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Ploughing friction and nanohardness dependent on the tip tilt in nano-scratch test for single crystal gold

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ABSTRACT

Different from macro-scale scratch, in nano-scale scratch test, the scratching tip is easily tilted, which may display a considerable change of the friction behavior. The ploughing friction and nanohardness dependent on the tip tilt in nano-scratch test for single crystal gold is studied in this paper by using molecular dynamics simulations. The results show that tilting forward (backward) to the scratch direction has a larger effect on the friction coefficient than the case of tilting laterally to the scratch direction. Scratch hardness is also sensitive to the tip tilting forward (backward), while it is insensitive to the tip tilting laterally. Moreover, the local plastic behaviors near tip (pile-up, plastic area, and dislocation evolution) are also dependent on the tip tilt, which may be a major contribution to the mechanism of the nano-scale wear.

1. Introduction

In the nano-scratch test, both contact force and contact area are very sensitive to the local contact conditions such as the nanoscale roughness [1,2], which leads to the difficulty in the measurement with high resolution. As a result, in the nanoscale friction, the study of the relative position between the tip and the sample is of great importance. During nano-scratch process, the tip is not strictly perpendicular to the scratch surface due to the following three main factors: beam bending of the Atomic Force Microscope (AFM), substrate with a tilt angle, as well as roughness of the sample surface. Experiment [3] showed that tilt angle of the tip has significant effects on the size and shape of wear debris during nano-scratching tests. The tip tilt effects on indentation [4,5] and scratch tests [6] have been studied by using finite element method, and the results show that the tip tilt leads to the change of the indentation load, contact area and contact stiffness. The change of contact area caused by the tilt is not included in Sneddons equation, commonly used in nano-indentation analysis.

Studies from continuum mechanics show, a tilt of 5° can cause approximately 12% error and 30% error in measurement of hardness [5] and friction coefficient [6], respectively. These studies mostly attribute the influence to the difference of macro-scale yielding pattern, which is not a proper concept for nano-scale contact. In nano-scale, pile-up of material plays a critical role, different from the case in macro-scale. In order to study ploughing, Szlufarska et al. [7,8] proposed an analytical model taking account of ploughing friction for single-asperity contacts, and they considered the effects of both elastic recovery and atomic pileup, but without taking account of the tip tilt effect on friction coefficient. Different from macro-scale friction, friction behavior of nano-scratch is sensitive to the detailed contact geometry: Gao et al. [9] investigated the effect of asperity shapes on the wear of nickel thin film by using molecular dynamics (MD) simulations, their results reveal that the sharp surface asperities cause more friction than that of the blunt asperities. Zhu et al. [10] gave different results, by studying the effect of indenter shape on the nanometric scratching process of copper, they showed the blunt asperities may result in more friction if the asperities are rather small. Besides, the nano-scale yielding has extra high strength, Kiely and Houston [11] showed the yield strength of gold is as high as $\sigma_p = 7.8$ GPa, which is much larger than the value of yielding at macro-scale [4–6].

Thus, it remains unknown that how the nano-friction behavior is related to the local contact condition by effects of atomic pileup, dislocation movement, and contact geometry, while these factors can be significantly changed by the tilt of the tip. Also, the tip tilt effect on scratch hardness at nano-scale has various mechanisms. These effects will be studied in this work.

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2. Methodology

MD simulations are carried out to study the scratch test of a conical tip over the single crystal Au (see in Fig. 1 for section views). In the present study, the package LAMMPS [12] is used for all the simulations. Tip consists of carbon atoms with diamond cubic structure, it has a much larger rigidity compared with the tested samples, thus is considered as not deformable. The tip has a cone shape with a semi-cone angle $\theta = 40.0°$. At the contact point of a real AFM tip, it always has a hemisphere with the radius in the range of nano-meters as a result of fabrication. Correspondingly, in our model, the tip curvature radius is taken as $R = 10$ nm. In order to study the effect of tilt angle, tips with different tilt angles (η_x or η_z) are selected during nano-scratch process.

During indentation, periodic boundary conditions are applied in the x and z directions, while the bottom atoms (in the y direction) are fixed, the top atoms are in a free surface (see in Fig. 1). The y and x directions are the indentation and scratch directions, respectively. The substrate is a single crystal (Au), which has a approximate size of $250 \times 200 \times 150$ Å^3. The Embedded-Atom Method (EAM) potential for Au is taken from Ref. [13], simulations with other EAM potentials [14,15] are also compared in the study. Morse potential between the tip and the substrate is adopted according to Refs. [16,17], but with only repulsive interaction considered [7]. The Morse potential is written as:

$$\phi(r_{ij}) = D\{\exp[-2\alpha(r_{ij} - r_0)] - 2\exp[-\alpha(r_{ij} - r_0)]\} \quad (1)$$

where $\phi(r_{ij})$ is the pair potential energy function. D, α, and r_0 correspond to the cohesion energy, the elastic modulus and the atomic distance at equilibrium, respectively. The potential parameters are set as $D = 0.1$ ev, $\alpha = 1.70$ Å^{-1}, $r_0 = 2.20$ Å for the interaction between the tip and substrate. The forces are recorded as the summation of interaction forces between the tip and the substrate.

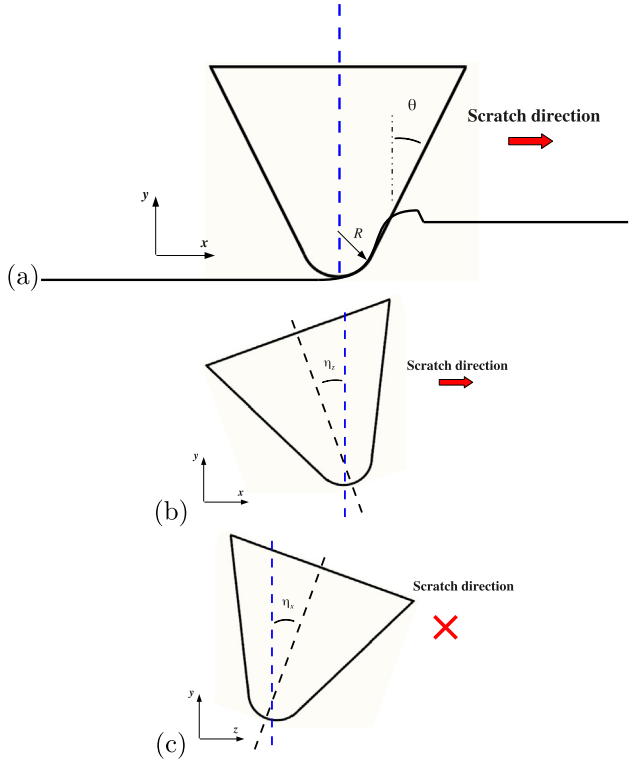

Fig. 1. Sketch of the simulation model (a) section view of x–y plane (b) section view of x–y plane with tilting backward ($\eta_z > 0$) (c) section view of z-y plane with tilting laterally (changing η_x). The tilt angles shown here are in the positive direction. The cross is defined as the scratch direction is perpendicular to the paper.

Table 1
Crystal orientations of 11 simulation sets.

Case ID	β (°)	Orientations					
A	0.00	x:	$\langle 00\bar{1}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}0\rangle$
B	8.05	x:	$\langle 1\bar{1}\bar{1}0\rangle$	y:	$\langle 110\rangle$	z:	$\langle 55\bar{1}\rangle$
C	10.03	x:	$\langle 1\bar{1}\bar{8}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 44\bar{1}\rangle$
D	13.26	x:	$\langle 1\bar{1}\bar{6}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 44\bar{1}\rangle$
E	19.47	x:	$\langle 1\bar{1}\bar{4}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 22\bar{1}\rangle$
F	35.26	x:	$\langle 1\bar{1}\bar{2}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}1\rangle$
G	54.74	x:	$\langle 1\bar{1}1\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}2\rangle$
H	64.76	x:	$\langle 3\bar{3}2\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}1\rangle$
I	74.21	x:	$\langle 5\bar{5}2\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}5\rangle$
J	79.98	x:	$\langle 44\bar{1}\rangle$	y:	$\langle 110\rangle$	z:	$\langle 1\bar{1}8\rangle$
K	90.00	x:	$\langle 1\bar{1}0\rangle$	y:	$\langle 110\rangle$	z:	$\langle 001\rangle$

Before the indentation process, each simulation process includes several steps: generation of samples from the perfect crystal lattice, energy minimization of sample by using conjugate gradient method, relaxing at the temperature of 600 K with pressure of 0 Pa under NPT ensemble (number of molecules N, pressure P and temperature T are conserved) for 50 ps, system cooling down to 1 K in 50 ps under NPT, and the finally system being relaxed for another 50 ps at the temperature of 1 K under NVT ensemble (number of molecules N, volume V and temperature T are conserved), The size of the box can be obtained by using NPT ensemble. Both indentation and nano-scratch are performed at the temperature of 1 K so that the thermal effect on micro-scale plasticity can be eliminated. The indentation is carried out at a penetration speed of 50 m/s. Before scratch, another 50 ps relaxation is applied (Longer relaxation time (100 ps) is also carried out, it does not change the structure). From our verification tests, we find that the indentation rate does not influence the scratch process.The scratch velocity is taken as 15 m/s, which is relatively slow compared to most of the previous nano-scratch simulations [7,9,10]. The scratch depth is defined as the distance between the lowest atom of the tip and the height of the sample surface after scratch, the depth is taken as 24 Å in all the later simulations.

The anisotropy of friction is an intrinsic property for all crystalline solids [18]. In the present work, we focus our major attention on studying the tip tilt effect on friction behavior, thus, in order to minimize crystal orientation effect on the friction, we choose eleven crystal orientations on $(1\,1\,0)$ surface for attaining an average estimate. These orientations are shown in Table 1. Because of the two-fold symmetry of $(1\,1\,0)$ surface, the rotation angle (β) of each set, with respect to the reference frame[1], is evenly distributed from 0.00° to 90.00°. The tip is tilted either around x axis (lateral to scratch direction) or z axis (along the scratch direction), with angle defined as η_x and η_z, respectively. The signs of tilt angle (η_x and η_z) are defined according to right hand rule for angular quantities.

3. Results and discussions

3.1. Ploughing friction response with tilt angle

In most of the previous MD simulations, the friction curve has large fluctuations, it leads to the difficulty of quantitatively analyzing the results and comparing with experimental results. The physical origin of large fluctuation basically comes from the thermal dynamical characteristics of atomic interactions (high frequency vibration), thus it needs averaging process to minimize the effect

[1] Case A in Table 1 is selected as the reference frame