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Molecular dynamics simulation of mechanism of nanoparticle in improving load-carrying capacity of lubricant film

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ABSTRACT

The properties of base oil and nano-lubricant film confined between two approaching walls under boundary lubrication were studied using molecular dynamics simulation. The nano-lubricant consists of one Cu nanoparticle and *n*-octane as base fluid. The load-carrying capacity of nano-lubricant was found to be much higher than that of the base oil. The nanoparticle improved the load-carrying capacity before rupture of the lubricant film. The effect of nanoparticles on lubricant film structures was analyzed to determine mechanisms responsible for these results. Firstly, because of an adsorption layer around the nanoparticle, the nano-lubricant molecules become more organized and compact compared with base oil. Secondly, the soft Cu nanoparticle is deformed by the structural characteristics of the nano-lubricant film, which provides good support for the lubricant film.

1. Introduction

Recently, the use of nanoparticles as lubricant additives has attracted considerable attention because of their remarkable tribological properties. Many researchers have proven that nanoparticle additives can reduce wear and friction in mechanical systems [1–8]. Compared with traditional additives, nanoparticles are relatively insensitive to temperature and their tribochemical reactions are limited [9,10]. Moreover, a wide variety of nanoparticles exist, including those from metals, metal oxides, sulfides, nonmetals and rare earth elements. Therefore, nanoparticles are promising new lubricant materials.

When the mechanisms responsible for favorable friction properties of nanoparticles are studied, the main researcher concerns are whether protective films are formed and the film chemical composition. By analyzing scanning electron microscopy images and energy-dispersive spectrometry patterns of the wear surface, several mechanisms have been proposed: (a) surface protective films [5,11,12], (b) third-body materials [7,13], (c) rolling friction [14–16], (d) and a self-repair effect [6,17]. However, these mechanisms are speculative based on experimental results and lack theoretical support and direct evidence. The lubrication state in an experiment represents, in general, a combination of boundary lubrication, thin film lubrication, and elastohydrodynamic lubrication. Moreover, the lubrication mechanisms of nanoparticles vary with lubrication state. As a result, mechanisms obtained from experimental results are general and vague. Therefore, more research is required to understand the anti-friction and anti-wear mechanisms of nanoparticles.

Under boundary-lubricated conditions, the lubricant film thickness is of the order of surface roughness. Lubricant film may be ruptured in rough areas because of high contact pressures, which cause direct contact of friction surfaces. Experimental results showed that nanoparticles are most efficient in boundary and mixed lubrication regimes [4,5,9,13,14,17–19]. The nanoparticles are so small that they can enter the contact area easily [3,20], as shown in Fig. 1a (ellipse domain). Asperity areas are locations where lubricant film would first be ruptured. An improvement in the tribology properties in asperity areas by nanoparticles is one of the reasons for a reduction in wear and friction. We infer that structures of lubricant films in asperity contact areas (ellipse domain in Fig. 1a) can be changed by nanoparticles, which influences lubricant film strength and load-carrying capacity. Most existing mechanisms are based on an improvement in worn surface morphology caused by nanoparticles. Minimal studies have been conducted on the properties of lubricant films with the addition of nanoparticles especially for boundary lubrication. Therefore, we have studied changes in physical properties of lubricant film by the addition of nanoparticles to reveal physical mechanisms that result in excellent tribological properties.

Because of the small scale of the nanoparticles and lubricant film, it is difficult to study the physical properties of lubricant film

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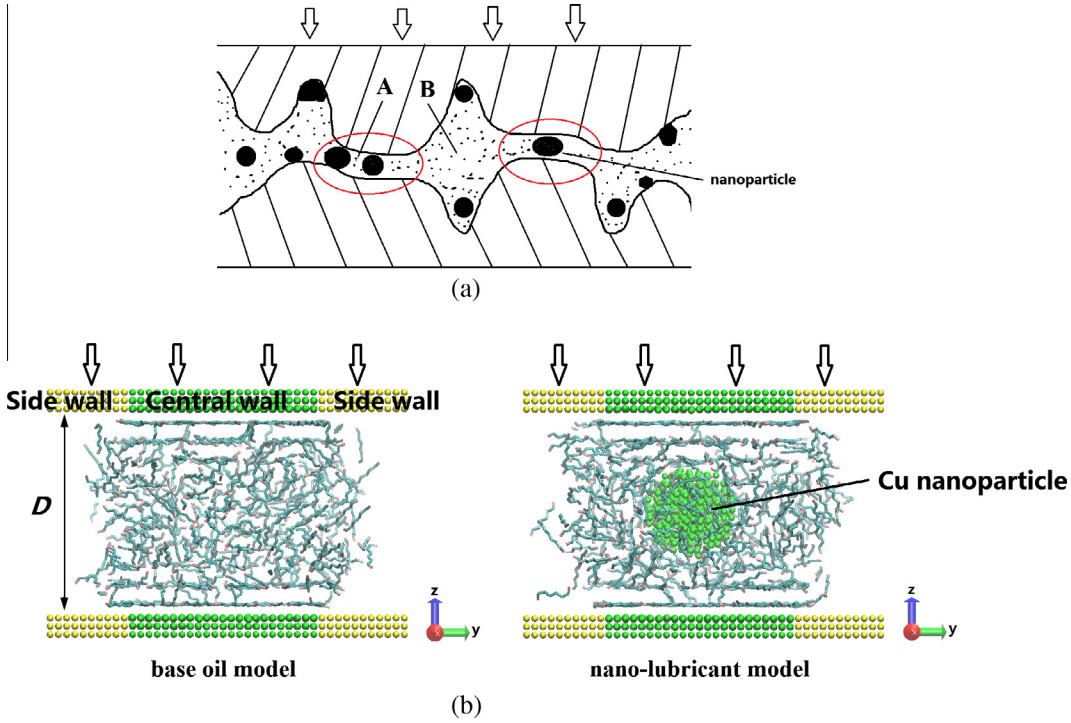

Fig. 1. Schematics for (a) the distribution of nanoparticles under boundary-lubricated condition and (b) MD simulation model.

experimentally. Fortunately, molecular dynamics (MD) simulation can compensate for the lack of experiments and provide an opportunity to understand friction processes at the atomic level. Persson et al. [21–23] have studied the properties of lubricant confined between two approaching solids using MD. Structures of lubricant films at different pressure are shown. Savio et al. [24] investigated the friction properties of the last lubricant layers prior to direct contact of surfaces by considering several parameters. Kalyanasundaram et al. [25] simulated the organizational behavior of *n*-decane for different gap separations (sub-10 nm) and found that the medium structures were affected by mechanical boundary conditions and crystallographic directions. Minimal investigations exist on anti-wear and anti-friction mechanisms of nanoparticles. Lv et al. [26] studied the friction behavior of copper (Cu)–argon nanofluids between two solid plates using MD. However, they only analyzed nanoparticle movement under different pressures and did not consider the interaction between nanoparticles and base fluid. In our previous work [27,28], we investigated the effect of Cu nanoparticles on thin-film lubrication and dry friction. But the intermediate lubrication state where the film thickness was close to the nanoparticle size was not considered.

We therefore simulated properties of lubricants confined between two approaching surfaces using MD. Changes in physical properties of lubrication film (asperity contact areas) caused by the addition of a nanoparticle were investigated. The base oil and nanoparticle were *n*-octane and a Cu nanoparticle, respectively. A comparison of load-carrying capacity and lubricant film structure between the base oil and nano-lubricant (containing a Cu nanoparticle) is discussed.

2. Model and simulation details

2.1. Simulation model

Fig. 1a shows a schematic of the distribution of nanoparticles under boundary-lubricated conditions. The nanoparticles are so small that they can enter the contact area (ellipse domain) easily [3,20]. We mainly investigated changes in physical properties of the lubrication film (asperity contact areas) caused by the addition of a nanoparticle before rupture of the lubricant film. With the increase in load, the film thickness is reduced and some lubricant molecules are squeezed out of the asperity contact region. The lubricant density is a function of pressure and temperature [29]. Under the state of boundary lubrication (Fig. 1a), the pressure in the asperity contact region (region A) is much higher than that in region B. A higher pressure leads to a greater lubricant density. So the lubricant density in region A is higher than that in region B. Moreover, because of the smaller space, the effect of solid walls on the film structure in region A is stronger than that in region B.

To reflect these properties, the MD simulation model was built, as shown in Fig. 1b. The thin lubricant films are confined by solid walls. Periodic boundary conditions are imposed in the *x*- and *y*-directions. Simulation model lengths in the *x*- and *y*-directions are 4.7 nm and 8 nm, respectively. Initially, the lubricant film thickness D is 4.5 nm. The liquid lubricants (C_8H_{18}) and 2-nm-diameter Cu nanoparticle are confined by the two walls. The wall material is the same as that of the nanoparticle. The lower wall is stationary and the upper wall moves down toward the lower wall at a constant squeezing speed v. The outermost layers of the two walls are frozen to prevent deformation. The temperature of the other two layers is maintained the same as the lubricant by using Nose–Hoover thermostat baths [30]. Each wall is composed of a central and two sidewalls. The Lennard-Jones (LJ) potential is used to describe the lubricant–wall interaction. The interaction between the sidewall and lubricant is one-fortieth that between the central wall and the lubricant. The central and sidewall regions are used to represent regions A and B, respectively (Fig. 1a). When the upper wall moves down, the sidewall regions can hold the lubricants squeezed out of the central wall region. The sidewall-lubricant interaction strength ensures that lubricants do not penetrate the walls and that the simulation processes are smooth. As the load increases, it is realistic that the film thickness can be decreased gradually. The film structures in the central wall region are mainly analyzed.