

## A MOLECULAR DYNAMICS SIMULATION OF A LIQUID DROPLET ON A SOLID SURFACE

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### ABSTRACT

A liquid droplet placed on a solid surface was simulated by the molecular dynamics method to study the microscopic aspects of the solid-liquid contact. Four hundred argon molecules were employed to create a liquid droplet and the surrounding vapor. The solid surface was represented by a single layer of fcc lattice made of fixed Lennard-Jones particles. The energy scale  $\epsilon_{sl}$  of the inter-molecular potential between solid and liquid molecules and the system temperature  $T$  were changed to reproduce various shapes of droplets. Two-dimensional density and potential energy distributions obtained for various values of the solid-liquid potential parameter  $\epsilon_{sl}$  showed a strong dependency of the droplet shape on the magnitude of the interaction of solid and liquid molecules. The density distributions revealed the layered structure of the liquid molecules near the solid surface. However, the dependency of the estimated contact angle on various parameters was not far from the simple energy balance concept of a macroscopic liquid drop.

### NOMENCLATURE

$h$	= height measured from the surface
$N_v$	= the number of vapor molecules
$R$	= radius of droplet
$r$	= radius measured from the center of droplet
$T$	= temperature
$\epsilon$	= energy scale of L-J potential
$\epsilon^*$	= non-dimensional energy scale, $\epsilon_{sl}/\epsilon$
$\phi(r)$	= potential function
$\gamma$	= surface free energy
$\theta$	= contact angle
$\sigma$	= length scale of L-J potential

### Subscripts

c	= center of droplet
g	= vapor
l	= liquid
s	= solid

### INTRODUCTION

The microscopic mechanism of solid-liquid contact is the fundamental issue to understand the phase change phenomena such as the dropwise condensation on a solid surface and the collapse of film boiling leading to the transition boiling. The physical mechanism of solid-liquid contact is, however, not sufficiently understood. Recently, the simulation of the liquid-vapor interface by the molecular dynamics method has become the powerful technique to get physical insights into the interface properties such as surface tension (Maruyama et al., 1994a; Maruyama et al. 1994b; Matsumoto, 1994; Nijmeijer et al., 1992) and condensation coefficient (Matsumoto and Kataoka, 1992). However, little is known about the microscopic dynamics of the solid-liquid contact where three phases: solid, liquid and vapor coexist.

In this paper, we report our attempts to investigate the microscopic mechanism of solid-liquid contact using molecular dynamics simulations of a tiny liquid droplet placed on a solid surface. For the purpose of obtaining a basic knowledge on the phenomena, we have chosen a rather simple system as the calculation model. The system included two groups of molecules: one was for the liquid droplet and its vapor, the other for the solid surface. Only the molecules of the former group were computed; the molecules for the solid were fixed at grid points. Although our model of the solid surface does not seem realistic, our preliminary simulations with several types of surface models have suggested that the complicity of the solid model was not so important as far as the results discussed in this

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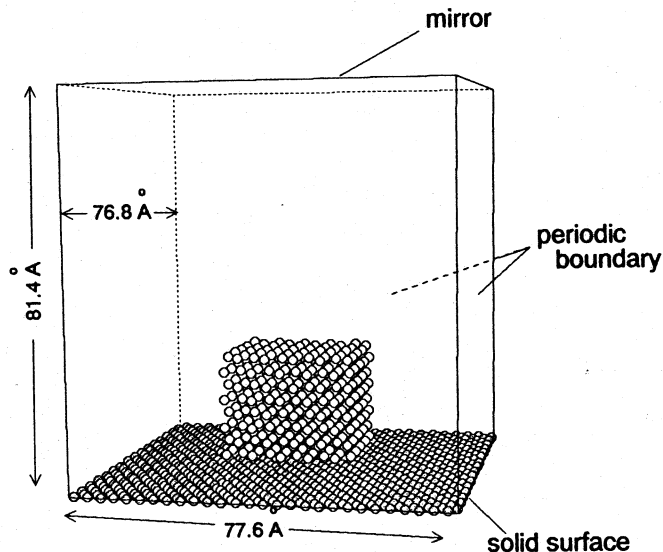


FIG. 1 CALCULATION REGION AND THE INITIAL CONFIGURATION OF MOLECULES

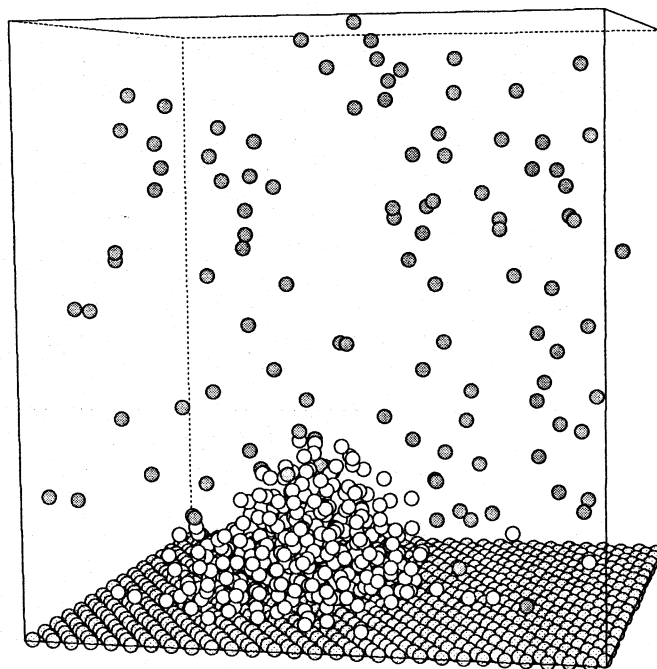


FIG. 2 A SNAPSHOT OF A GENERATED DROPLET ON THE SOLID SURFACE (E2:  $T = 95\text{K}$ ,  $\epsilon^* = 0.344$ )

paper were concerned. We assumed Lennard-Jones potential functions for both liquid-liquid and solid-liquid interactions. The parameter  $\epsilon_{sl}$  for the solid-liquid potential function can be regarded as a measure of the affinity between the solid and the liquid. Thus we have paid the special attention on the effect of the solid-liquid affinity on the states of contact, including the structure of the interface region and the shape of the droplet as a whole, by applying various values for this parameter. The effect of the temperature was also speculated from simulations of two different system temperatures.

### DESCRIPTION OF SIMULATIONS

The molecular dynamics simulation was designed to achieve a stable equilibrium state of liquid droplet and its vapor on a solid surface under the *NVE* ensemble, i.e. the number of molecules, volume and total energy of the system were kept constant. Fig. 1 illustrates the calculation region and the initial configuration of molecules. The region had a mirror boundary (or a hard wall boundary) for the top wall and periodic boundaries for the four side walls. The solid surface located at the bottom of the calculation region was represented by one layer of molecules on a (111) plane of the fcc lattice structure. The lattice constant  $2.77 \text{ \AA}$  was employed after that of the platinum. We ignored the motion of these particles and the influence from the molecules beneath the one layer. It is noteworthy that this stationary molecules was an adiabatic boundary since there was no energy transfer through the surface.

The liquid drop and the vapor were formed of argon molecules. The interactions between molecules were expressed by the following Lennard-Jones potential function.

$$\phi(r) = 4\epsilon \left\{ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right\} \quad (1)$$

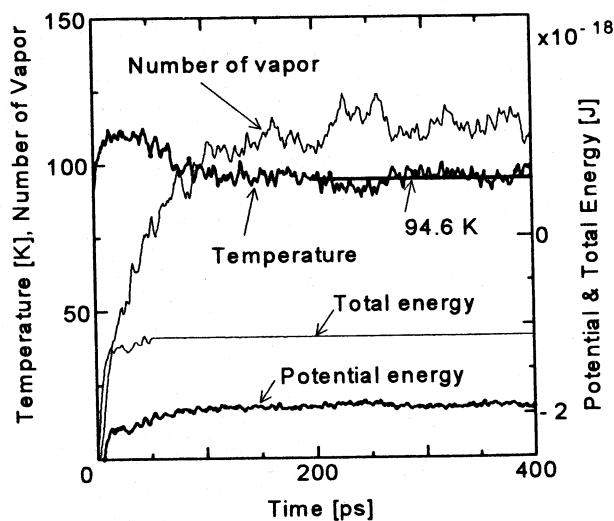


FIG. 3 NUMERICAL EVAPORATION AND EQUILIBRIUM OF A DROPLET (E2:  $T = 95\text{K}$ ,  $\epsilon^* = 0.344$ )

Values of parameters were  $\sigma_l = 3.4 \text{ \AA}$ ,  $\epsilon_l = 1.67 \times 10^{-21} \text{ J}$  for liquid-liquid interaction. As for the solid-liquid interaction,  $\sigma_{sl}$  was determined by taking average of the lattice constant of the solid and  $\sigma_l$ . On the other hand,  $\epsilon_{sl}$  was implicitly specified through a non-dimensional parameter  $\epsilon^* = \epsilon_{sl} / \epsilon_l$  as one of the calculation conditions.

The system contained four hundred argon molecules which

