Normal Contacts of Lubricated Fractal Rough Surfaces at the Atomic Scale

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1. Introduction

The friction of contacting interfaces is a function of surface roughness and applied normal load. Under boundary lubrication, this frictional behavior changes as a function of lubricant wettability, viscosity, and density, by practically decreasing the possibility of dry contact. Many studies on contacts with atomic scale roughness adopt simplified sinusoidal shapes for the roughness, comprising a deformable surface in contact with a rigid flat; however, roughness has a fractal nature. In this paper, molecular dynamics is used to simulate the three-dimensional contact between atomically rough fractal surfaces of nickel lubricated with different volumes of hexadecane molecules. Results show that the contact force on the solid surfaces decreases and changes in the surface RMS roughness diminish with increasing lubricant volume.

2. Methodology

A pair of incommensurable fractal surfaces [1] was generated with an RMS roughness and correlation length of 10 Å and 8 Å, respectively. Two atomic blocks of fcc-nickel were constructed below and above them with the (100) lattice planes normal to the *z* direction. The solid structure was built with a length of approximately 14.1 nm in the lateral directions, and a minimum thickness of 2.5 nm for each block. Each of the two bodies was divided into three layers: rigid, thermostatic, and free deformable. These were modeled with an embedded-atom-method (EAM) potential [2]. The rigid layer of a block was fixed, and of the other was moved to apply a pressure of 0.5 KPa. Different numbers of hexadecane molecules (0, 192, 576, and 960) were used as a lubricant, modeled through a united atom formulation. The optimized potentials for the liquid simulations [3] were applied for the intramolecular interactions. The interactions between non-bonded atoms of the lubricant molecules were calculated via the Lennard-Jones (LJ) potential [3]. Moreover, other needed interactions were computed via LJ potentials directly, or by applying mixing rules.

The simulations were performed with LAMMPS [4]. The equations of motion were solved using the velocity-Verlet algorithm [5], with the rRESPA method [6]. Periodic boundary conditions were applied to the lateral directions. The weak coupling thermostat [7] was applied to the thermostat layers to keep the temperature at 300 K. Determinations of the contacted atoms and area were done in post-processing with atoms closer than 3 Å being considered as contacting. Considering an effective radius of 1.24 Å for nickel, the projected area on the XY plane was used to estimate the percentage of real contact area using OVITO [8], and ImageJ [9].

3. Results and discussion

Figure 1 shows the decreasing contact area (A_c) with increasing number of molecules (lubricant volume).

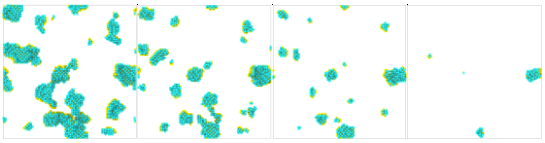

Figure 1: Projection of the contacted atoms for systems with 0, 192,576, and 960 lubricant molecules, respectively from left to right.

The compression pressure along the *z* axis was found to be ~123 MPa. The normal force was calculated as $F=P\times A_c$ and the results were plotted in figure 2. This figure also shows the changes in topography quantified by the change of RMS roughness. The changes suggest that even a small number of lubricant molecules can dramatically decrease the flattening of rough surfaces.

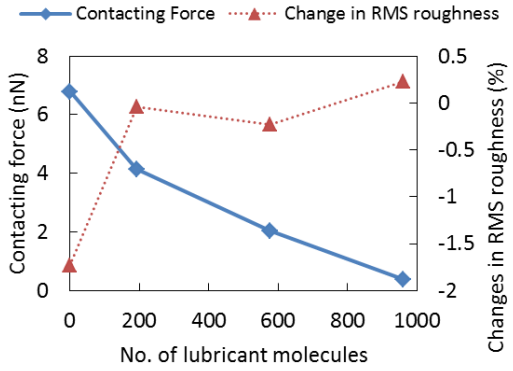

Figure 2: Calculated contacting force (solid line), and changes in surface RMS roughness (dotted line) as functions of No. of lubricant molecules.

4. References

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