Tribology International 81 (2015) 169–178

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

Interference effect on friction behavior of asperities on single crystal copper

Xiaoming Liu [a,*], Bin Zhang [b], Yueguang Wei [a]

[a] LNM, Institute of Mechanics, Chinese Academy of Sciences, 100190 Beijing, China
[b] State Key Laboratory of Mechanics and Control of Mechanical Structures, College of Aerospace Engineering, Nanjing University of Aeronautics and Astronautics, 210016 Nanjing, China

ARTICLE INFO

Article history:
Received 15 July 2014
Received in revised form
8 August 2014
Accepted 16 August 2014
Available online 2 September 2014

Keywords:
Friction transition
Plastic behavior
Green function molecular dynamics
Asperity interference

ABSTRACT

By using Green function molecular dynamics method, we systematically study the friction behavior of a single asperity and asperity array over the (1 1 1) surface of single crystal copper. We find that internal plastic behavior (burst of stacking faults, dislocation emission and propagation) is a promising reason for the higher value of static friction coefficient than that of dynamics friction in non-adhesive scratch. For the rough surface, however, the difference between static and dynamic friction coefficients disappear due to the interference between asperities. The interference dramatically increases the friction coefficient by introducing atomic scale plastic features (pile-up atoms, stacking faults, and U-shape dislocation loop).

1. Introduction

Friction and wear at nano-size contacts are not the same as those in macroscale, since surface and interfacial phenomena becomes dominant in nanoscale. Measurements of nano-tribology properties (such as the friction coefficient, wear rate) depend highly on the surface structure, elastic/plastic/creep properties of material, and physical and chemical environments. The single asperity apparatus has been developed for providing mechanical properties of the surface with characteristic size from a few hundred nanometers to several microns. Experiments with single asperity apparatus such as the scanning force microscope (SFM) and atomic force microscope (AFM), are widely used in investigating friction behavior at nanoscale.

Continuum theories (Hertz, JKR [1], and DMT [2]) have been successfully used to explain adhesive or non-adhesive single asperity contact and friction. However, these theories aren't always precise. The study [3] by Mo et al. demonstrated the breakdown of continuum mechanics at nano-scale, which is explained by the rough (multi-asperity) nature of the contact. They showed that roughness theories of friction should be applied at the nanoscale. Further study [4] showed that roughness theories captured the correct physics of deformation at the nanoscale, and the number of atoms interacting across the interface actually dominated the nano-friction behavior. Experiment [5] observed that the size of nanoscale asperities distributed on the AFM diamond tip is in the order of few nanometers. The nanoscale roughness can be represented by an array of asperities in multi-scale models [6] which extract the force–displacement data of a single asperity from molecular simulations. Pile-up of nano-scale material plays a similar important role as the nanoscale roughness factor, Mishra et al. [7,8] developed an analytical model to study plowing friction for the single-asperity contact at nanoscale, their results proved that the material pile-up has a large contribution to nano-friction. Local roughness may affect frictional strength by multi-scale nature [9,10] or flattening characteristics [11], its effect on dislocation pattern has been studied during nano-scale metallic contacts [12,13], but has not been presented for nano-scratch process.

Another interesting topic has been discussing for decades: Why is the coefficient of static friction normally higher than the value of dynamic friction? The reasons which have been discovered include several factors as following: *The adhesive interaction* between the surfaces is well established when the surfaces are at rest, the relative motion gives less time for those stronger bonds to form; *The inertia effect* is one factor, the applied force has to overcome both friction and the inertia for the start of sliding in the case of static friction; *The surface roughness* is another factor, irregularities between surfaces make the fitting of two surfaces by peaks and valleys, thus a larger applied force is needed for starting the body's motion. While the surfaces are moving, all asperities are hopping along, skipping along the surface; *The third body* explanation is that elastic particles tend to deform and lock themselves together, thus the two sliders form a

* Corresponding author.
E-mail addresses: xiaomingliu@lnm.imech.ac.cn (X. Liu), beenchang@nuaa.edu.cn (B. Zhang), ywei@imech.ac.cn (Y. Wei).

http://dx.doi.org/10.1016/j.triboint.2014.08.007
0301-679X/

kind of ratcheting effect when there is no relative movement. *In this work*, we study the effect of internal plastic behavior on the transition from static to dynamic friction. The obvious reason for this factor is that plastic behaviors (stacking fault burst, dislocation nucleation and propagation) are all rate dependent, and are very sensitive to the local instability caused during friction contact. And also, discrete behavior of dislocation is much more critical in small scale deformation than macro scale [14,15]. But to authors' knowledge, no study has ever discussed about the contribution of internal friction of material on this topic, the contribution can be more critical during the nano-scratch process since the discrete effect plays a more important role.

In our study, we use Green function molecular dynamics (GFMD) method to study the effect of internal plastic behaviors (stacking fault, dislocation emission and propagation) on nano-friction behavior, its contribution for the higher value of static friction coefficient is discussed. The interference effect between asperities is also studied for understanding roughness effect.

2. Method

Studying indentation or scratch using molecular dynamics normally requires very high computational cost. However, the cost can be largely reduced. Because according to Hertz contact theory [1], the deformation field decays with the increase of the distance from the contact point, with a $1/r$ law. Thus full scale computation is not necessary because plastic deformation only appears near the scratch surface. The GFMD can be used to take account of the long-range interaction from atoms in the area far from the contact points. The computational cost can be reduced by replacing atoms in those areas with GFMD. This method has been effectively applied as a seamless boundary condition for cases where near-surface deformation are dominated, such as surface relaxation [16], contact [17], or calculation of surface phonon dispersion [18].

We use the method developed by Campaná and Müser [19], and further implemented by Kong et al. [17], the scheme of the method is shown in Fig. 1, which is divided to two steps. First, the effective elastic stiffness coefficients of the GFMD atoms, from the bottom block in Fig. 1, are calculated by using the fluctuation–dissipation theorem. In another word, the layer of GFMD atoms is connected with a layer of nonlinear springs, with stiffness matrix provided by using Green function method. Simulation of 500,000 time steps (time step of 1*fs*) is used to obtain the Green function matrix (elastic stiffness) in the reciprocal space. Second, in the scratch simulation, a single layer of the GFMD atoms are set at the bottom of the z direction, which reproduces the effective elastic force from the bulk material by using the Green function matrix in the reciprocal space. This method significantly reduces the computational cost for indentation and scratch test, by considering only atoms near the surface.

During indentation or scratch simulation, boundary conditions are applied as follows. The top asperities are fixed, while one layer of atoms (set as Green function atoms) at the bottom is uniformly applied with normal force (F_n) and horizontal force (F_t). The force boundary conditions are similar to literature [20]. First, the normal force is applied piecewise in 300 ps (time step 1*fs*). Then the whole system is relaxed under NVT for a period of 100 ps before scratch. Simulations under various normal forces are conducted, and it has been verified that the system is fully relaxed before scratch that the indentation rate has no effect on the friction behavior.

In the simulation, we use force boundaries instead of velocity control [21]. The disadvantage of velocity control is that it leads to the inaccuracy of measuring the initial sliding force (static friction force). Theoretically, the acceleration is infinity once the velocity jumped from zero to the applied value at the initiation stage of sliding. The initial acceleration will cause an artificial contribution on the static friction force (the initial force required for sliding). Thus, in friction simulation, we gradually apply the friction force with a constant rate 0.03 nN/ps while keep F_n as a constant value. The time evolution of the sliding distance, measured as the distance between the asperities and bottom slabs, is recorded. In order to eliminate thermal effect on the plastic behavior during scratch, the whole system is kept at a temperature of 10 K via an external Nose–Hoover thermostat. It should be noted that, the Green function matrix is also calculated at 10 K. The scratch speed is not a constant but is below 150 m/s during the scratch distance of 40 nm, which is in the range normally used in MD simulations [22,23].

The simulation model consists of a crystal block at the bottom and a 2×2 asperity array (or just one asperity in single asperity test) at the top (see in Fig. 2). *The bottom block* is a single crystal copper with orientations as: x-$\langle 1\,1\,\bar{2} \rangle$, y-$\langle \bar{1}\,1\,0 \rangle$ and z-$\langle 1\,1\,1 \rangle$. The x and y directions are periodic, while top of z direction is treated as the surface for scratch, and the bottom side of z direction has atoms with Green function boundary condition applied. The dimension of the substrate in x and y direction is approximately 64 nm and 33 nm, respectively, while the dimension in z direction has different values in present study in order to check the dimension sensitivity in z direction. *The asperity array* is composed of 4 rigid spheres with a square pattern as shown in Fig. 2, the alignment of the array is measured quantitatively by the rotation angle θ. Our main concern is to investigate the

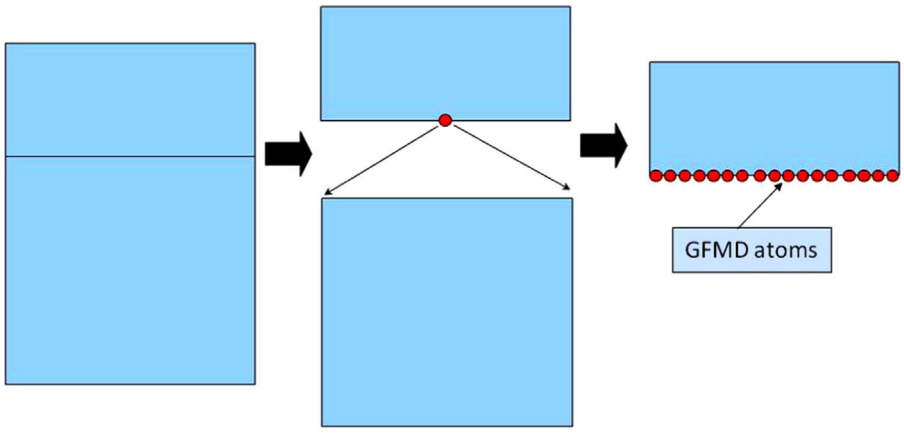

Fig. 1. Illustration of applying boundary atoms by using Green function molecular dynamics method. Instead of simulating the infinite half space (left), few layers of atoms are integrated in the computation (right) by using GFMD atoms to reproduce the effective elastic force from the lower bulk material (middle). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)