# Molecular Dynamics Study of Lubrication Phenomena of Nanoscale Liquid Bridge between Surfaces

T. Tokumasu[1*], M.-H. Meurisse[2] , N. Fillot[2] , P. Vergne[2]

[1)] Institute of Fluid Science, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan.
[2)] Universite de Lyon, CNRS, INSA-Lyon, LaMCoS UMR5259, F-69621 Villerubanne Cedex, France.
[*]Corresponding author for tokumasu@ifs.tohoku.ac.jp

I

## 1. Introduction

When the lubricant supply is not sufficient to fill the gap between the solid surfaces in a lubricated contact, or when the wettability conditions are insufficient, the lubrication film can fractionate into disjointed liquid bridges. In these circumstances, surface tension of the liquid at the menisci and the behavior of mobile contact lines may strongly influence the friction between surfaces [1]. Especially, when the width of the liquid bridge is in the order of nanometers, such as in thin film or boundary lubrication regimes, the effect of the interfacial region cannot be disregarded. The phenomena occurring in a nanoscale liquid bridge must be analyzed from a microscopic point of view. Molecular dynamics (MD) is an effective tool for analyzing the molecular mechanisms of such nanoscale transport phenomena. From this point of view, we already observed the characteristics of lubrication phenomena of nanoscale liquid bridge without surfaces and it is found out that the momentum flux through the interfacial region is 1/4-1/3 of that through bulk region.

In this paper, the momentum transport phenomena in a nanoscale liquid bridge between surfaces are simulated using MD method and the effect of surfaces, such as wettability, on the momentum transport phenomena of liquid bridge are analyzed in detail.

## 2. Simulation method

In this paper a steady momentum flux in a nanoscale liquid bridge made of water between Si surface was generated by nonequilibrium molecular dynamics method. The schematic diagram of the simulation system is shown in Fig. 1. The dimension of the simulation system was set at $L_x$ =80 Å, $L_y$ =120 Å and $L_z$ =30 Å in $x$, $y$ and $z$ direction, respectively and periodic boundary condition was assumed in all direction. Silicon surfaces consisted of 1152 Si atoms and the number of water molecules was changed to express the difference of the width of liquid bridge. The S-W potential and the SPC/E potential was used as an interaction between Si atoms and water molecules, respectively. The interaction potential between Si atoms and water molecules were obtained as

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

and $\alpha$ was changed to express the difference of wettability. Fennell method was used to consider the coulomb interaction between water molecules. A cutoff distance was set at $R_c$=15 Å. Time integration was performed by Velocity Verlet method and time interval was set at $\Delta t$=1 fs.

Upper Si surface moved to $+y$ direction at the velocity of $V$=50 m/s and the lower surface moved to $-y$ direction at $V$=50 m/s to maintain the velocity gradient. During the simulation the temperature in the bottom layer of these surfaces were controlled to $T$=300 K by velocity control. All cases of simulations were performed 200,000 steps and data were sampled except for the temperature control region.

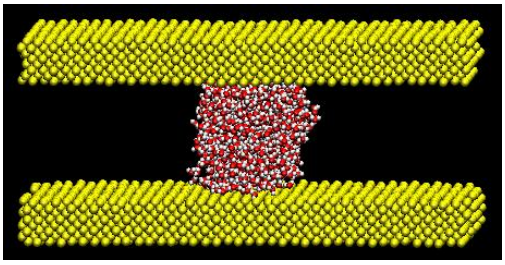

Fig. 1. Schematic diagram of this simulation

## 3. Results and discussion

By this simulations momentum fluxes through liquid bridges are obtained from the tangential force acting on the surface from the liquid bridge and contact area between liquid bridge and the surfaces. The momentum flux decreases with the decrease in the width of liquid bridge. Moreover the momentum flux depends on the wettability of the surface. Comparing these results with those obtained by the simulations without surfaces[2], we will obtain the effect of the surface on the characteristics of momentum transport in the future.

## 4. Acknowledgement

Part of the work was carried out under the Collaborative Research Project of theInstitute of Fluid Science, Tohoku University.

## 5. References

[1] Israelachvili, J. N., “Intermolecular and Surface Forces: 2nd Edition”, Academic Press, 1992.
[2] Tokumasu, T, Meurisse, M.-H., Fillot N. and Vergne P. “A Molecular Dynamics Study of a Nanoscale Liquid Bridge under Shear,” Trybology International, 59, 2013, 10-16.