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# A molecular dynamics simulation of boundary lubrication: The effect of *n*-alkanes chain length and normal load

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## ABSTRACT

A molecular dynamics simulation of confined *n*-alkanes has been conducted to investigate the effects of the chain length of lubricant molecule and normal load on friction and asperity contact. The density distribution and surface coverage of lubricant atoms were calculated. The simulation results indicate that longer chain *n*-alkanes can provide more atoms for the mono-layer in the asperity contact interface than shorter ones, which, as a result, significantly reduce the friction force when the asperity contact occurs. C64-alkanes molecules can form a mono-layer of lubricant to avoid direct asperity contact at pressures up to 1000 MPa.

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## 1. Introduction

Over the last two decades, molecular dynamics (MD) simulations of confined thin film lubricant have been conducted to investigate its rheological behaviours between atomic flat or rough crystalline walls. It has been found that a layered structure of thin film [1] and stick-slip motion [2] existed in thin film lubrication. There have also been wide discussions about the effects of the chain length of lubricant molecule [3,4], chain branch [5–8] and roughness of wall surfaces [9–12] on viscosity, distributions of lubricant density and velocity, but these works ignored asperity contact and deformation of the wall.

Real tribology inevitably involves surface roughness and asperity contact. It is important to investigate the surface contact between tribo-pairs at the atomic scale with or without lubricant. Zhong and Adams [13] introduced a MD simulation to analyse the effects of sliding velocity, crystal orientation, and asperity shape in aluminium asperity shearing without lubrication. They concluded that the most significant factor in determining the wear process is inter-asperity bonding. Lin et al. [14] identified the dynamic process of dry interfacial friction between Cu/Fe and Cu/Ag metal tribo-pairs, and demonstrated that a rapid increase in temperature occurred when two blocks were sheared, and also observed that extensive plastic deformation and material transfer between blocks occurred. Spijker et al. [15] carried out an atomic simulation of dry sliding contact with 3D rough surfaces and found that by varying the surface roughness,

sliding speed, and applied normal load, the friction force increased with a larger wall roughness. Surface flattening played an important role in reducing the friction force after repetitive sliding. However, there is a limited number of works on boundary lubrication by MD simulation that take the asperity contact with lubricant into account. Eder et al. [16] proposed a smooth particle approach to define and calculate the asperity contact area and lubricant cavity volume. The influence of different shaped asperities and normal load on the contact area and friction force was discussed. However, the effects of lubricant properties, such as the chain length of lubricant molecule, were not considered. Furthermore, Sivebaek et al. [17] carried out a MD simulation in squeezing thin *n*-alkanes films between curved solid surfaces. It was clear that lubricant molecules with a longer chain can provide a better lubrication effect than with a shorter chain.

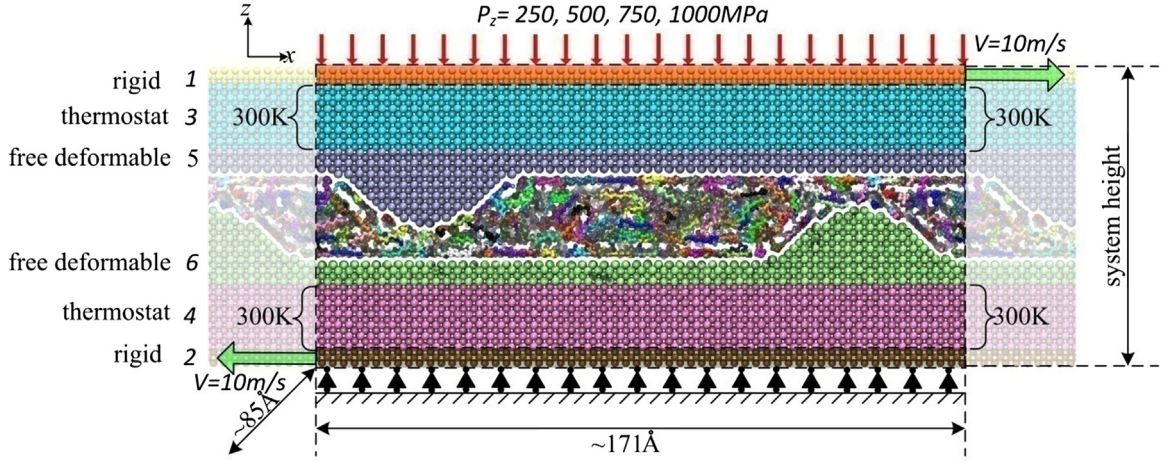
In this paper, a molecular dynamics simulation model with bcc iron as the rough walls and *n*-alkanes as the lubricant was established to investigate the effects of the chain length of lubricant molecule and load on the asperity contact and friction force. It will provide a fundamental understanding of the characterisation of lubricant in boundary lubrication, which can help to design a proper lubricant for metal tribo-pairs in practice.

## 2. Methods

### 2.1. Model setup

The simulation was carried out with the Larger-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) MD code [18]. As shown in Fig. 1, the model consists of upper and lower bcc iron

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**Fig. 1.** A snapshot of the simulation model with *n*-alkanes confined between the bcc iron walls. The lighter shaded regions are periodic images of the simulation box. The external loads ( $P_z$ ) were only applied on the rigid upper layer 1, while the rigid lower layer 2 was fixed in *y*- and *z*-directions. The arrows with  $V=10$  m/s indicate the sliding speed imposed on the rigid layers.

walls with (0 0 1) surfaces, and randomly distributed *n*-alkanes with the chain length in the range of 8, 16, 32 and 64. The bcc iron wall could be further divided into six layers: rigid layers (1, 2), thermostat layers (3, 4), and free deformable layers (5, 6). A sinusoid curve with an amplitude of 15 Å and period of 92 Å was used to construct the asperities of the upper and lower iron walls. Periodic conditions were applied to the *x*- and *y*- directions. The normal direction (*z*) was allowed to vary because the film thickness fluctuated during the compression and shearing under different normal loads, such as 250, 500, 750 and 1000 MPa. The number of atoms in the iron walls was kept constant at 74340. There were 5400, 21600 and 10170 atoms for rigid, thermostat and free deformable layers in the upper wall and the lower counterparts had the same atom numbers. The upper and lower walls slid against each other along the *x*-direction at the same but opposite speed of 10 m/s. In this work, 9600 united atoms ( $\text{CH}_3$  and  $\text{CH}_2$ ) were used to construct *n*-alkanes, which satisfied the following conditions: (1) the asperity peaks do not touch the opposite wall's surface during compression, and (2) the upper and lower asperities contact each other during shearing. It must be noted that the number of lubricant molecules varied with different chain lengths (8, 16, 32 and 64) although the number of lubricant atoms was fixed at 9600.

## 2.2. Force field

The bcc iron walls were modelled by the Finnis-Sinclair (FS) EAM potentials [19] which can represent the properties of solid Fe better than Lennard-Jones (LJ) or Morse potentials. It was crucial to introduce a realistic force potential for solid walls in the current research because the asperity contact involves a severe plastic deformation and transfer of atoms, which depends entirely on a proper force field.

The *n*-alkanes were represented by a United-Atom (UA) model (TraPPE-UA [20]). The TraPPE-UA model uses pseudo-atoms representing all  $\text{CH}_x$  groups that are located at the position of carbon atoms. The molecular potential includes bond stretching, angle bending and torsion angle. Interactions between all non-bonded pairs, as well as the solid-liquid potential, were modelled by LJ potential, as shown in Eq. (1).

$$E_{\text{nonbonded}} = 4\epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad (1)$$

where,  $r_{ij}$ ,  $\epsilon_{ij}$ , and  $\sigma_{ij}$  are atom to atom separation, LJ well depth and diameter, respectively. The parameters of unlike

**Table 1**

Potential parameters used in this work.

LJ 12–6 potentials	$\sigma$ (Å)	$\epsilon$ (eV)	Mass(g/mole)	
$\text{CH}_3^a$	3.75	0.0084449	15.0351	
$\text{CH}_2^a$	3.95	0.0039639	14.0272	
$\text{Fe}^b$	2.20	0.0294720	55.8450	
Bond	$K_b$ (eV/Å <sup>2</sup> )	$r_0$ (Å)		
C–C <sup>a</sup>	39.0279464	1.54		
Angle	$K_\theta$ (eV/rad <sup>2</sup> )	$\theta_0$ (degrees)		
C–C–C <sup>a</sup>	5.3858393	114		
Dihedral	$C_0$ (eV)	$C_1$ (eV)	$C_2$ (eV)	$C_3$ (eV)
C–C–C–C <sup>a</sup>	0	0.0305941	–0.0058761	0.0681907

<sup>a</sup> taken from Ref [20].

<sup>b</sup> taken from Ref [21].

interactions were computed with the Lorentz–Berthelot combining rules in Eq. (2).

$$\sigma_{ij} = \frac{1}{2} (\sigma_{ii} + \sigma_{jj}) \epsilon_{ij} = \sqrt{\epsilon_{ii} \epsilon_{jj}} \quad (2)$$

Intra-molecular potentials include bond stretching, angle bending, and torsion angle are given by Eqs. (3–5). All the potential parameters are summarised in Table 1.

$$E_{\text{bond}} = \frac{K_b}{2} (r - r_0)^2 \quad (3)$$

$$E_{\text{bend}} = \frac{K_\theta}{2} (\theta - \theta_0)^2 \quad (4)$$

$$E_{\text{torsion}} = c_0 + c_1 [1 + \cos(\alpha)] + c_2 [1 - \cos(2\alpha)] + c_3 [1 + \cos(3\alpha)] \quad (5)$$

## 3. Simulation procedure

Each simulation consists of three steps: relaxation for 0.2 ns, compression for 0.6 ns and shearing for 1.2 ns. In the relaxation step, the atoms of the upper and lower rigid layers 1 and 2 were fixed to keep the system height at 111 Å, which allowed the lubricant molecules to fully relax. After that, a uniformly distributed load ranged in 250, 500, 750 and 1000 MPa was applied to the atoms of the rigid upper layer 1 while the atoms of the rigid lower layer 2 were constrained from moving in the *z*-direction, thus compressing the lubricant. At this stage, it began to apply a

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