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Study of nanocontact and incipient nanoscratch process using the quasicontinuum method

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ABSTRACT

As a developed multiscale method, the quasicontinuum(QC) method is introduced to investigate the process of nanocontact and incipient nanoscratch between a large tip and a single crystal aluminum substrate with low computation cost. Through an analysis of the simulation result, microscopic mechanisms of deformation are studied and revealed. In the nanocontact process, it is found that the normal force of the tip shows stair-like increase with increase of indentation depth in the elastic deformation stage. The asymmetrical strain energy accumulation under both sides of the tip beneath substrate surface produces small fluctuations in friction force at the stage of plastic deformation. In the nanoscratch process, the elastic recovery of the scratched surface starts to appear obviously when the scratching distance is of 3.8 nm with the glide band expanding and localized strain sharply increasing. As a result, part of the dislocations underlying surface extend to the surface and form twinning deformation. Meanwhile, the crystal lattice deep beneath the surface undergoes severe distortion and rotation. A comparison of friction coefficient for the scratch process is also made between theoretical values and our numerical results. The effect of elastic strain energy feedback on friction coefficient in elastic recovery of the scratched surface is quantitatively analyzed.

1. Introduction

It is well known that one of the major breakthroughs in modern tribology should be the adhesion model of friction established by Bowden and Tabor more than 50 years ago [1]. As a matter of fact, many friction phenomena happen in our daily life, in addition to the plastic deformation of surface materiel, surface structure damage or wear and plastic adhesion, but also with ploughing, plastic deformation of subsurface, dislocation, crack initiation and propagation, cleavage of covalent bonding and ionic bonding [2]. Nowadays, as the gaps of tribo-pairs in modern precision machine and micro-machine are always in micro/nano scale, it is obvious that the classic friction theory based on the analysis of macro roughness of surface and phase transition is no longer available. Furthermore, the impact of contact friction force far exceeds bulk force due to the influence of dimension effect in micro-machine. Above all, reducing the friction to save energy consumption becomes the crucial issue.

With the improvement of experimental technique and advent of nanoscale sophisticated instruments such as AFM (atomic force microscope), FFM (friction force microscope) and STM (scanning tunneling microscope), the experimental research methods have obtained enormous development. Xiao et al. have carried out microscratch tests on Cu–graphite composites by using scanning electron microscope (SEM). The study has found that the dominant wear mechanism transits from ploughing to micro-cutting with increasing the normal loads [3]. Consiglio et al. have measured the accurate characterization of elasticity, hardness, adhesion and mechanical integrity in coated systems by nano-scratch tester using scanning force microscope (SFM) [4]. In spite of much research on the process of nano-friction being carried out by many domestic and overseas scholars, the real-time dynamic process of micro-deformation still could not be observed. In addition, because of factors such as the initial imperfection of the test sample, the defect of the tip of probe and the experimental environment, which have a great impact on the experimental results, the experimental results have high dispersibility.

The improvement of computer hardware has significantly promoted the application of molecular dynamics (MD) in the study of contact and friction in nanoscale. Aiming at making a thorough inquiry into the main theoretical calculation method of

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micro-friction and wear mechanism, the MD method has the ability to research the process of material deformation, transfer and scratch in atomic scale. There is no doubt that it is considered as one of the most perspective theoretical calculation methods in simulating and analyzing mechanical effect principle in micro/nano scale as it can solve the troubles of studying friction and wear in micro/nano scale with the experimental research method. According to a lot of reference literatures published in journals at home and abroad, the MD simulation method has been widely used to study the friction behavior in nanoindentation and nanoscratch. Jun et al. have simulated the scratching process by high-speed ploughing on the Al(111) surface applying the MD simulation method. The simulation results showed that the shape of the AFM tip directly influences the facet formation on the scratched groove. The penetration depth into the substrate during scratching has been further verified to affect both surface pile-up and residual defect generations [5]. Smith et al. have inserted a sharp pyramidal diamond tip into the (100) surface of Ag at various depths and for different temperatures and pulled across the surface and investigated the mechanisms behind the stick slip and wear events utilizing MD simulations. The result indicated that dislocation propagate in the 〈110〉 direction from the tip as the scratch develops and the pile-up patterns are shown to be in good agreement with experimental observation. Meanwhile, higher temperature simulations showed less pronounced dislocation emissions than at 0 K and pile-up which is spread further away from the scratch [6]. In addition, Gao et al. and Liu et al. have investigated the friction behavior in nanoscratch of Ni thin film by the MD method. Gao et al. focused around the effects of the indenter shape on the nanoscratch deformation. Two cases were considered in the simulation: a sharp indenter and a blunt one. It has shown that the vertical forces of shape one are larger than those of the blunt one while the scratching forces are similar during scratch [7]. Liu et al. have mainly researched the combination effects of both scratching depths and film thicknesses. It has been proved that friction coefficient decreases with decrease in both the scratch depth and film thickness [8].

Although striking achievements have been gained in modeling materials and obtaining real-time characteristics by using the MD simulation method, in reality a normal desktop computer can model material only a few hundred nanometers across by considering millions of atoms in the MD model, which is still smaller than the grain size that has a range of about several microns in traditional metal. Therefore, the MD simulation method is still difficult for meeting calculation requirements. Because some limitations exist in the MD simulation method [9], the multiscale method has evoked much attention of scholars at home and abroad. By coupling macro scale research methods such as the finite element (FE) method, the meshless method and the boundary element method with microscale research methods such as the MD simulation method and the quantum-mechanical method through a certain mathematical model, not only could the multiscale method expand the computation scale, but also guarantee the physical and mechanical properties of the considered problems. Up to now, the studies focus on computation materials science, which involves frictional contact problems with multiscale method, are still insufficient.

As the multiscale methods are more and more extensively applied to observe the detail characteristics in the crystal of specific regions in materials science field to understand the essence of many physical phenomena, several valid multiscale methods have emerged. For instance, the bridging domain (BD) multiscale method proposed by Liu et al. [10], which could couple particles (atoms/molecules) computation region with continuum computation region effectively by establishing appropriate boundary conditions. Another important multiscale method is the quasicontinuum (QC) method, which is put forward by Tadmor et al. [11]. The QC method simplifies particle system instead of considering the number of numerous molecules/atoms, which still has the ability to shed light on the information and physical properties of the original particles. In recent years, Sauer et al. have proposed a contacting mechanics model based on the QC method, which has been utilized to settle adhesion contact problems of carbon nanotube in large deformation and contact processes [12,13].

The application of multiscale methods to nanoscratch has been rare in the past reports. Zhu et al. [14] have constructed a three-dimensional multiscale nanoindentation and nanoscratch model between a spherical indenter and a single crystal copper by coupling the MD regions with finite element (FE) regions employing the coupling method proposed by Luan et al. [15]. Compared with those using the pure MD model, the advantages of the multiscale method have been elucidated. Even though the deformation of substrate and forces in the nanoscratch process have also been investigated and a great achievement has been made by the work, the insight provided into the micro-mechanism such as dislocation formation, atomic migration is not full enough. In this paper, a multiscale model of nanocontact and nanoscratch between a rigid spherical indenter and a single crystal aluminum substrate has been established using the QC multiscale method. Through the analysis of the simulation results, the atoms' movement and state, dislocation nucleation and emission have been studied. Finally, comparisons to the theoretical calculation results and experimental results have also been made and micro-deformation mechanisms in the nanocontact and nanoscratch process have been illustrated.

2. Methodology

2.1. Coupling algorithms

The quasicontinuum (QC) method is a comparatively mature multiscale simulation method that has far-reaching influences, which is proposed by Tadmor et al. [16] based on the constitutive rule of Cauchy–Born [17] in 1996.

The key idea of zero-temperature QC is the selective representation of atomic degrees of freedom. Instead of treating all the atoms that make up the system, a small relevant subset of atoms is selected to represent, by appropriate weighting, the energetics of the system as a whole. Based on their kinematic environment, the energies of individual 'representative atoms (repatoms)' are computed either in nonlocal fashion in correspondence with straightforward atomistic methodology or within a local approximation as befitting a continuum model. The representation is of varying density with more atoms sampled in the highly deformed regions and correspondingly fewer in the less deformed regions that are closely approximated by a uniformly strained crystal. The model is adaptively updated as the deformation evolves. In fact, the nonlocal representative atomic region is essentially the atomic region defined in other multiscale methods while the local repatoms coincide with finite element nodes in the continuum regions. Thus if the exact energy of a collection of N atoms in the model is given by [18]:

$$E_{tot} = \sum_{i=1}^{N} E_i \tag{1}$$

where E_i is the energy of atom i, with the QC method, a small subset of atoms is selected as repatoms to calculate the energy of the model. The crystal is then divided into disjointed cells each containing a single one of these selected atoms whose energetics are assumed to represent those of all the other atoms in its cell. Therefore, a reduced potential is defined, such that

$$E'_{tot} = \sum_{i=1}^{S} n_i E_i \tag{2}$$