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Frictional properties of multi-asperity surfaces at the nanoscale

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ABSTRACT

Asperities are considered as unevenness of surfaces, or surface roughness. Surfaces that are finely polished are still considered uneven at the nanoscale. This unevenness of surface reduces the actual contact area when two surfaces come into contact. Understanding surface asperities are very important because the friction and wear properties of two materials depend on the nanoscale contact between the material surfaces. Many experimental studies have concluded that surface texture can help improve contact characteristics and reduce the frictional forces between surfaces. We use molecular dynamics simulations to study the frictional and mechanical response of an aluminium surface with cylindrical and spherical asperities that resemble true surfaces. Nanoindentation and scratch tests are carried out using different indenter radii on spherical and cylindrical asperities, and the results are compared to surfaces without asperities. When comparing the spherical and cylindrical asperities, we observe that the coefficient of friction (COF) is lower for spherical asperity surfaces, if the indenter radius is less than or equal to 4 nm, and the COF is lower for cylindrical asperity surfaces, if the indenter radius is greater than or equal to 5 nm. Finally, the COF decreases with increasing indenter radius for the surface geometries studied here. The atomic mechanisms corresponding to the observed frictional response of the surfaces are explained by dislocation nucleation and propagation in the system. These studies could perhaps be used to guide experiments to design multi-asperity surfaces for tribological applications.

1. Introduction

The mechanics behind surface deformations have been of interest for researchers over the past few decades. Surface properties such as adhesion, friction, and wear are all important aspects for understanding and addressing the surface behavior of materials. Multi-asperity surfaces have gained tremendous interest in engineering due to tribological properties associated with them. With the availability of nanolithography [1], development of surfaces with nanoscale asperities of different shapes, and size are possible for various engineering applications. For example, researchers have recently shown that multi-asperity surfaces have application in cancer research [2], where they have shown that the malenoma cells migrate on a surface with cylindrical asperities based on the distance between asperities. Similarly, neuro cell [3,4] growth depends on the geometry (cylindrical or spherical shape) of the surface with which the cell come into contact. It should be noted that depending on the application, the asperity size varies from micro to nano meter length scales. The deformation of the asperities plays a critical role towards surface properties due to contact with either probes (such as AFM) or other surfaces. Hence, understanding the properties of surfaces with different asperities has interdisciplinary application. Many continuum-based models have been proposed to understand the phenomenon of contacts between two surfaces. Hertz (1882) [5] describes the deformation of two elastic bodies; DMT theory [6] describes adhesive contact between spheres without elastic deformation. Unlike DMT theory, Johnson et al. (1971) [7] (JKR) theory considers elastic deformation. Maugis (1992) [8] proposed a model which gives transition between DMT-JKR. All these continuum-based models have limitations when they are applied to micro or nano length scales [9].

Recent advances in the development of micro and nanoelectromechanical systems (MEMS/NEMS) demand better understanding of the contact mechanics in micro and nanoscale surfaces [10]. Surface measuring technologies such as atomic force microscopy, frictional force microscopy (FFM) and lateral force microscopy (LFM) [11] are used to study the frictional and wear properties at the nanoscale. Developments in computational materials modeling have paved the path to use methods such as molecular dynamics

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(MD) which allow us to predict atomic level properties. This method has been widely used in exploring the surface properties of various materials [12–20]. Moreover, the results obtained by MD can guide the experimental research by providing the details of asperity shape, asperity size, and distance between asperities for specific application [20].

Cheong and Zhang (2003) [21] were the first to study the effect of relative position and orientation of asperities on the nanoscale wear mechanisms of silicon (Si) surfaces using MD simulations. They found that forces experienced by the asperities are independent of their relative positions and that there were no dislocations when the indentation depth is small. Cha et al. (2004) [22] investigated single asperity surface and its deformation when two surfaces come in contact. According to their study, JKR theory is not applicable to the loading condition of the asperity, but is applicable to unloading, and the deformation of the asperity is considered to be nearly elastic. Liu et al. (2009) [23] performed MD simulations to study contact between a rigid cylindrical probe and an elastic Cu substrate with and without adhesion by varying the radius, size, shape and number of asperities on the cylindrical probe. This study showed that the adhesive effect is stronger when surfaces have smaller and more numerous asperities in contact with the substrate. Similarly, Jacobs et al. (2013) [20] studied atomic scale roughness on adhesion between carbon based materials and nanoscale asperities of either diamond like carbon (DLC) or ultra nanocrystalline diamond using MD and experiments; they found that adhesion decreased more than an order of magnitude as roughness increased. Si and Wang (2014) [18] conducted MD studies on surface roughness and on adhesion between a spherical tip with single asperity and on smooth surfaces. The study was carried out by varying height, radii, and nanoindentation velocity, with both the spherical tips and surfaces made of Si. Their results led to the conclusion that the adhesion force decreases when the asperity size is at the nanoscale. However, the adhesion forces obtained are larger than the Rumpf [24] and Rabinovich [25] models, which they explain is due to not considering the chemical bonds.

Multiscale approaches have been performed by various researchers to address the nanoscale contact information using molecular dynamics and the finite element method [26–29]. Using the multiscale approach Tong et al. (2011) [26] studied 2D nano scale sliding contact between a rigid cylindrical tip and an elastic copper substrate with a textured surface. In their research, the adhesive effects are considered using different asperity shapes, height, and spacing between asperities; this allowed them to find the optimal asperity height and spacing between asperities on the copper substrate; however, the effect of the indenter radius or dislocation mechanisms were not investigated. They concluded that with the proper asperity height and spacing, surface texture can reduce frictional forces effectively. Tong et al. (2012) [27] using multiscale approach, studied the contact between a rigid cylindrical tip and a smooth surface. They conclude that the compressive force of textured surfaces increases with either increasing asperity height, or decreasing the asperity distance. This indicates that an appropriate spacing between the asperities could help in getting the required contact force. Similarly, Zhu et al. (2011) [28] and Anciaux et al. (2010) [29] has performed multiscale simulations, where Zhu et al. (2011) [28] revealed that indenter velocity and radius significantly affects the nanoindentation process; and Anciaux et al. (2010) [29] implemented a bridging domain method coupled with FEM and MD which developed promising strategy for analysis of sliding contacts.

The current study focuses on multi-asperity surfaces of spherical or cylindrical shape which will reduce the surface friction, and provide a better understanding of microscopic plastic deformation and its relationship to frictional properties. We perform nanoindentation and scratch tests on an aluminium (Al) surface with and without asperities using molecular dynamics simulations. We investigate how the coefficient of friction (COF) changes with the asperity geometry (sphere and cylinder), and the indenter radius. In this study, we propose model surfaces that can be used to identify the suitable asperity shape (cylinder or spherical asperities) that reduces the COF. This study also reveals microscopic deformation mechanisms, such as dislocation nucleation and propagation, for both spherical and cylindrical asperities during nanoindentation and scratch tests.

2. Methodology

We use molecular dynamics simulations to predict the COF on surfaces without asperities (Fig. 1a), as well as those with equally-spaced spherical (Fig. 1b) and cylindrical asperities (Fig. 1c). All samples used in this study are single crystal Al with dimensions of 40, 20 and 25 nm along x $[1\,1\,\bar{2}]$, y $[1\,1\,1]$ and z $[1\,\bar{1}\,0]$ directions respectively. The spherical and cylindrical multi-asperities are created on top of the x-z plane, as shown in Fig. 1 (b) and (c) where spacing between the asperities is 2 nm. The spherical asperity has a radius of 2 nm, and the cylindrical asperity has a radius and height of 2 nm and 4 nm respectively. An initial spacing of 2 nm between the asperities is chosen to avoid interaction between the asperities during nanoindentation and scratch process. For example, as observed by Tong et al. (2011) [26] the deformed neighboring asperities could come in contact to form another asperity of higher radius. We also study different asperity distances for both cylindrical and spherical cases. We use spherical indenters with radii of 3, 4, 5 and 6 nm for nanoindentation and scratch tests. The indenter radii are considered such that it is greater than the asperity size, and the indenter is in contact with more than one asperity at a given time during nanoindentation. We chose a thickness of 20 nm for the substrate to avoid the boundary effects. We also study two more asperity spacing at 1 and 3 nm with the indenter of radius 6 nm, to see the effect of COF on different spacing between the asperities. During the nanoindentation and scratch process, the bottom 8 atom layers are fixed and all other atoms are mobile. The periodic boundary conditions are employed along x and z directions and shrink-wrapped boundary conditions are employed in the y direction. Atomic interactions between Al atoms are governed by the embedded atom method [30].

The samples are first minimized and then equilibrated at 300 K by maintaining zero pressure along the x and z directions using NPT (isothermal and isobaric) ensemble for a duration of 350 ps. The indenter is lowered to the surface along the y direction and the samples are indented to a depth of 1.8 nm, and then scratched along the x direction over 10 nm. The velocity of the indenter is maintained at 5 m/s during nanoindentation and scratch tests. We use the LAMMPS [31] software package to perform MD simulations. For all simulations, we use a hard spherical indenter (with force constant, $K = 10$ eV/Å^3) as implemented in LAMMPS [26]. The indenter implemented in LAMMPS describes the interaction between the indenter and surface atoms using a repulsive L-J potential. Common neighbor analysis and dislocation analysis (DXA) is performed using OVITO [32], which allow us to visualize defects, dislocations or stacking faults during the simulations.

We start the indentation such that the indenter is in contact with at least two asperities, which reflect experimental conditions where two surfaces of different asperities are in contact with each other. For indenter radii of 3, 4, 5 and 6 nm the center of indenter is in between the two neighboring asperities. To study the effect of location of indenter on COF, we study an additional case, where the center of indenter of 6 nm radius is in between four neighbor-