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Quasicontinuum investigation of the feedback effects on friction behavior of an abrasive particle over a single crystal aluminum substrate

Congcong Fang [a,b], Xianghui Meng [a,b,*], Youbai Xie [a,b], Bo Zhao [a,b]

[a] State Key Laboratory of Mechanical System and Vibration, Shanghai Jiaotong University, Shanghai 200240, People's Republic of China
[b] School of Mechanical Engineering, Shanghai Jiaotong University, Shanghai 200240, People's Republic of China

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ABSTRACT

A multiscale model is developed to investigate the effects of energy feedback on frictional behavior in non-adhesion sliding problems. Released elastic strain energy beneath the scratched surface is termed as the feedback energy here. The analyses are carried out from the perspectives of the surface microstructural evolution and mechanical friction coefficient prediction. Captured mechanisms indicate that the scratched surface undergoes a series of plasticity events (lattice-distortion-induced amorphization, twining formation) on account of the energy feedback. The friction coefficients from this model are compared with those in the relevant plowing model and viscoelastic model. The comparisons reveal that the effects of elastic unloading caused by the energy feedback would be weakened by the gathering of dislocation and intensifying of plastic deformation.

1. Introduction

Tribological failures are identified from quality changes of the lubricants and particle-wear analysis. Three important wear mechanisms, corrosion, abrasion, and adhesion, have been mentioned over the years. Abrasive wear occurs when asperities of a tough, hard surface or hard particles slide over a softer surface and damage the interface by plastic deformation or fracture. Abrasive wear may be the most common and the most rapid form of wear in industry. For example, in premature engine failures, abrasive wear could be as much as about 44% of overall wear [1]. Real wear progression is quite complex and is a function of several factors, such as metallurgy of the contacting materials, surface finish, and integrity [2]. To fundamentally understand interfacial phenomena in macro-structures, it is essential to conduct a deeper study of the friction and wear processes at the micro- and nano-scales. It will provide a bridge between the science and the engineering [3].

In most abrasive wear situations, scratching is observed as a series of grooves parallel to the direction of sliding or plowing. The micro/nanoscratch technique has been commonly used for the estimation of material properties, including hardness and wear resistance. As the deformation mechanism in micro/nanoscratching is not yet fully understood, much research is being devoted to elucidating it. From the results of nanoscratch tests carried out with a nanoindenter coupled to an atomic force microscope (AFM), Lafaye et al. explained the non-linear behavior of the lateral force with the applied load [4]. In their study, the indenter was not perfectly sharp but had a rounded extremity. Microscratch tests on Cu–graphite composites have been carried out by Xiao et al. using a scanning electron microscope (SEM). In that study, the authors found that the dominant wear mechanism transitions from ploughing to micro-cutting as the normal load increases [5]. However, experimental results at the microscale are limited by the high dispersion of the data. Moreover, it is hard to observe the real-time dynamic deformation and wear process through experiments. Therefore, molecular dynamics (MD) simulation has been an important complementary tool in providing insights into the details of the friction and the wear mechanisms at the nanoscale. Utilizing MD simulations, Smith et al. have inserted a sharp pyramidal diamond tip into the (100) surface of Ag to various depths and at different temperatures and then pulled it across the surface to investigate the mechanisms behind stick slip and wear events. The simulation results indicated that a dislocation propagates in the ⟨110⟩ direction from the tip as the scratch develops. Meanwhile, simulations at higher temperature showed a less pronounced dislocation emission than that at 0 K [6]. Also, the pile-up was spread further away from the scratch. Zhu et al. performed a three-dimensional MD simulation to investigate the

* Corresponding author at: State Key Laboratory of Mechanical System and Vibration, Shanghai Jiaotong University, Shanghai 200240, People's Republic of China.
E-mail addresses: fongtsung@sjtu.edu.cn (C. Fang), xhmeng@sjtu.edu.cn (X. Meng).

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nanoscale scratching process. By distinguishing the ploughing-friction coefficient and the adhesion-friction coefficient, they concluded that the macroscale theory slightly overestimates the ploughing-friction coefficient for the various scratching depths simulated, while the adhesion-friction coefficient is almost constant and independent of the scratching depth [7]. Mishra et al. modeled the elastic–plastic sliding friction of a rigid particle on SiC and Cu. They demonstrated that although the microscale models correctly describe the elastic recovery behind a sliding nanoscale particle, they fail to predict the corresponding coefficient of friction [8]. In addition, Yang et al. performed a MD simulation to investigate the material deformation, the abrasion mechanism, and the lattice defects during the contact and the sliding friction process between a diamond tip and a single crystal copper surface [9]. Their comparison showed that there exist deviations between the classic theoretical results and the computational results. They attributed the differences to the fact that the classical friction theory is based on an ideal plastic contact model that ignores the effect of the elastic recovery. Some other scholars attempted to address the issues considering the elastic recovery at the rear part of the contact after passage of a moving tip through a more accurate estimation of the ratio between the cross-section and the normal section of the contact area [10,11]. However, it remains unknown how the friction coefficient can be correlated with material properties, dislocation movement and even energy evolvement.

Despite the fact that the computation power of modern computers has grown immensely, some limitations still exist in the MD simulation method [12]. In general, the atomistic simulations are carried out at shearing velocities of above 1 m/s, which is orders of magnitude faster than nanoscale tribological experiments [13]. In addition, the MD technique is computationally expensive and limits the system size and duration of simulations. For the current hardware level, a high-performance desktop computer only has operation capabilities of a MD model with the size range of a few hundred nanometers. It is much smaller than the grain size, which has a range of about several microns. Such small model systems can also cause unrealistic boundary conditions, which artificially change the dislocation dynamics [14]. In this situation, the multiscale analysis methods are more and more extensively applied with low computation cost [15]. The multiscale method couples the macroscale research methods such as the finite element method (FEM) and the boundary element method (BEM), with the microscale research methods such as the MD simulation method and the quantum-mechanical method. However, the investigation of the micro/nano-scratch using the multiscale method is rarely reported. Zhu et al. have constructed a three-dimensional multiscale nanoindentation and nanoscratch model of copper through coupling the MD and finite element (FE) regions with the handshake regions [16]. Compared with those using the full MD model, the advantages of the multiscale method including high computational efficiency and satisfactory simulation accuracy have been elucidated. However, the insight provided into the micromechanisms such as dislocation formation and stacking fault burst is not sufficient. The authors of this study have performed a multiscale simulation of the indentation and the sliding friction continuous process between a large rigid nano-particle and a single aluminum plane [17]. A mathematical model was derived to evaluate the proportion of deviations between the ploughing friction coefficient and the numerical friction coefficient caused by the elastic recovery of the scratched surface. However, the conclusions were drawn for a single specific scratching depth. Being the direct driving force of the elastic recovery, the correlation of energy feedback with frictional behavior remains unclear. The applicability and reliability of the theoretical models at the nanometer scale have not been extensively verified yet. This work intends to probe complex mechanical phenomena in the nanoscratch for clarifying these issues with more sophisticated analytical techniques.

2. Methods

Among the existing multiscale methods, the energy-based quasicontinuum (QC) method is comparatively mature and has far-reaching influences. The QC method was conceived and proposed by Tadmor et al. based on the constitutive rule of Cauchy–Born [18,19]. The core idea of the QC method is the selective representation of atomic degrees of freedom. Only a small relevant subset of atoms is selected to represent the whole system. Based on their kinematic environment, the energies of individual "representative atoms (repatoms)" are computed either in nonlocal fashion with a straightforward atomistic methodology or in a local approximation with a continuum model. Then the whole equilibrium configuration is obtained through energy minimization. As more atoms will be sampled in highly deformed regions, the representation is of varying density. In the less deformed regions, which are closely approximated by a uniformly strained crystal, fewer atoms will be sampled. The Cauchy–Born rule is employed to calculate the density function of the strain energy in the finite element region. Because the model is adaptively updated as the deformation evolves, the Cauchy–Born rule provides an adaptive refinement strategy and enlargement of the atomic region to track the details of the material deformation [19]. By adopting the combination of computation methods outlined above, the QC method is able to save a great deal computation cost and time while maintaining adequate calculation accuracy. Further technical details of the QC methodology can be found in the reviewed literature [20].

Fig. 1 is a schematic illustration of the scratch between a rigid particle and a single-crystal Al substrate in the case of two-body abrasion. The dimensions of the single crystal Al substrate are 200 nm wide and 100 nm thick. It has a minimal periodic length in the out-of-plane direction (along the z-axis) with periodic boundary conditions applied. Displacements of atoms can be in all three directions, but the periodicity out-of-plane means that the deformations can only vary in-plane. The radius of the rigid particle in this model is 10 nm, which is much larger than most of scratch indenters used in the MD simulations as far as we know. In order to capture the essential physics of the process, the crystal directions of the Al substrate along the x- and y-axes are chosen to be [110] and [001], respectively. The boundary conditions are applied as follows. At the bottom edge, the displacement degrees of freedom are fully constrained. At both side edges, the x and z components of the displacement degrees of freedom are constrained. The interatomic potentials between the same types of

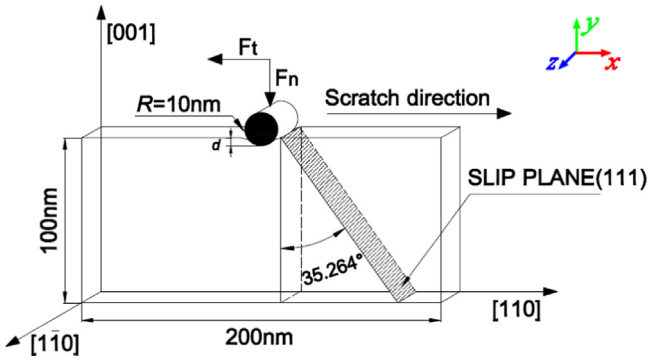

Fig. 1. Schematic representation of the model.