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The study of anisotropic behavior of nano-adhesive contact by multiscale simulation

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ABSTRACT

Quasi-continuum method is applied to investigate the anisotropic behavior of nanoscale adhesive contact when a Ni tip indents into and then pulls out of single crystal Cu substrates. For $(\bar{1}10)$ substrate, the Ni tip exhibits excellent brittle behavior. Interface fracture is mainly characterized by atomic rearrangement since few slip planes are available. For (001) substrate, Shockley partials and deformation twins are both observed during the indentation process. Interface fracture is dominated by atomic slip which leads to the ductile fracture of the interface. As for (111) substrate, the nanocontact leads to significant plastic deformation of the substrate and the piling up of Cu atoms as well as the wetting of the Ni tip. This is because the Ni tip and Cu substrate share the same crystal orientations and the misfit effect between them is less evident. These anisotropic adhesive behaviors illustrate the importance of choosing a proper crystal contact surface to prevent wearing in micro-electro-mechanical systems. Distinctive nanocontact-induced deformation mechanisms and fracture mechanisms are revealed and analyzed. We found that available slip systems should be paid enough attention to for adhesive contact at nanoscale. It is recommended that adhesive contact between the Ni tip and Cu substrate with the same orientations should be avoided in order to reduce wearing. Some of the results found in our work are also validated by similar or related experiments by other researchers.

1. Introduction

With the miniaturization of electronic devices such as micro-electro-mechanical systems, the influence of surface properties on the mechanical, physical and chemical behaviors of such devices plays a growingly important role [1,2]. For instance, plastic deformation and material transfer should be paid enough attention to as a result of high surface energy at nanoscale. On the other hand, modern manufacturing technologies including nanoimprint lithography call for continuous improvement on surface sticking problem at small scale in order to uncover the potential of lithographic patterning [3]. Therefore, the fundamental physical and mechanical contact behaviors at nanoscale need to be investigated in detail for the potential application of these devices.

Both experimental and numerical researches have already been carried out to investigate nanoadhesive contact. With the help of the latest experimental techniques [4,5] such as atomic force microscopy, the scanning tunneling microscope, high-resolution transmission electron microscopy [6–8] and the mechanically controllable break junction [9], the interaction between tips (asperities) and substrates are studied. Nevertheless, it is difficult to characterize the tips and asperities used in experiments properly. Also, real-time atomic scale details of nanocontact are still difficult to capture in experiments. Recently, atomic scale resolution experiments are done by some researchers [7,8]. However, they mainly focus on the conductance aspects of nanocontact. When it comes to numerical methods, the molecular dynamics (MD) simulation method is extensively used nowadays to investigate nanocontacts for its potential to reveal detailed deformation mechanisms at atomic scale. The earliest pioneering MD simulations of nanocontact were carried out by Landman et al. [10,11] using Ni tips; Song and Srolovitz [12,13] investigated the influence of the work of adhesion on material transfer when single asperity contact occurs; Jiang et al. [14] studied the effects of strain rates on the plastic flow during nanoindentation by using molecular dynamics. Hagelaar et al. [15] examined different types of contact behavior at low temperature when a tungsten tip moves into a tungsten substrate under different combinations of crystal directions. It is worth noting that the substrate used by Hagelaar is one order of magnitude smaller than the models we are going to investigate.

It is well accepted that special attention should be paid to anisotropic behaviors of materials at small scale. Several researchers [16,17] have demonstrated the orientation effects through nanoindentation of single crystals. Recent research [8] discloses that different crystal orientations of metals lead to quite different mechanical and electrical behaviors at atomic scale. As a consequence, a general description of adhesive contact used at macroscale might be inadequate to reveal nano-adhesive contact behaviors. Unfortunately, among all available related

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experimental researches, limited attention is paid to the anisotropic adhesive behavior of nanoscale crystals primarily because of technical difficulties of carrying out such kind of experiments. Among numerical simulations, only several reports [15] on anisotropic adhesive nanocontact are available. In our previous research [18], we have studied the nanocontact interaction between a Ni tip and a Cu substrate through which important contact-induced deformation mechanisms were revealed. However, only one specific crystallographic orientation was considered and anisotropic behaviors of the Cu substrate are not investigated. Here, in the framework of multiscale methodology, we focus on the influences of crystal orientations on nanocontact behaviors when a Ni tip indents into and then retracts from Cu substrates. Different deformation and interface fracture mechanisms are illustrated and analyzed. Furthermore, some common characteristics shared between our research results and some general related experiments are emphasized.

When it comes to simulation methodology, it must be admitted that it is rather expensive both in terms of time and computational cost to simulate contact models even at the scale of hundreds of nanometers. What's more, related research [19] reveals that the MD model with below 4 million atoms could not eliminate the boundary effect while most of the models [10–13] used by previous nanocontact researchers have less than a million. As a result, one should be very careful about interpreting previous MD results. With the help of multiscale approaches, contact models which are orders of magnitude larger than MD models could be studied easily without introducing any boundary effect. Most importantly, contact problems are best suited for the application of multiscale approaches since only the atomic details near contact surfaces are needed. Most of the bulk of a substrate that is far from the surface only goes through uniform deformation and a general description is enough. Therefore, the Quasi-continuum (QC) method, an effective multiscale approach that couples continuum and atomic simulation is used in our research.

2. QC method and multiscale model

2.1. QC method

The QC method is an effective multiscale approach that couples continuum and atomic simulation. It is established that atomic description is only necessary at a highly deformed region and in the vicinity of defects or interfaces. Representative atoms in the QC method are divided into local atoms and non-local atoms. The local atoms capture the behavior of atoms that undergo slowly varying deformation based on Cauchy–Born rule. The nonlocal atoms are treated by discrete atomistic lattice statics in areas where severe plastic deformation occurs. Using an adaptive refinement strategy, the QC method automatically reduces the degrees of freedom and computational demand without losing atomistic detail in regions where it is required. Similarly, Karpov et al. [20] presented a systematic approach to treat the interfaces between the localized and peripheral domains in atomic scale simulations of crystalline solids. More details of the QC method can be found in Refs. [21,22].

Tadmor et al. [23] studied the incipient plasticity during nanoindentation with both rectangular and cylindrical indenters applying the QC method. Smith et al. [24] extended the QC method to simulate complex crystal structures. Knap and Ortiz applied the streamlined theory to investigate the effect of indenter-radius size [25]. The QC method has been applied to study the deformation mechanisms of nanocrystalline metals, such as nanoindentation [26–29], nanoscale contact [30–33], fracture [20,34,35], mechanical behavior of grain boundary [36,37], nanovoid cavitation [38,39] and phase transformation [40].

2.2. Multiscale model

The schematic illustration of a nanocontact model is shown in Fig. 1(a). As the deformation of the tip is not the main concern and

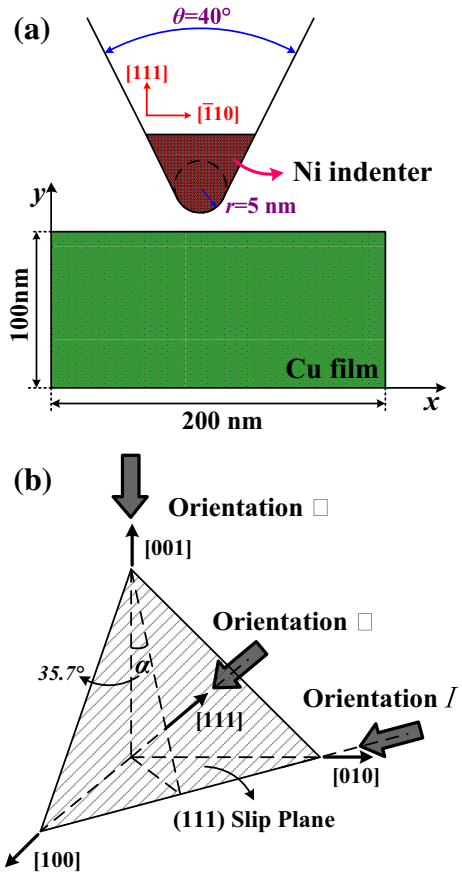

Fig. 1. Schematic illustration of nanocontact model (a) and schematic diagram of the various crystallographic orientations for nanocontact (b).

the tips used in experiments are generally much harder than substrates, a single crystal Ni tip whose Yong's modulus is larger than that of the Cu substrate is used. The crystal orientations of the tip along the x and y axes are chosen to be $[\bar{1}10]$ and [111] respectively. In this case, it is difficult for the Ni tip to have plastic deformation. The geometry of the tip is shaped like a wedge with a tip radius of 5 nm. There are two main reasons for the selection of the tip radius. First, the smallest AFM tip radius is around 5 nm [41]. Second, MD simulation [42] reveals that when contact size is around 5 nm, strong adhesive contact behavior is observed. Our treatment of the shape of the indenter may be simple, but what we focus on is the anisotropic behavior. As investigated by Borodich FM et al. [43], the geometry shape effect of the indenter is another important field of research. In this paper, the single crystal Cu substrates used are 200 nm in width and 100 nm in thickness with periodic boundary conditions in the out-of-plane direction. The size of each Cu substrate studied here is one order of magnitude larger than typical models used in MD [44] to avoid boundary effect. Three kinds of substrates with different crystal orientations are examined. The crystal orientations of each substrate with respect to their loading directions are schematically shown in Fig. 1(a) and their specific crystal orientations are listed below:

Orientation I x [111], y $[\bar{1}10]$ and z $[\bar{1}\bar{1}2]$. In this case, the Ni tip is pushed into the $(\bar{1}10)$ surface parallel to the (111) slip plane of a Cu substrate. Along this orientation, the favorable slip direction is <110> direction.

Orientation II x [110], y [001] and z $[\bar{1}10]$. A Ni tip pushes into the (001) plane of the Cu substrate. The two possible slip directions are $[\bar{1}\bar{1}2]$ and $[11\bar{2}]$. The Ni tip is pushed