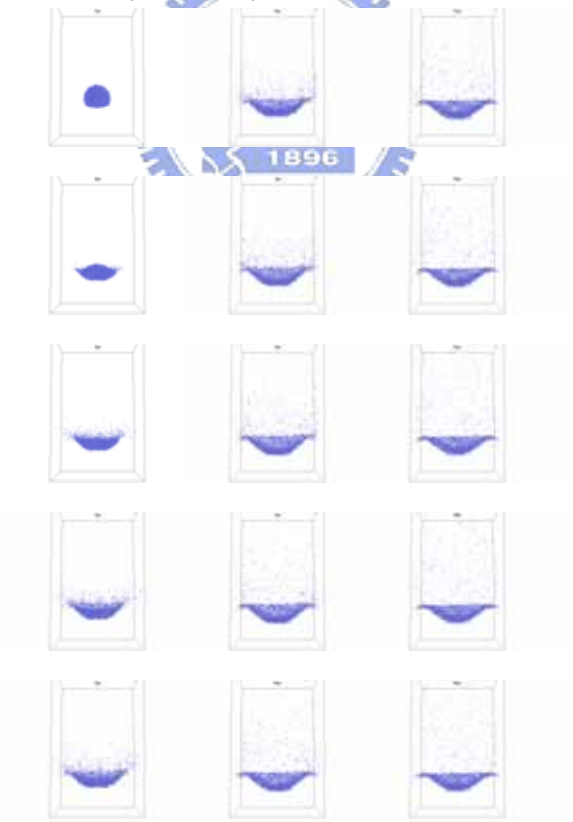

Figure 3.76 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =11 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

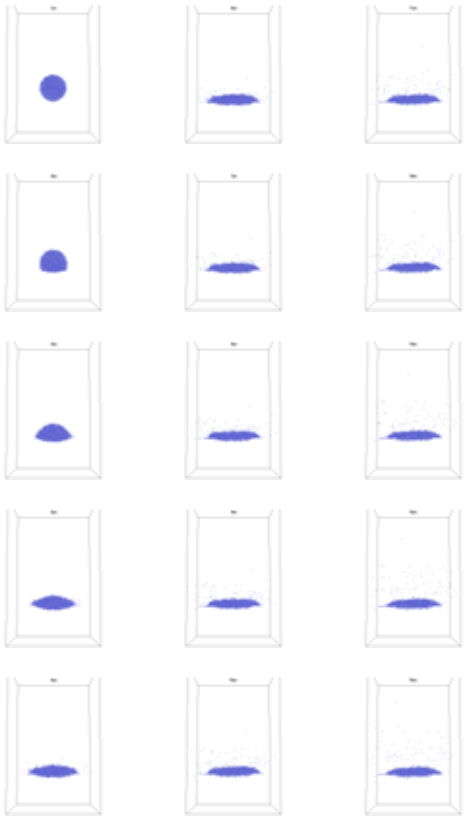

Figure 3.77 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =11 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

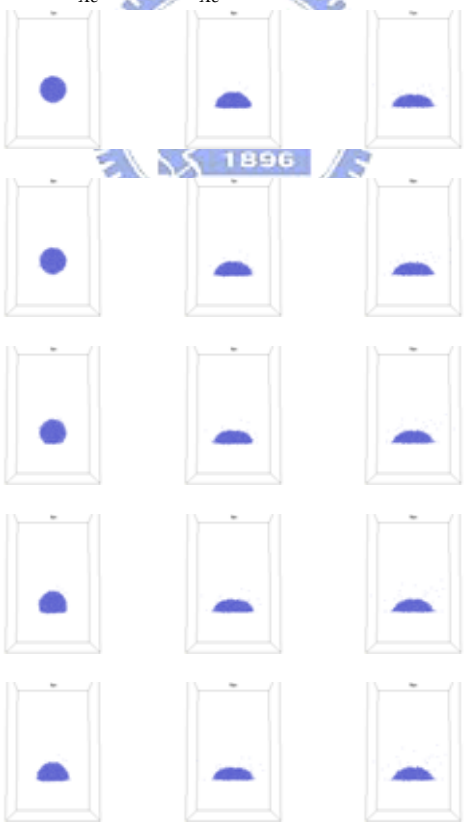

Figure 3.78 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =11 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

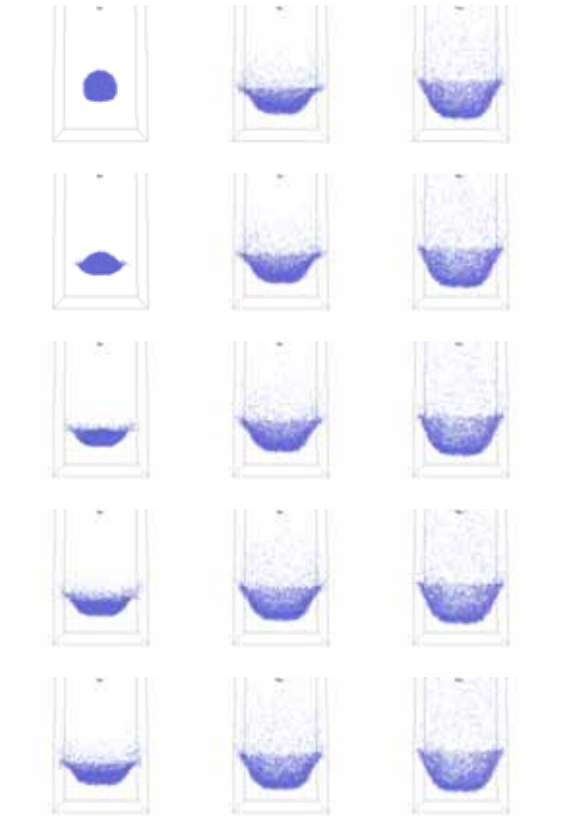

Figure 3.79 The evolution of the droplet impinging on the liquid film with the velocity 2000m/s, droplet radius =14.5 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

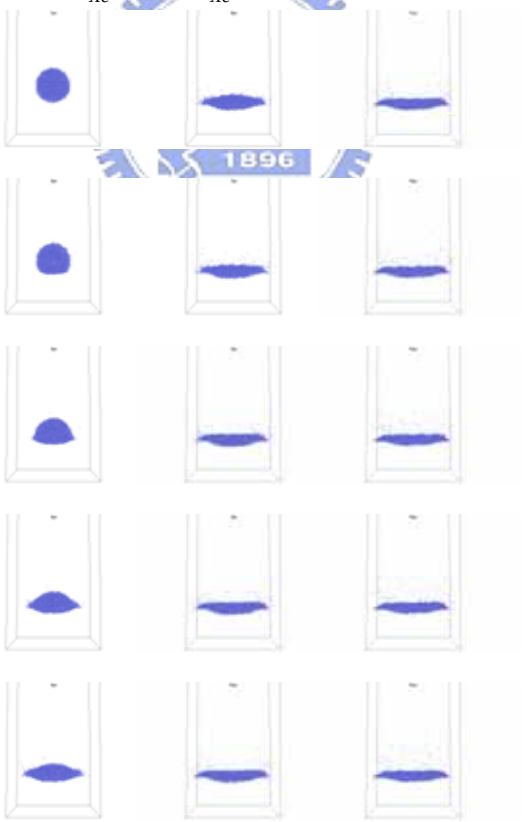

Figure 3.80 The evolution of the droplet impinging on the liquid film with the velocity 1000m/s, droplet radius =14.5 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

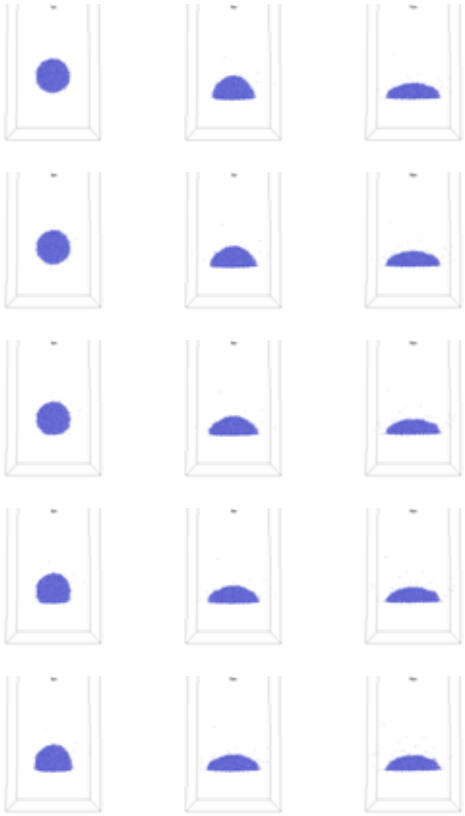

Figure 3.81 The evolution of the droplet impinging on the liquid film with the velocity 500m/s, droplet radius =14.5 σ_{Xe} for 16 σ_{Xe} film thickness. Time increment: 1 time step

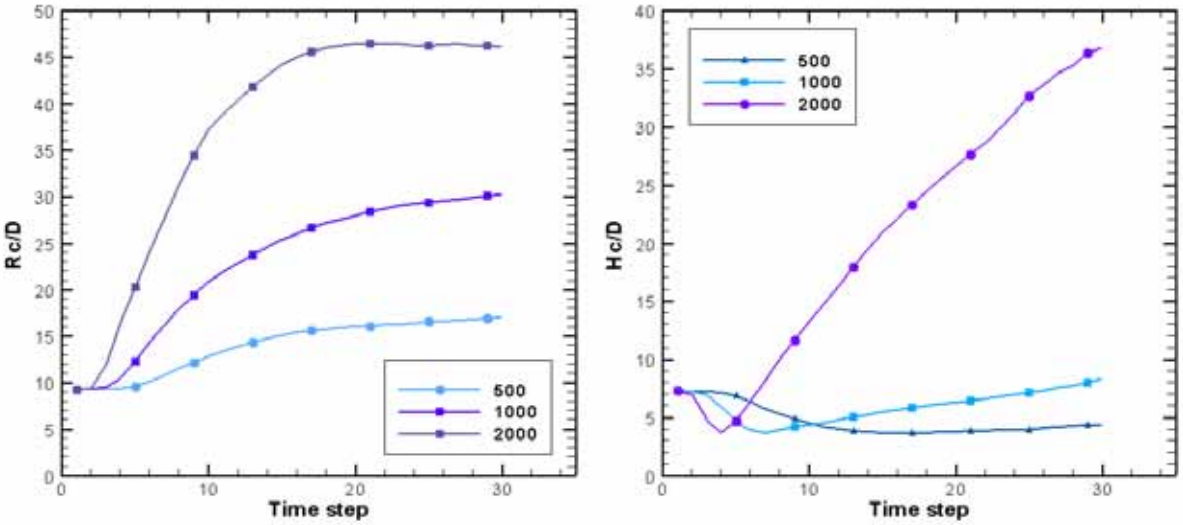

Figure 3.82 Comparison of non-dimensional deformation radius and height of droplet with different impact velocity (a) 500m/s (b) 1000m/s (c) 2000m/s (film thickness=8 σ_{Ar} and droplet size=11 σ_{Ar})

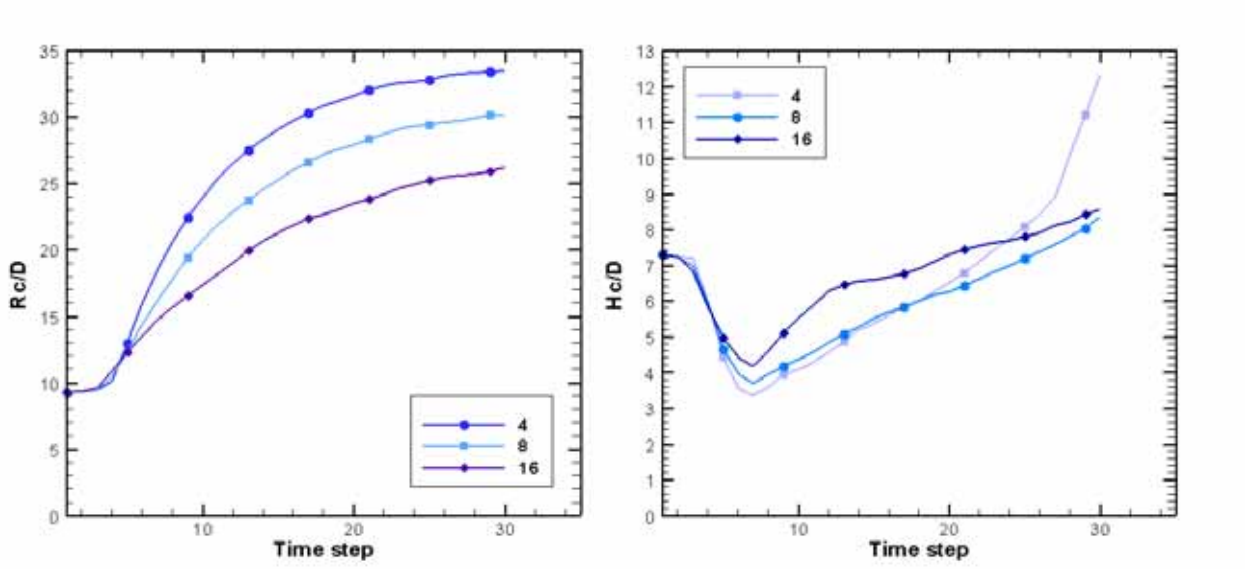

Figure 3.83 Comparison of non-dimensional deformation radius and height of droplet with different film thickness (a) $4\sigma_{Ar}$ (b) $8\sigma_{Ar}$ (c) $16\sigma_{Ar}$ (droplet size=$11\sigma_{Ar}$ and impact velocity=1000m/s)

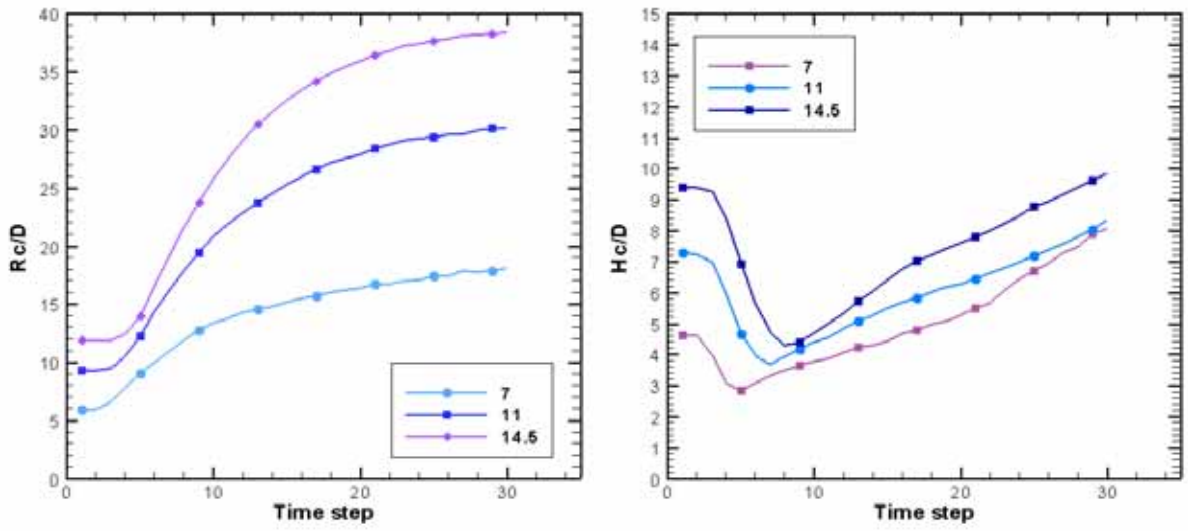

Figure 3.84 Comparison of non-dimensional deformation radius and height of droplet with different droplet size (a) $7\sigma_{Ar}$ (b) $11\sigma_{Ar}$ (c) $14.5\sigma_{Ar}$ (film thickness=$8\sigma_{Ar}$ and impact velocity=1000m/s)