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Friction and wear reduction via tuning nanoparticle shape under low humidity conditions: A nonequilibrium molecular dynamics simulation

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ABSTRACT

Because of the excellently thermal and chemical stabilities, nanoparticles have been considered as a potential lubricant additive to reduce friction and wear. In this study, nonequilibrium molecular dynamics simulations are used to reveal the friction and wear reduction mechanisms of diamond nanoparticle confined between the monocrystalline copper (Cu) slabs under low humidity conditions. The results indicate the movement pattern of nanoparticles can be changed from sliding to rolling by tuning the nanoparticle shape from a flat ellipsoid to a sphere. The sliding of sharp nanoparticles causes the water films being squeezed out from the worn region, which increases the surface friction and wear dominated by the polishing effect but impedes the formation of defects within Cu substrates. Contrarily, in the rolling process controlled by the rolling effect, a lot of water molecules remain in the worn region and thereby stop the surfaces from contacting with nanoparticles, which dramatically improves the friction and wear reduction. The interactive forces manifest the water films can transfer the normal force from slabs to nanoparticles during the rolling process. Therefore, by tuning the shape of nanoparticle additives to facilitate the rolling effect is helpful to reduce friction and wear in boundary or mixed lubrication.

1. Introduction

Lubrication is of vital importance for numerous tribological systems, which cannot only extend the lifetime of individual components and entire systems, thus improving durability and reliability, but also boost energy conversion efficiency [1,2]. It is well known that the lubrication can be classified into four regimes: boundary lubrication, mixed lubrication, elastohydrodynamic lubrication and hydrodynamic lubrication. Among them, the boundary and mixed lubrication shows particularly high friction and wear [3]. In such conditions, to add the friction or wear modifier additives (like organic friction modifiers and nanoparticles) to lubricants is the best-applied method to reduce friction and wear [2–5]. Wherein, the nanoparticles are considered thermal stable at elevated temperatures that make them favorable as solid lubricants and as lubricant additives in comparison with organic additives and have started to play more important roles for their potential in emission reduction and improving fuel economy [5].

There have been many studies on nanoparticles used as the solid lubricants and lubricant modifiers for friction modification and wear resistance. Particularly, the nanoparticles based on carbon compound, metal, metal oxide, metal borate, metal carbonate, fullerenes, and silica have been investigated [3,6–14]. The tribological properties of the lubricant additives of Fe, Cu, Ni and Co nanoparticles in mineral oil were investigated and each set of nanoparticles significantly reduced the coefficient of friction and wear of friction pairs due to the formation of a tribo-layer composed of the elements from the nanoparticles [6,7]. The metal oxide nanoparticles, such as CuO, ZrO_2 and ZnO, showed a good friction and wear-reducing performance, which was produced by tribo-sintering [8]. Wu et al. considered that the anti-wear mechanism was the deposition of CuO nanoparticles on the worn surface, which may decrease the shearing stress, thus improving the tribological properties [9]. Recently, many types of carbon-based nanoparticles have attracted interest for use as boundary lubricant additives since they have a high degree of structural and chemical stability and do not contain some elements like sulfur, phosphor and plumbum, which are environmentally harmful and poisonous for engine exhaust after-treatment devices [5,10]. For instance, Gupta et al. indicated that the improvement in wear by using fullerene (C60) nanoparticles was due either to the transfer-film formation in contact area or to the C60 clusters acting as "tiny ball bearings" [11], while the formation of C60 tribofilm was confirmed by Ginzburg et al. [12]. Similarly, the dispersed carbon nanoonions showed a friction reduction at least as

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effectively as graphite particles [13]. When Nano-Diamond was used as the additives for the SF oil and Base oil, the worn scar depths were reduced by 43.3% and 62.1%, respectively, as compared to the oil without nanoparticles [9]. Before that, Tao et al. found that the ball-bearing effect of diamond nanoparticles existed between the rubbing faces, the surface polishing and the increase in surface hardness effects of the diamond nanoparticles were the main reasons for the reduction in wear and friction [14]. Based on the previous research, the mechanisms of friction reduction and anti-wear of nanoparticles are usually attributed to rolling effect, tribofim formation, mending effect and polishing effect [3,5,9,10]. In addition, it is worth to note that the tribological performances of nanoparticles as friction and wear modifiers are dependent on the individual features of the nanoparticles, such as size, shape, concentration and physicochemical nature [2,4,9].

However, there is still much uncertainty about the relationship between the friction reduction mechanisms and the individual features. During boundary lubrication, the shape of nanoparticles is able to determine the particles' movement pattern related to the friction mechanisms [15–18]. In particular, the nanoparticles are required to be hard enough not to be plastically deformed under the high uniaxial pressures, which maintains the separation of surface asperities [4,10]. On the one hand, the rolling resistance of the approximately spherical nanoparticles may decrease energy losses relative to the sliding friction, as is the case for most macroscopic systems [10,19,20]. On the other hand, the non-spherical nanoparticles may reduce friction through polishing effect, whereby it is possible to shift the system from boundary to mixed lubrication conditions [21]. Therefore, the nanoparticle geometry plays an important role in the friction and wear process, whereas, it is not very clear about how the nanoparticle shape influences the friction and wear behaviors.

In order to further shed light on the friction and wear behaviors and the corresponding friction reduction mechanisms of nanoparticle, the nonequilibrium molecular dynamics (NEMD) simulations are performed, where the diamond ellipsoid is chosen as a hard nanoparticle additive and the metal surfaces are represented by Cu. The particles' size, although rather small because of computational constraints, still lies well within the experimentally relevant range [10]. This will be helpful to give insights into the nanoscale tribological behavior of nanoparticles confined between asperities, which is hard to be derived from experiments.

2. Simulation details

This work was carried out by the NEMD simulations with classical molecular dynamics code LAMMPS [22]. In all simulations, two atomically smooth slabs of monocrystalline Cu with 321,440 atoms and size of $80a \times 25a \times 40a$ (a = 3.615 Å is the lattice constant of Cu) for each one along x-[1 0 0], y-[0 1 0] and z-[0 0 1] crystal orientations were used as the substrates, representing the asperity contact, as shown in Fig. 1. The Cu substrates were composed of boundary zone, thermostat zone and Newtonian zone. The boundary zone containing 5 atomic layers was rigid to provide structural stability, the thermostat zone containing 6 atomic layers was kept at a constant temperature of 300 K to mimic the heat dissipation, and all atoms in the last zone freely moved according the Newton law. The diamond nanoparticles, with various axial ratio (γ) from 0.70 to 0.90 to reflect the change in shape of nanoparticles as listed in Table 1, were confined between the two slabs. The size or volume of nanoparticles would be changed as the axial ratio was adjusted, simply by changing values of b, which means that the change of nanoparticle shape was accompanied by a variation of nanoparticle' size as reported in references [15,18]. As reported by Ewen et al. [10,23,24], the base oil molecules with relatively large volume and long chains were omitted in these simulated systems because most of them will be squeezed out from the contact area of asperities in boundary lubrication. Contrarily, due to the small volume and strong polarity, the ultrathin water molecules can be more easily absorbed on the monocrystalline Cu surfaces to reveal the tribological properties under low humidity or wetting conditions. Here, the initial water films were constructed by Materials studio software and then translated to the data file used in LAMMPS.

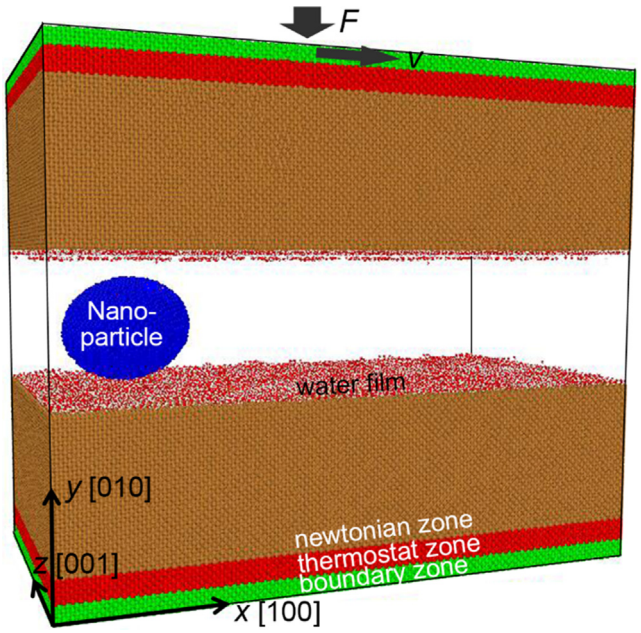

Fig. 1. Schematic of the MD simulation model for monocrystalline Cu with water film.

Table 1
Geometry parameters of nanoparticles with different semi-axes a, b and c along x-, y- and z-directions, respectively.

$\gamma = b/a$	0.70	0.80	0.85	0.90
a (x-axis)/Å	60	60	60	60
b (y-axis)/Å	42	48	51	54
c (z-axis)/Å	60	60	60	60

The interactions between Cu atoms were modeled using the embedded atom method (EAM) potential to accurately reflect plastic deformation within the slabs [25]. The interactions between Cu atoms and C atoms of the diamond nanoparticles were modeled using Morse potential [26] in which the corresponding parameters have been validated in previous results [27–29]. The interactions between C atoms were omitted due to the treatment of a rigid body [27]. The rigid TIP4P model was used to describe the condensed phase of the water film [30]. The interactions of H atoms in water molecules with other types of atoms were neglected due to the weak influence of H atoms [29]. The Cu-O and C-O interactions were modeled by Lennard-Jones (12–6) potential. All the relevant parameters were shown in Table S1 (in Supplementary Materials) [27–29,31–33].

The friction and wear process with diamond ellipsoidal nanoparticles was simulated through three stages: (i) optimizing system energy and configuration at NVT ensemble with Nose-Hoover thermostat for 100 ps. The relaxation performed an energy minimization of the system, by iteratively adjusting atom coordinates with the steepest descent algorithm, and iterations were terminated when one of the stopping criteria is satisfied, where the stopping tolerance for energy is 0.0, the stopping tolerance for force is 10^{-12}, the max iterations is 1000, and the max number of force/energy evaluations is 10,000. In addition, the initially atomic velocities obeying the gaussian distribution were generated using a random number generator with the specified seed at the specified temperature (300 K), and the position and velocity were updated for all atoms each timestep (1.0 fs); (ii) exerting