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Atomistic simulation of the effect of roughness on nanoscale wear

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ABSTRACT

At the macroscale, it is expected that surface roughness decreases adhesive wear and increases abrasive wear, and both increase with load. Here we evaluate whether these trends are also applicable to nanoscale contacts. Molecular dynamics simulation is used to model dry sliding of Si atomic force microscope tips with varying roughness on a Cu substrate at a range of normal loads. Surface wear is quantified as the number of substrate atoms displaced during steady-state sliding and characterized as a function of tip roughness and load. The interaction energy between the tip and substrate and a geometric roughness factor are used to investigate the contributions of adhesive and abrasive wear. By predicting how roughness affects nanoscale wear, and isolating the adhesive and abrasive wear modes, it is possible to describe the relationship between roughness, load and wear and, further, to determine an optimum tip roughness that will minimize wear at a given load.

1. Introduction

The atomic force microscope (AFM) is widely used to investigate surface and material properties at the nanoscale. The AFM also enables nanoscale manufacturing. During AFM-based measurement and manufacturing processes, contact between the tip and sample can result in wear of the sample, tip or both [1]. Although the tip is nanoscale, it is not ideally smooth, and the roughness can affect the nature of the contact between tip and substrate [2–10]. These contact features in turn affect nanoscale wear. Thus, a fundamental understanding of the effect of nanoscale roughness on wear is critical to enabling reliable and precise measurements at the nanoscale, as well as tip-based nanomanufacturing methods.

Previous studies have shown that roughness significantly affects the adhesive strength of nanoscale contacts. Such studies showed that adhesive strength decreases with increasing nanoscale roughness, due to the reduction in real contact area between the two surfaces [11–14]. It has also been found that adhesion can be minimized at an optimum surface roughness and that roughness can be tuned by the size or density of asperities or particles on the surface [15–19].

Adhesive strength is known to play a significant role in determining wear in nanoscale contacts [20–25]. Studies have reported that there will be a larger number of atoms transferred from one surface to another when there are more interfacial bonds formed between the surfaces [20] or when the adhesive strength is stronger [21–24]. This was corroborated by studies that showed adhesion and wear decreased or increased together when different tips were used in AFM measurements [26,27]. However, although nanoscale wear increases with adhesive strength and roughness decreases adhesive strength for small surface roughness, wear has been found to increase with roughness [28]. This observation suggests that nanoscale wear is not solely determined by adhesion and, like at the macroscale, both adhesion and abrasion contribute, and both are affected by roughness. Although this is a reasonable assumption, it has not been systematically studied.

To address this, here we use molecular dynamics (MD) simulation to characterize the wear between a model Si AFM tip and a Cu substrate using tips with different degrees of roughness at different loads. Then we analyze the relationship between the tip roughness and wear in terms of adhesion and abrasion, which are assumed to be the two major wear mechanisms during nanoscale dry sliding [21,25,29,30]. Macroscale wear theories that relate adhesive and abrasive wear to sliding distance, load and roughness are used to isolate the contributions of the two wear modes. To apply these expressions to describe nanoscale wear, we introduce an additional term to capture the effect of adhesion on contact size and redefine the wear coefficients in terms of atom–atom interaction energy. The resulting expression makes it possible to predict the effects of load and roughness on nanoscale wear and to determine the roughness of scanning probe tips that will minimize that wear.

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2. Methods

The MD model consists of a Si tip, which has a diamond crystal structure, and a face-centered-cubic Cu (100) surface, as shown in Fig. 1(a). To model rough tips, we superimpose a spherical cap, which has a radius of 29 nm and a height of 3 nm, with a cosine wave along the x-direction and another cosine wave along the y-direction. The inset of Fig. 1(a) shows a schematic of this process. The amplitude of the cosine wave is varied from 0.01 nm to 1 nm while the wavelength is kept at 4 nm to obtain tips with different roughness. Seven different tips are obtained by setting the amplitude of the cosine wave to 0.01, 0.2, 0.35, 0.5, 0.6, 0.8 and 1 nm, which correspond to root mean square roughnesses R_q of 0.184, 0.214, 0.271, 0.352, 0.409, 0.526 and 0.638 nm, respectively. We calculate the roughness as the root mean square of the difference between the z-direction position of each atom on the surface of the tip and that on an ideal sphere with the same center and radius. A few of the model tips with different roughness are shown in Fig. 1(b). The substrate lattice orientations along the x, y and z directions are [100], [010] and [001], respectively. The dimensions of the Cu substrate are $60 \times 40 \times 2.2$ nm in the x-, y- and z-directions, respectively. Periodic boundary conditions are applied in the x- and y-directions. The atoms in the top three layers of the tip and the bottom two layers of the substrate are fixed. All interatomic interactions within the model are described by the Modified Embedded-Atom Method [31] with reported parameters in [32]. The Nosé–Hoover thermostat is applied to the free atoms in the system with a target temperature of 300 K. All simulations are performed using LAMMPS simulation software [33,34] with a time step of 1 fs.

Sliding simulations are conducted with each model tip to investigate the effect of tip roughness on wear. A constant normal load W (10, 25, 50 or 100 nN) is maintained on the rigid top layers of the tip and the system is allowed to relax for 0.05 ns. Then the tip slides along the x-direction through a distance of 34 nm. A sliding speed of 100 m s^{-1} is applied on the tip during the first 14 nm sliding to decrease the time required for the run-in stage, and then the sliding speed is reduced to 50 m s^{-1} for the remainder of the simulation. Both of these speeds are fast compared to typical AFM experiments, but necessitated by the small time step of the simulations and the relatively large model system. We observe that the vertical position of the tip is constant after 24 nm of sliding and so identify from 24 to 34 nm as steady-state sliding.

Wear predominantly occurs on the substrate in our model, as expected since the Si tip is harder than the Cu substrate. We therefore quantify wear in terms of plastic deformation of the substrate during sliding. Because MD simulation makes it possible to know the exact position of the atoms in the model, we can calculate the displacement of each substrate atom at each moment in time to quantify wear [35]. When the displacement of an atom is greater than the Cu lattice constant (0.361 nm), it is identified as displaced (worn). To characterize wear only in steady-state, a displaced atom is assumed to be one whose position at some sliding distance x ($x > 24$ nm) has changed by more than 0.361 nm compared to its position at a sliding distance of 24 nm. The total number of displaced substrate atoms N at a given sliding distance is a measure of substrate wear.

To assess the adhesive strength of the interfaces between different rough tips and substrate, we calculate the interaction energy E between each rough tip and substrate before sliding:

$$E = E_1 + E_2 - E_{12} \tag{1}$$

where E_{12} is the total energy of the interface (consisting of the tip and substrate) at equilibrium, and E_1 and E_2 are the total energies of the tip and the substrate at equilibrium, respectively [36]. E_1 and E_2 are calculated from energy minimization after the tip and substrate are relaxed separately. To obtain E_{12}, the tip is placed 0.3 nm above the substrate surface and then the system is relaxed without applied load for 0.05 ns. The tip is allowed to move freely in response to the interaction with the substrate during this relaxation stage. Then the system energy is minimized to calculate E_{12}.

3. Results and discussion

Fig. 2 shows wear, quantified as the number of displaced substrate atoms, increases with sliding distance for the different tips and at a range of normal loads; recall that x and N are by definition zero at the beginning of steady-state wear. Wear increases with sliding distance in all cases. If we take the last point on this plot, i.e. wear after 10 nm of steady-state sliding, we can analyze the effects of roughness and load. Fig. 3 shows the number of displaced substrate atoms as a function of tip root mean square roughness R_q at applied loads of 10, 25, 50 and 100 nN. At any load, wear increases with tip roughness.

The results are replotted as a function of load for the $R_q = 0.214$ nm case in the inset of Fig. 3. It can be observed that wear increases with applied load, consistent with previous observations of nanoscale dry sliding [37,38]. The increase of wear with load is associated with an increase in contact area. At the nanoscale, the contact area is expected to be non-zero at zero externally applied load due to the adhesion between tip and substrate [39]. To illustrate the effect of this on wear, a linear fit is used as a rough approximation of the load-wear trend in the inset of Fig. 3. We observe that the number of atoms displaced does not go to zero at zero load. This is consistent with the behavior observed for all model tips.

Adhesive and abrasive wear are typically the two dominant wear mechanisms in dry sliding. Adhesive wear evolves through the formation of adhesive junctions, their growth and their fracture. An expression for adhesive wear at the macroscale is [40],

$$V_{adh} = \frac{k_1 W x}{R_q} \tag{2}$$

where V_{adh} is adhesive wear volume; k_1 is an adhesive wear coefficient which, at the macroscale, is related to the correlation length of the surface and the effective modulus of elasticity. Eq. (2) predicts that adhesive wear is proportional to applied load W, sliding

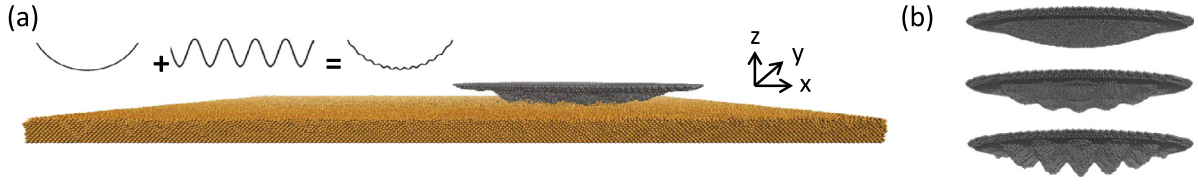

Fig. 1. (a) Snapshot of the simulation system consisting of a Si tip and Cu substrate during sliding. The inset shows the geometry of a rough tip created by superposing a spherical cap with a cosine wave. (b) Snapshots of a few of the model tips with different roughness: R_q = 0.184, 0.352 and 0.638 nm, from the top to the bottom image. Cu atoms are shown in orange, Si atoms in gray.