

Molecular Dynamics Simulations of a Liquid Droplet in Contact with a Solid Surface

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ABSTRACT

Adequate treatments of phase interfaces are crucial for the sound microscopic modeling of multiphase flows. Especially when phase change phenomena such as evaporation and condensation are involved, consideration of molecular scale phenomena may be necessary to predict the kinetic behavior of interfaces. Hence, an example of the molecular dynamics simulation of phase interfaces is described for a tiny liquid droplet which is in contact with a solid surface. Here, we encounter three different kinds of phase interface, the liquid-vapor interface of the same molecular species, liquid-solid and vapor-solid interfaces of different species.

Molecular dynamics simulations were performed with typically 400 Lennard-Jones molecules for liquid and vapor as well as up to 4 layers of molecules with harmonic potential representing the solid surface. Lennard-Jones molecules were initially placed at fcc crystal lattice points adjacent to the solid surface. With a given temperature the L-J crystal would melt and evaporate to a L-J liquid droplet surrounded by its vapor. The interaction potential between L-J molecules and solid surface molecules was represented by the Lennard-Jones potential with various length scale σ_{sl} and energy scale ϵ_{sl} . When the potential parameters, σ_{sl} and ϵ_{sl} were within the certain range, the liquid droplet was in contact with the surface.

Using a cylindrical coordinate system from the center of the liquid droplet, the two-dimensional (radius and height) density profile was calculated. Furthermore, the contact angle was measured just like the experimental evaluation, spherical curve fit to the density profile. The two-dimensional potential profile measured in the same manner exhibited almost the same contact angle. From simulations for various length scale σ_{sl} and energy scale ϵ_{sl} of the potential between L-J molecules and solid surface molecules, it was found that cosine of the measured contact angle was correlated as a linear function of σ_{sl} and ϵ_{sl} . These linear dependencies along with the effective one-dimensional potential energy of the surface suggest that the over all shape of the droplet can be determined by the simple energy balance concept similar to the macroscopic relation.

Two interesting aspects revealed from simulations are discussed. Even though the over all two-dimensional density profile was in rather good agreement with the spherical fit, there observed the clear layered structure in the density profile. Furthermore, the nearest liquid layer to the surface was considerably expanded from the spherical fit, so that the contact line in the macroscopic sense could hardly defined in the profile. Another feature was the random movement similar to the Brownian motion of the mass center of the droplet along the surface.