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Molecular dynamics investigation of the effect of copper nanoparticle on the solid contact between friction surfaces

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ABSTRACT

This study investigated the effect of copper (Cu) nanoparticles on the solid contact between friction surfaces by applying a molecular dynamics method to reveal the mechanisms responsible for the favorable friction properties of nanoparticles. Two models were built, which were named model A (without Cu) and model B (with Cu), respectively. The differences in the mechanical properties between these two models were compared. The simulation results demonstrated that the improvement in friction properties by Cu nanoparticles was more obvious at low velocity than at high velocity. At low velocity, a Cu nano-film was formed on the friction surface, which accommodated the velocity gradient and plastic deformation. Due to the good lubrication effect of the nano-film, the plastic deformation, defect structures and friction force of model B were improved compared with model A. Under high velocity conditions, a transfer layer appeared adjacent to the interface in both models. Because of this, the friction forces of the two models decreased with increased velocity. The fluid mechanics theory was used to explain why the friction force in model B was lower than that in model A at high velocity. The effect of the load on friction properties was also analyzed and the results showed that the mechanisms of anti-wear and friction reduction by Cu nanoparticles under a low load were the same as those under a high load.

1. Introduction

The addition of nanoparticles to lubricants is effective in reducing friction and wears [1–25], and has become an increasingly hot research topic in recent years. The number of publications in the literature on nanoparticle tribology has increased dramatically. There are a wide variety of nanoparticles, including metals [11,13,14,16,20–23], metal oxides [4,5,7,8,10,12,18], sulfides [2,9,17], nonmetals [1,3,5] and rare earth elements [19]. Currently, researchers use small sized manipulation and measurement equipment (such as atomic force microscopy, electron microscopy and energy-dispersive X-ray analysis) to study the tribology properties of nanoparticles and speculate on the anti-wear and friction reduction mechanisms based on the experimental results. Several mechanisms have been proposed in the literature: (a) rolling friction [1–7], (b) third body material [2,8–10], (c) surface protective film [9,11–15,24], (d) a self-repair effect [16–18]. However, these mechanisms are speculative based on experimental results and lack theoretical support and direct evidences. As a result, these mechanisms are still not well known. Ghaednia et al. [26] reported that there is some debate regarding the active and dominant mechanisms responsible for the favorable friction properties of nanoparticles. Therefore, it is essential to study the mechanisms of friction reduction and anti-wear of nanoparticles in detail.

Many studies have demonstrated that gold, silver, palladium, copper, nickel, lead and tin nanoparticles all improve the tribology properties of lubricants [11,13,14,16,20–23]. Most research has been based on the anti-wear and friction reduction properties of copper (Cu) nanoparticles. These soft metal nanoparticles have common characteristics in the lubrication mechanisms. In the present study, we will focus on the effect of Cu nanoparticles in improving tribology properties.

To obtain direct evidences of the mechanisms of dispersing nanoparticles in lubricants which result in lower friction and erosion, we aim to study the mechanical properties of nanoparticles and the effect of these nanoparticles on the mechanical properties of the friction pair. Due to the small scale of nanoparticles, it is difficult to obtain this information in experiments. Therefore, a molecular dynamics (MD) simulation method, which is usually considered a very useful complementary tool to experimental studies on friction mechanisms, provides an opportunity to understand the

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friction process at the atomic level. Lee et al. [27] investigated the rolling friction of a sphere on an atomically flat surface. The results showed that sphere size, penetration depth, and adhesion at the rolling interface strongly affected the rolling friction. Karthikeyan et al. [28] and Lin et al. [29] studied the friction characteristics between metal tribopairs and evaluated the dynamics processes of atomic-scale interfacial friction. Hammerberg et al. [30] studied the metallic friction at Ta/Al and Cu/Ag interfaces and found that the sliding velocity had a significant effect on the friction properties. Kim et al. [31] simulated the process of sliding between crystalline materials and provided insight into the evolution of material structure during sliding. Spijker et al. [32] used MD simulations to model the friction of two rough deformable surfaces and found that friction increases with roughness and decreases to zero after repetitive sliding. However, investigations on the anti-wear mechanisms of nanoparticles are scarce. Lv et al. [33] studied the friction behaviors of Cu–argon nanofluids between two solid plates using MD methods. However, they analyzed the movement of nanoparticles under different pressures and did not study the mechanical properties of the friction system. In a previous study [34], we simulated the effect of nanoparticles on the rheological properties of lubricant film. However, the effect of nanoparticles on the solid contact between friction surfaces was not considered.

In boundary and mixed lubrication, there are not enough liquid lubricants in the contact area to prevent direct metal/metal contacts [35]. Nanoparticles used as lubricant additives can improve direct contacts of friction surfaces. In light of the above, we will investigate the effect of Cu nanoparticles on the solid contact between friction surfaces using MD simulations. The changes in mechanical properties of the friction system caused by the presence of Cu nanoparticle will be discussed. The cooperation between nanoparticles and lubricants will not be considered, thus no lubricant was included in the models built in this study.

2. Model and simulation details

2.1. Model setup

All the simulations were performed using the classical open source MD LAMMPS code [36]. The simulation models are shown in Fig. 1 and were named model A (without Cu) and model B (with Cu), respectively. Periodic boundary conditions were imposed in the *x*- and *z*-directions. The *x*- axis, *y*-axis and *z*-axis were the [1 0 0], [0 1 0] and [0 0 1] orientation, respectively. The friction pair consisted of two similar iron (Fe) blocks. When no nanoparticles were present, the two blocks came into direct contact with each other (Fig. 1a). As shown in Fig. 1b, one Cu nanoparticle with a diameter of 40 Å was placed between the two blocks to avoid direct contact of the friction pair. The two blocks were divided into six layers: rigid layers (1, 6), thermostat layers (2, 5), and free deformable layers (3, 4). The temperature of the thermostat layer was fixed at 300 K using Nose–Hoover thermostat baths [37]. The atoms in each rigid layer were frozen. All the atoms in the free deformable layers were unconstrained and moved freely due to the forces between atoms. The two rigid layers slid in opposite directions at velocity *v*. In order to simulate normal external compressive loads, a normal load (P) was applied to the upper rigid layer. The lower rigid layer remained still in the *y* direction. The total number of atoms in the two models was 56,448 and 59,277, respectively.

2.2. Molecular dynamics

The interactions between solid atoms (Fe–Fe, Cu–Cu, Fe–Cu) were described by embedded atom method (EAM) potential:

$$U = \sum_i F_i \left(\sum_{j \neq i} \rho_i \left(r_{ij} \right) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{ij} \left(r_{ij} \right) \quad (1)$$

where F_i is the embedding energy which is a function of the atomic electron density ρ, ϕ is a pair potential interaction, and i and j represent atoms i and j, respectively. The EAM potential parameters used in the study were developed by Bonny et al. [38].

2.3. Simulation procedure

Each simulation consisted of four steps: relaxation for 200 ps, compression for 200 ps, relaxation again for 200 ps and sliding for 1600 ps. Initially, the system was relaxed adequately to reach an equilibrium state. During compression, the load *P* was applied to the upper rigid layer gradually and the systems were subsequently equilibrated again. The upper and lower rigid layers were then pulled in opposite directions at velocity *v*. The simulation time step was 0.002 ps. In this study, we used the velocity Verlet algorithm [39] to calculate the atomic motions. During the sliding simulation, evolution of friction was tracked by monitoring the tangential *z*-direction forces required to maintain the constant velocity of rigid atoms.

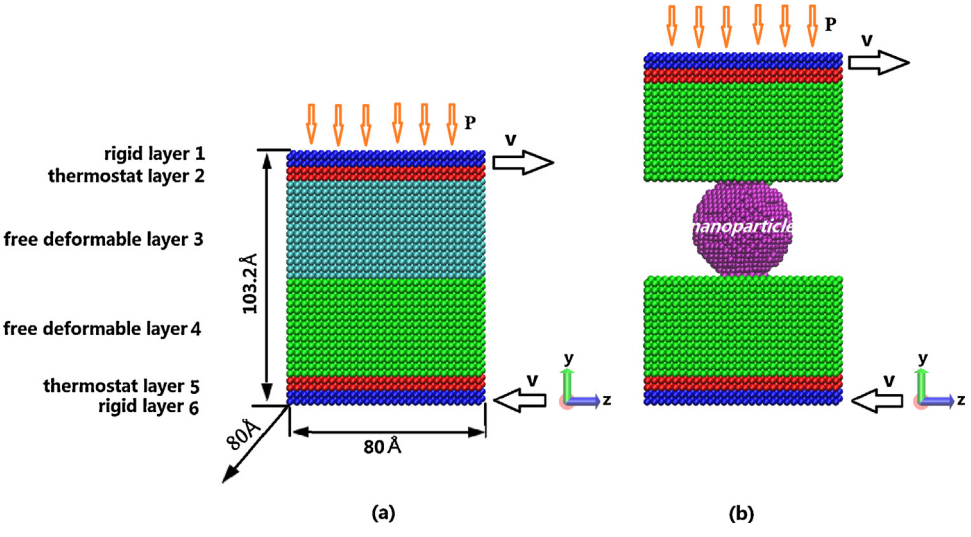

Fig. 1. MD simulation models. (a) Without Cu nanoparticle and (b) with Cu nanoparticle.