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Study of the minimum depth of material removal in nanoscale mechanical machining of single crystalline copper

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ABSTRACT

It is widely believed that the minimum depth of material removal of single crystalline workpieces is one single atomic layer in nanoscale mechanical machining. However, direct evidence for this is still lacking. In this work the minimum depth of material removal of single crystalline copper in nanoscale mechanical machining is investigated through nanoscratching using molecular dynamics simulations. We demonstrate that the minimum depth of material removal of copper workpiece can achieve a single atomic layer under certain machining conditions in nanoscale machining process. It is found that the minimum depth of material removal is closely associated with the crystal orientation and scratching direction of copper workpiece. Our results also demonstrate that even when the depth of material removal is a single atomic layer of copper workpiece under certain machining conditions, the workpiece material is not removed in a layer-by-layer fashion, which rejects the hypothesis that single crystalline metal materials can be continuously and stably removed one layer of atoms after another in nanoscale mechanical machining. These understandings not only shed light on the material removal mechanism in nanoscale mechanical machining but also provide insights into the control and optimization of nanoscale machining process.

1. Introduction

In the last two decades miniaturization toward nanoscale has been the trend of technological development in a variety of industries such as mechanical, optical and electronic applications. The ever-increasing demand for devices and systems with nanoscale size and/or nanoscale accuracy (such as micro- and nano-electro-mechanical systems (MEMS and NEMS)) has motivated the development of nanoscale manufacturing technologies [1–3]. Among the nanoscale manufacturing technologies nanoscale mechanical machining processes such as cutting, grinding and tip-based nanomanufacturing have been attracting much attention since they can machine a wide range of materials and produce three-dimensional complex nanoscale devices with high accuracy controllably and stably [4–6]. However, as the nanoscale mechanical machining involves only the removal of a few atoms or layers of atoms, the nanoscale material removal mechanisms cannot be accurately described by the conventional macroscale machining theory based on continuum mechanics due to the discrete nature of materials at the nanoscale [7–10]. At this stage the material removal mechanisms in the nanoscale mechanical machining processes are still not fully understood. Many researchers assume that the nanoscale material removal takes places via chip formation as in macrosale machining process [4,5]. However, Komanduri et al. demonstrated that most of the material removal in the nanoscale machining process occurs by ploughing instead of chip formation in front of the tool as in macroscale and microscale machining [10]. In addition, Fang et al. proposed a new cutting model that material removal in the nanoscale machining process is based on extrusion rather than shearing in macroscale cutting process [7,8]. In a word, owing to the complexity of nanoscale machining process, there are still many fundamental questions concerning the material removal that need to be urgently addressed. One of the most important questions is: what is the limit of nanoscale mechanical machining? That is, what is the minimum depth of material removal in nanoscale mechanical machining? The minimum depth of material removal can be defined as the minimum depth above which the workpiece atoms can be removed stably from the workpiece surface under perfect machining conditions. As the minimum depth of material removal is a measure of the extreme accuracy achievable in nanoscale machining, investigation of the limit of nanoscale mechanical machining can not only contribute to the understanding of nanoscale material removal

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mechanisms, but also offer insights into the control and optimization of nanoscale machining process [4,11,20].

However, despite its importance, little attention has been paid to the study of the minimum depth of material removal in nanoscale machining process, although many researchers have been focusing on the investigation of minimum depth (thickness) of cut under which no stable chip formation in front of the tool would occur in microscale machining during the past decades [15–19]. A pioneering study employing molecular dynamics (MD) simulations and experiments by Shimada et al. showed that the minimum thickness of cut is about 1 nm [11,20]. It is obvious that the minimum depth of material removal could be expected to be less than 1 nm. Another significant study using MD simulations found that the minimum wear depth of Cu(1 1 1) surface is equal to the critical indentation depth (0.65–0.87 nm) associated with the first force-drop in the force-depth curve of nanoindentation [21]. However, the friction model ignores atomic-scale surface roughness of probe produced by discrete atoms and adhesion interaction between the probe and Cu(1 1 1) surface [21], both of which have considerable effect on contact area and stress distribution in the nanoscale contact and should be taken into consideration [22–25]. Another inspiring simulation work presented a monoatomic layer removal mechanism in chemical mechanical polishing (CMP) by modeling the nanoscratching process of single crystalline silicon using a spherical silica tool [26]. It is assumed that in CMP process the material was removed one atomic layer after another. But in their work the material removal is neither continuous nor stable. In fact, it is very natural to hypothesize that the minimum depth of material removal is one atomic layer of workpiece for single crystalline materials such as copper and silicon. The demonstration of atom-by-atom manipulation [12–14] and recently proposed atom-by-atom wear mechanism [27–29] make this hypothesis even more convincing. However, so far, although a great many experiments and simulations have been widely carried out to investigate the nanoscale machining mechanisms [4–6,30–38], a study verifying the hypothesis that the minimum depth of material removal is one single atomic layer of workpiece in nanoscale mechanical machining process is still lacking. Furthermore, the view that single crystalline metal materials can be continuously and stably removed one layer of atoms after another in nanoscale mechanical machining has never been demonstrated.

This work intends to fill this gap. As it is rather difficult to directly observe the nanoscale machining process by *in-situ* experiments with atomic-scale resolution, MD simulation that can capture atomic details provides a powerful tool to gain deeper insights into the minimum depth of material removal and fundamental machining mechanisms of nanoscale machining process. Therefore, in this study MD simulations of the nanoscratching process of single crystalline copper using diamond tool are preformed to explore the minimum depth of material removal in the nanoscale machining process. Copper is chosen as the workpiece since it is a common and typical metal and has numerous applications in various fields such as integrated circuits, MEMS and NEMS [39,40]. In this work we demonstrate that the minimum depth of material removal of copper workpiece can achieve a single atomic layer under certain machining conditions in nanoscale machining process, but the workpiece material is not removed in a layer-by-layer fashion. Our results reject the hypothesis that single crystalline metal materials can be continuously and stably removed one layer of atoms after another in nanoscale mechanical machining.

2. Methods

In this study, we use MD simulations to investigate the nanoscratching process of single crystalline copper. The MD Simulations are conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [41]. The simulation model consists of a hemispherical rigid diamond tool and a single crystalline copper workpiece (see Fig. 1). Since single crystalline copper exhibits significant anisotropic effects in deformation behavior under nanoindentation [42] and nanomachining [9,43], we perform MD simulations of nanoscratching on three different surfaces of Cu (0 0 1), (1 1 0), and (1 1 1) planes. For Cu(0 0 1) surface, the coordinate systems are taken as x-[1 0 0], y-[0 1 0] and z-[0 0 1] and the size of workpiece is $21.69 \times 14.46 \times 2.89\ \text{nm}^3$. For Cu(1 1 0) surface, the coordinate systems are taken as x-[0 0 1], y-[$1\bar{1}0$] and z-[1 1 0] and the size is $21.69 \times 14.57 \times 2.81\ \text{nm}^3$. And for Cu (1 1 1) surface, the coordinate systems are taken as x-[$1\bar{1}0$], y-[$11\bar{2}$] and z-[1 1 1] and the size is $21.73 \times 14.61 \times 2.92\ \text{nm}^3$.

The Cu workpiece is composed of three kinds of atoms: boundary atoms, thermostat atoms and Newtonian atoms, as shown in Fig. 1. The two layers of atoms at the bottom of the workpiece are kept fixed in space as boundary atoms to prevent the workpiece from translating during the nanoscratching process. The next four layers of atoms adjacent to the boundary atoms are thermostat atoms which are kept at a constant temperature of 300 K by the velocity scaling method [44] to mimic the heat dissipation in real machining process. The remaining workpiece atoms are Newtonian atoms that are free of constraints and move freely according to the interatomic forces. The equations of motion are integrated with a velocity-Verlet algorithm with a time step of 1 fs. Periodic boundary conditions are imposed in the x and y directions.

Interatomic forces within Cu are derived from an embedded atom method (EAM) potential [45]. The EAM potential has been very successful in modeling the elastic properties, defect formation energies and fracture mechanisms of various metals [45,46]. It has also been successfully applied to describe the surface properties of metals such as surface energies and surface reconstructions [45–48]. As the tool is treated as a rigid body, the interactions between tool atoms are ignored. The interaction between Cu and tool is modeled by the widely used Morse potential [44]:

$$V(r) = D(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}) \quad (1)$$

where $V(r)$ is a pair potential energy function; D is the cohesion energy; α is the elastic modulus; r and r_0 are the instantaneous and equilibrium distance between two atoms, respectively. The cut-off radius of the Morse potential is chosen as 9.0 Å, which ensures that the calculations will not consume large amounts of computational time calculating the forces that are near zero. The standard Morse potential parameters [35–38,49] are given as $D = D^* = 0.087$ eV, $\alpha = 5.14\ \text{Å}^{-1}$ and $r_0 = 2.05$ Å. It should be noted that the interaction strength of material bonds generally increases with the increase of cohesion energy D [50,51]. It is well-known that adhesion plays an essential role in nanoscale machining process. Hence, in order to examine the effects of adhesion between tool and workpiece on the minimum depth of material removal, we also perform MD simulations of nanoscratching for different values of D [50,51].

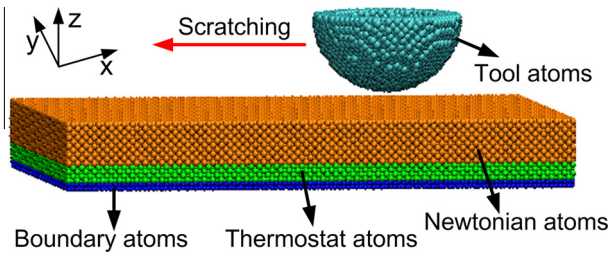

Fig. 1. Simulation model of nanoscratching process.