Tribology International 59 (2013) 10–16

Contents lists available at SciVerse ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

A molecular dynamics study of a nanoscale liquid bridge under shear

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ARTICLE INFO

Article history:
Received 13 October 2011
Received in revised form
16 August 2012
Accepted 20 August 2012
Available online 27 August 2012

Keywords:
Liquid bridge
Molecular dynamics
Momentum transport

ABSTRACT

The lubrication phenomenon occurring by shearing a nanoscale liquid bridge was simulated using the molecular dynamics method by varying the width of the liquid bridge, and the momentum transport phenomena of the liquid bridge were analyzed. The Fennell method was used to calculate the coulombic interaction and the Lees–Edwards method was used to maintain the velocity gradient in the liquid bridge. First, to estimate the overall viscosity coefficient of the liquid bridge, the width and interfacial region of the liquid bridge were determined. The overall viscosity coefficient was then modeled by considering two contributions from the bulk and interfacial region and the momentum fluxes or viscosity coefficients in the bulk and interfacial region were obtained. The model approximately expresses the simulation results, and the viscosity of the interfacial region was determined to be between one fourth and one third of that of the bulk. In addition, the partial momentum fluxes were calculated to verify the validity of the proposed model.

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. Lubrication phenomena by liquid bridges are often observed in everyday life, such as the ski–snow interface, brakes under wet conditions, or the water film between a windshield and wiper under drying conditions. 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 [1,2]. The classical theories of lubrication do not explain the load acting on the surfaces or the friction generated in liquid bridges, and that is why the analysis of the lubrication phenomena of liquid bridges is important.

As for previous research in the field of liquid bridges, Stark et al. [3] conducted a theoretical analysis of capillary condensation of the liquid between spherical particles and concluded that the shape of a liquid bridge depends on its size, which changes according to the interaction potential. Cheneler et al. [4] developed a method to measure the linear viscoelastic properties of a small volume of liquid contained within a capillary bridge between two flat smooth parallel plates using a microrheometer. Jang et al. [5] analyzed the condensation of a liquid meniscus between a curved tip and a completely wetted substrate using the grand canonical Monte Carlo method and discussed the dependence of the meniscus on the water saturation (relative humidity). Alguacil et al. [6] proposed a theoretical description of the capillary forces between two solid spheres connected by a liquid bridge, and the region where a concave liquid bridge can exist was determined in terms of volume and wetting angle. Meurisse et al. [7] introduced a theoretical analytical model to calculate the normal forces on a solid surface when squeezing a flat liquid bridge and the behavior of the forces was described. Zheng et al. [8] analyzed the interaction between two elastic spheres coupled via a small liquid bridge and the mechanical stability of the interface was examined. Such studies have gradually clarified the theoretical description of liquid bridges.

An interfacial region with a width in the order of nanometers is generated at the gas–liquid boundary in a liquid bridge [1], as shown in Fig. 1. The density and the structure of the liquid in the interfacial region is different from that of the bulk liquid [1], and therefore the momentum flux in the interfacial region is different from that in the bulk region. When the characteristic diameter of the liquid bridge is large enough, the width of the interfacial region is relatively small compared with the bulk, and therefore the momentum that transfers in the interfacial region can be ignored. Under these conditions, the characteristics of momentum transfer in a liquid bridge can be estimated from a macroscopic point of view. However, 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 can no longer be disregarded. The phenomena occurring in a nanoscale liquid bridge must be analyzed from a microscopic point of view. Fluid flow in liquid bridges at the nano/microscale is often observed in various nano/micro devices, and it can be formed from capillary condensation between rough surfaces.

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http://dx.doi.org/10.1016/j.triboint.2012.08.009

Nomenclature

$F_{ij\alpha}$	α component of the force acting on jth molecule from ith molecule
J	momentum flux that is transferred in a liquid bridge
L_α	α component of the simulation domain
M	momentum that is transferred in a liquid bridge
N	the number of molecules in a sampling cell
T	temperature
ΔV	volume of the sampling cell
V_y	shear velocity
W	half width of the interfacial region
K	Boltzmann constant
M	mass of a water molecule
n_α	α component of the number of molecules at initial condition
t	time
Δt	time step of simulation
$v_{i\alpha}$	α component of the velocity of ith molecule
x_0	half of the width of liquid bridge
μ	viscosity coefficient
ρ	density

subscript

b	bulk region
d	lower boundary
I	interfacial region
U	upper boundary

Molecular dynamics (MD) is an effective tool for analyzing the molecular mechanisms of such nanoscale transport phenomena. Of the published studies on the nanoscale flow of polymers confined between parallel solid walls, many have used nonequilibrium MD (NEMD) [9–19] and equilibrium MD (EMD) [9,14–16,20,21] simulations to discuss the "shear thinning" of viscosity, dynamical properties and relaxation of rotation. Ogata analyzed the morphology of hydrocarbon on a wall and quantified its characteristics [22]. The simulation methods to predict Newtonian and non-Newtonian viscosity are also discussed in detail [23–25]. Concerning previous studies of nanoscale liquid bridges, Busic et al. [26] simulated the squeezing motion of liquid bridges made of polymer, and they characterized and compared the time evolution of the liquid filament profile with experimental results. Cramer et al. [27] simulated the formation of a nanoscale liquid bridge submitted to an electric field using the MD method and described the threshold voltage and hysteresis behavior according to the formation of nanoscale liquid bridges. However, the characteristics of momentum flux and the viscosity of nanoscale liquid bridges under shear conditions were not analyzed in detail. The values of the momentum fluxes, or viscosity coefficients, in both bulk and interfacial regions are very important in the analysis of nanoscale flow phenomena.

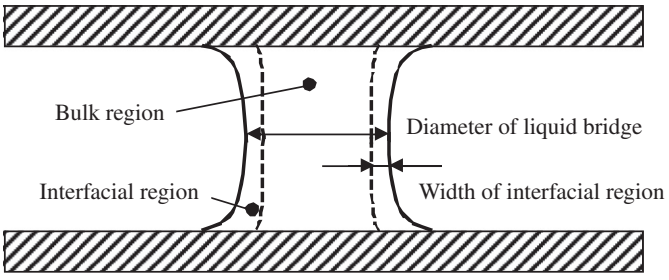

Fig. 1. Shape of a liquid bridge. The bulk and interfacial regions are also shown.

In this paper, the momentum transport phenomena in a nanoscale liquid bridge are analyzed using the MD method and water is used as the liquid. The details of the simulation method are reported in Section 2. In Section 3, the overall viscosity coefficient of a liquid bridge is modeled and the momentum fluxes and the viscosity coefficients in the bulk and interfacial regions are obtained. In Section 4, the partial momentum fluxes in the bulk and interfacial regions are introduced and the consistency with the model is analyzed. Finally, this research is summarized in Section 5.

2. Simulation method

In this paper, a steady momentum flux was generated in a 3-dimensional nanoscale liquid bridge made of water using the nonequilibrium MD method because water is a very important liquid to form a liquid bridge in nature. In real liquid bridge between surfaces, there are concave menisci at solid liquid interfaces, which can affect the behavior of liquid bridges. In this paper, however, we focus on the momentum transfer in both bulk and interfacial region of liquid bridge, which is also important to analyze the characteristics of a nanoscale liquid bridge, as well as meniscus. The analysis of momentum transfer is much easier by the simulation of liquid bridge without concave meniscus because the boundary between bulk and interfacial region becomes straight along z axis. For this reason we only analyze the momentum flux as a first step without concave meniscus toward a better understanding of real liquid bridge behavior. A schematic diagram of the simulation system is shown in Fig. 2. The left panel of Fig. 2 shows the view in the x–z direction and the right panel shows that in the y–z direction. The dimensions of the simulation

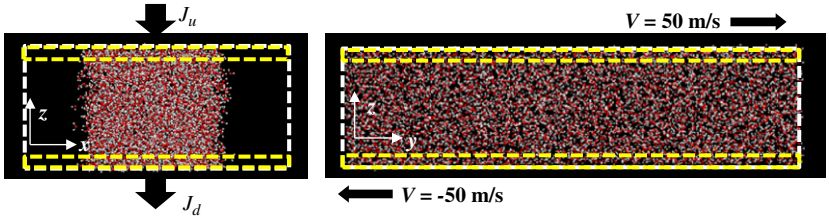

Fig. 2. Schematic diagram of the simulation system in the x–z (left panel) and y–z (right panel) directions. The upper and lower regions indicated by dashed lines are the temperature-control regions. This case is for n_x=8 and the time is 200 ps, where n_x means the number of molecules initially arranged in the x direction.