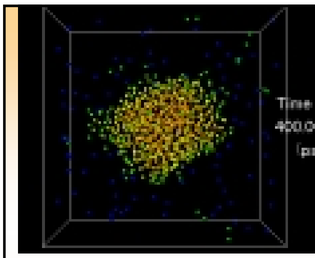
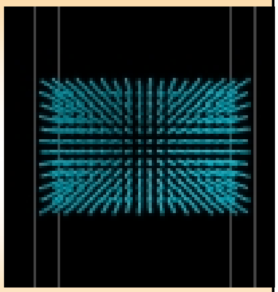
4. Molecular Dynamics of Phase-Interface

4.1 Liquid Vapor Interface
- Surface Tension
- Young-Laplace Equation
- Condensation Coefficient

4.2 Liquid-Solid-Vapor Contact
- Liquid Droplet on a Solid Surface
- Vapor Bubble on a Solid Surface
- Contact Angle and Young's Equation
- Thermal Boundary Resistance between Liquid and Solid

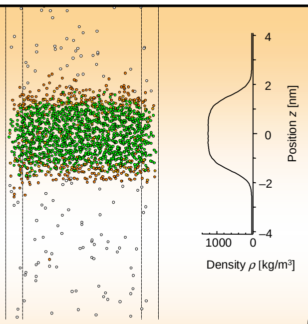


Liquid Droplet



Flat Interface

Liquid-Vapor Interface



$$\gamma_{LG} = \int_{z_L}^{z_G} \left[P_N(z) - P_T(z) \right] dz$$

Surface Tension

Young-Laplace Equation

$$\gamma_{LG} = \frac{(P_L - P_G)R}{2}$$

$$P_N(r) = k_B T \frac{\rho(r)}{m} - \frac{1}{4\pi r^2} \sum_k f_k$$

$$P_N(r) = k_B T \frac{\rho(r)}{m} - \frac{1}{4\pi r^3} \sum_k \left| \mathbf{r} \cdot \mathbf{r}_{ij} \right| \frac{1}{r_{ij}} \frac{d\phi(r_{ij})}{dr_{ij}}$$

Equilmolar Dividing Radius $\quad mN = \frac{4\pi}{3} R_e^{\,3} \rho_L + \left\{ L^3 - \frac{4\pi}{3} R_e^{\,3} \right\} \rho_G$

Tolman Length δ $\quad \gamma_{LG} = \gamma_{LG\infty} \left(1 - \frac{2\delta}{R_e} \right) + O\left(R_e^{\,-2} \right)$

Surface Tension of Droplet

Condensation coefficient α

$$\alpha = \frac{\textit{Condensation Molecule Flux}}{\textit{Incident Molecule Flux}}$$

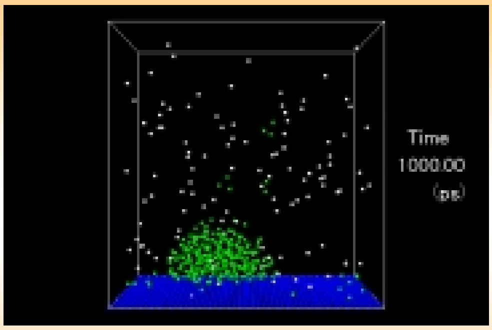
Matsumoto et al.

Molecular Exchange = Boiling off other molecules

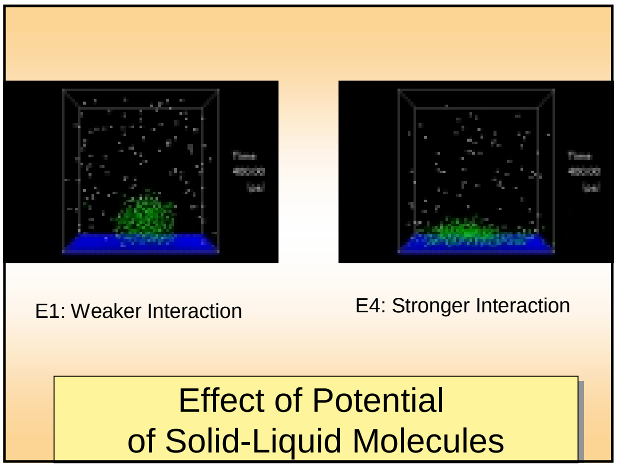
Tsuruta et al.

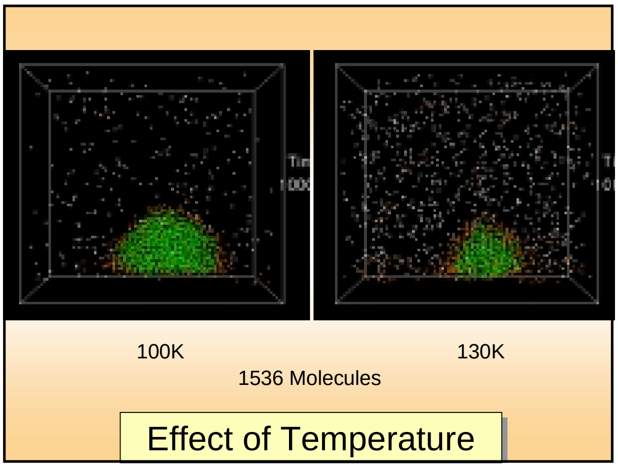
Connection to DSMC

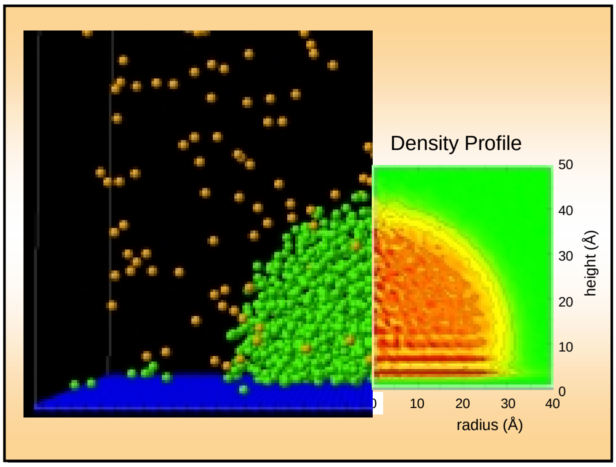
Condensation Coefficient

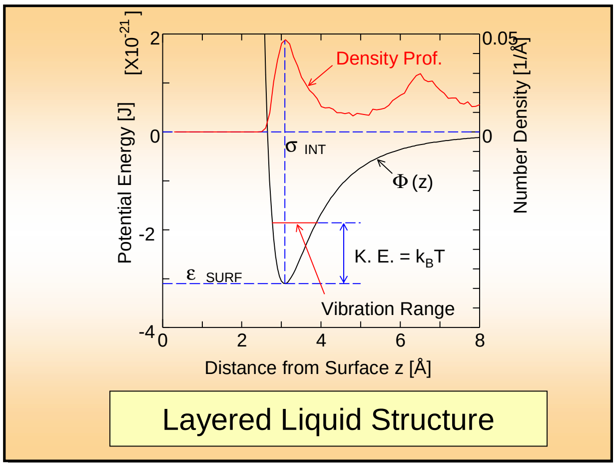


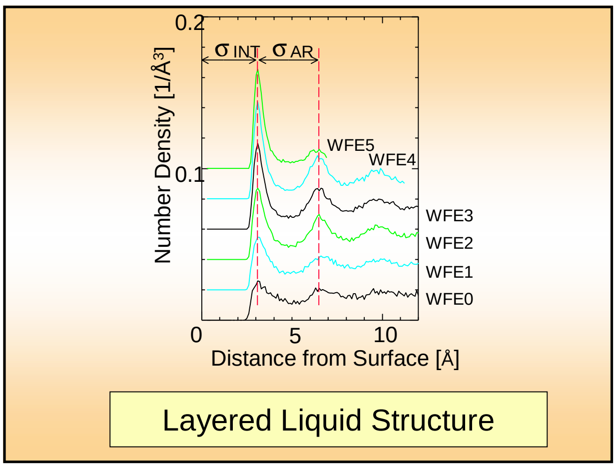
Liquid Droplet on Solid Surface

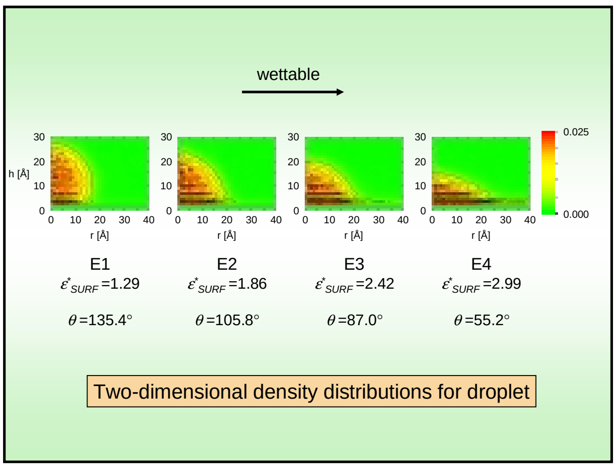

E1: Weaker Interaction
E4: Stronger Interaction
Effect of Potential
of Solid-Liquid Molecules

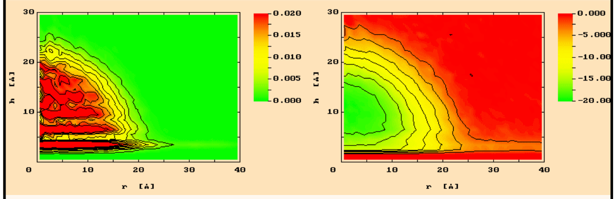

100K
130K
1536 Molecules
Effect of Temperature


Density Profile
height (Å)
radius (Å)
50
40
30
20
10
0
10
20
30
40

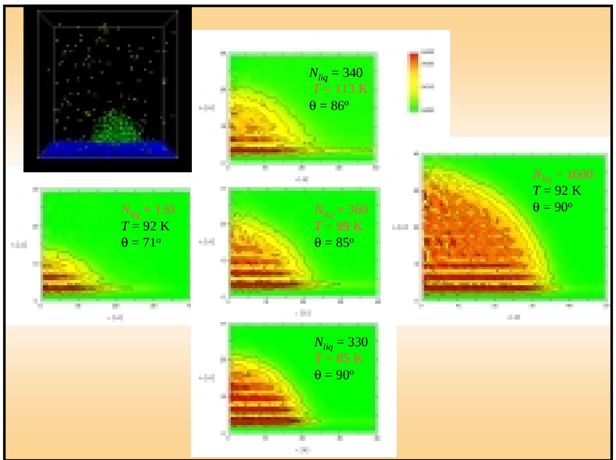

[X10^-21]
Potential Energy [J]
Number Density [1/Å³]
Density Prof.
σ INT
Φ (z)
K. E. = k_BT
ε SURF
Vibration Range
Distance from Surface z [Å]
2
0
-2
-4
0
2
4
6
8
0.05
0
Layered Liquid Structure

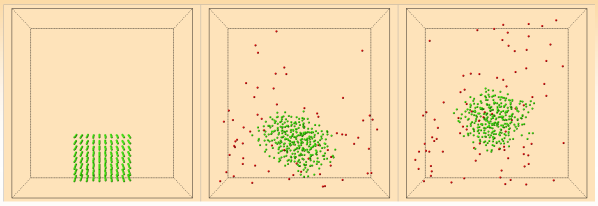

0.2
0.1
σ INT
σ AR
Number Density [1/Å³]
WFE5
WFE4
WFE3
WFE2
WFE1
WFE0
0
5
10
Distance from Surface [Å]
Layered Liquid Structure


wettable
h [Å]
r [Å]
0.025
0.000
E1
ε*SURF =1.29
θ =135.4°
E2
ε*SURF =1.86
θ =105.8°
E3
ε*SURF =2.42
θ =87.0°
E4
ε*SURF =2.99
θ =55.2°
Two-dimensional density distributions for droplet



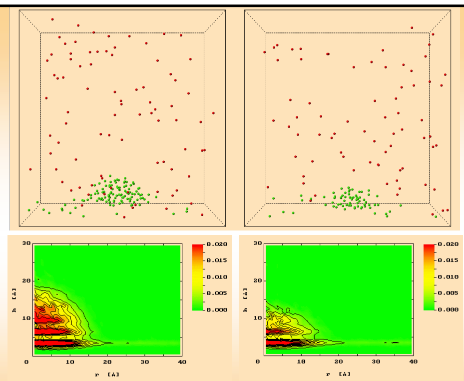
Density and Potential Profiles





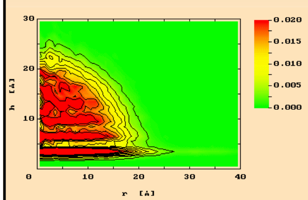
t = 0 ps   t = 30 ps   t = 60 ps

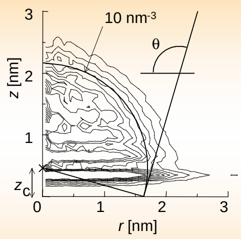
Departure of Droplet for $\varepsilon^*_{SURF} < 1.0$



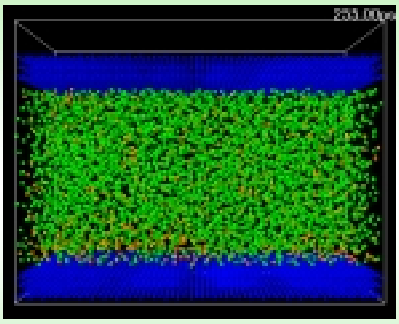
N = 200, N_{Liquid} = 114   N = 144, N_{Liquid} = 66

Smaller System ε^*_{SURF} =1.86

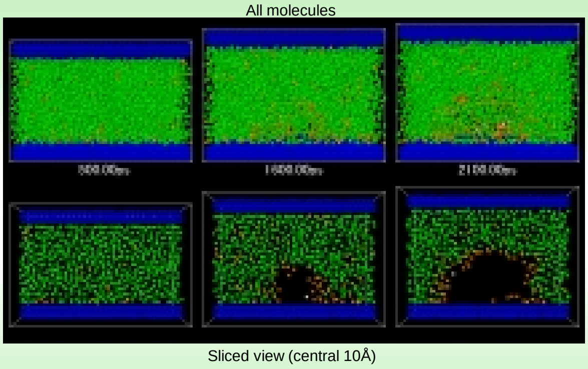




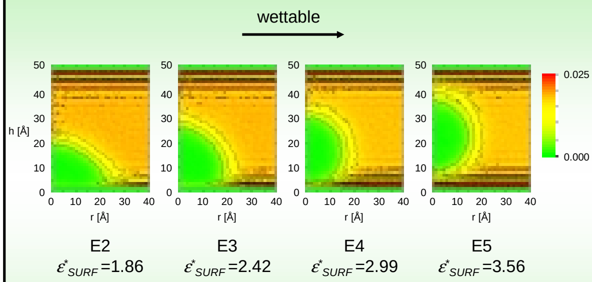
Density and Potential Profiles



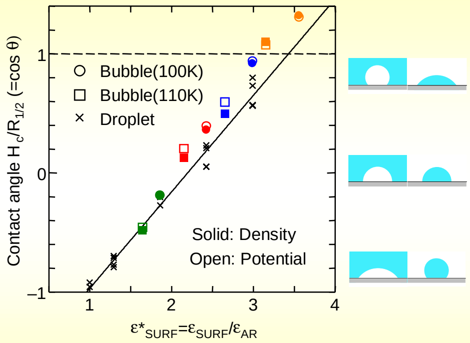
Vapor Bubble on Solid Surface



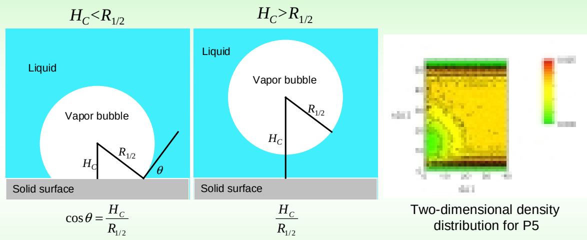
Snapshots of bubble formation for E3



Two-dimensional density distributions



Contact angle correlated with ε^*_{SURF}

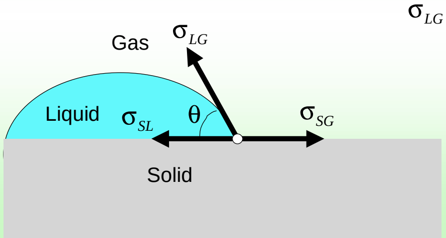


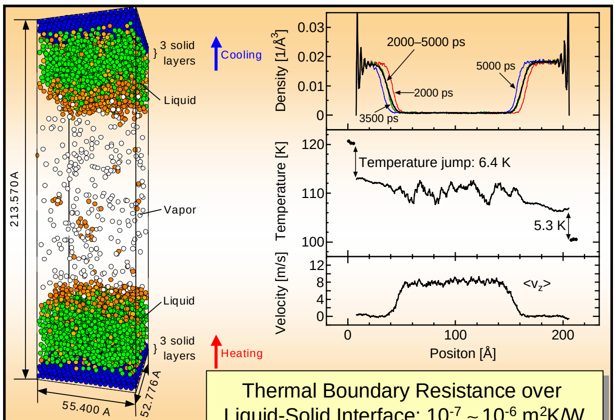
Definition of contact angle $\cos\theta$ for E5 and P5

Young's Equation (Macroscopic)

$$\sigma_{LG}\cos\theta + \sigma_{SL} = \sigma_{SG}$$

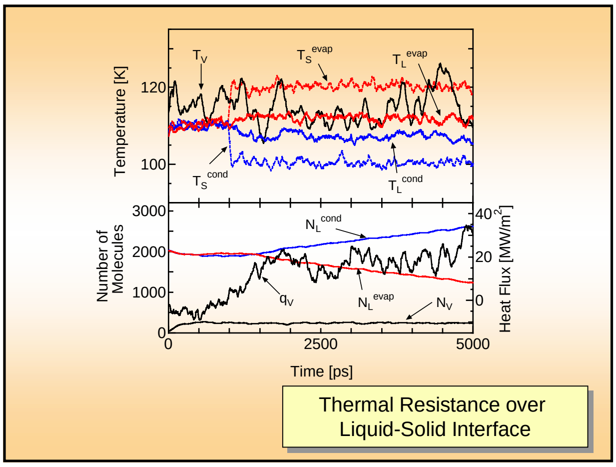
$$\cos\theta = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}}$$

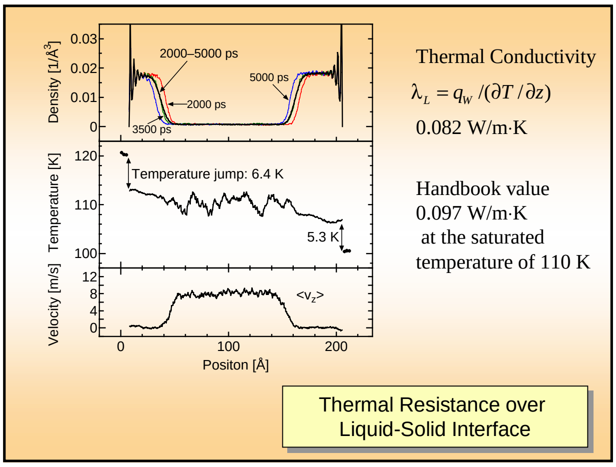


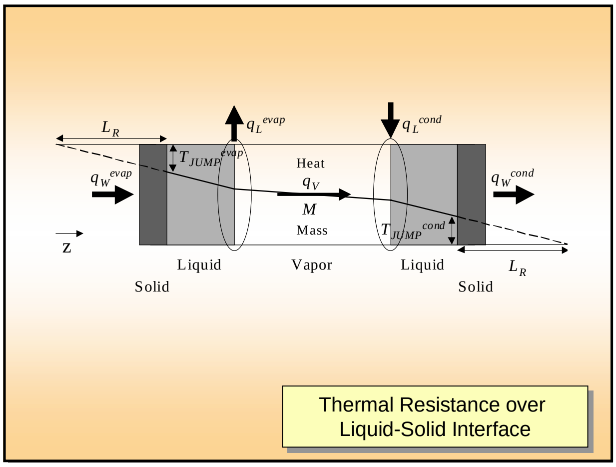


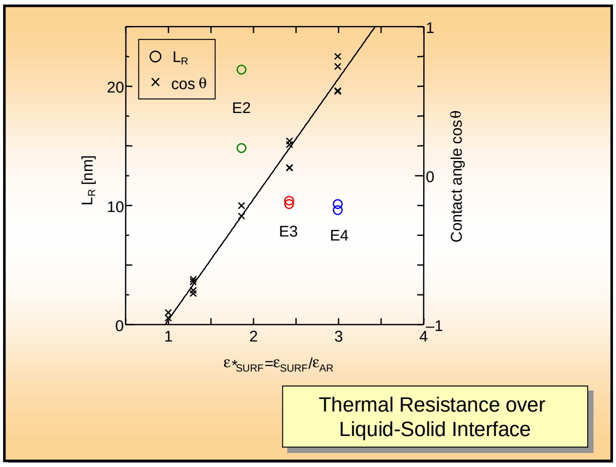
Thermal Boundary Resistance over Liquid-Solid Interface: $10^{-7} \sim 10^{-6}$ m²K/W

Therm. Sci. Eng., 1999, vol. 7, no. 1, pp. 63-68.


Temperature [K]
Number of Molecules
Heat Flux [MW/m2]
Time [ps]
Thermal Resistance over Liquid-Solid Interface


Density [1/Å3]
Temperature [K]
Velocity [m/s]
Positon [Å]
2000–5000 ps
5000 ps
2000 ps
3500 ps
Temperature jump: 6.4 K
5.3 K
<vz>
Thermal Conductivity
λL = qW /(∂T /∂z)
0.082 W/m·K
Handbook value
0.097 W/m·K
at the saturated
temperature of 110 K
Thermal Resistance over Liquid-Solid Interface


Heat
Mass
Liquid
Vapor
Liquid
Solid
Solid
Thermal Resistance over Liquid-Solid Interface


LR [nm]
Contact angle cosθ
LR
cos θ
E2
E3
E4
ε*SURF=εSURF/εAR
Thermal Resistance over Liquid-Solid Interface