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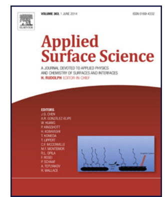

A molecular dynamics investigation into the mechanisms of subsurface damage and material removal of monocrystalline copper subjected to nanoscale high speed grinding

Jia Li[a,b], Qihong Fang[a,b,*], Youwen Liu[a,b], Liangchi Zhang[c]

[a] State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, Hunan Province 410082, PR China
[b] College of Mechanical and Vehicle Engineering, Hunan University, Changsha, Hunan Province 410082, PR China
[c] School of Mechanical and Manufacturing Engineering, The University of New South Wales, NSW 2052, Australia

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A B S T R A C T

This paper investigates the mechanisms of subsurface damage and material removal of monocrystalline copper when it is under a nanoscale high speed grinding of a diamond tip. The analysis was carried out with the aid of three-dimensional molecular dynamics simulations. The key factors that would influence the deformation of the material were carefully explored by analyzing the chip, dislocation movement, and workpiece deformation, which include grinding speed, depth of cut, grid tip radius, crystal orientation and machining angle of copper. An analytical model was also established to predict the emission of partial dislocations during the nanoscale high speed grinding. The investigation showed that a higher grinding velocity, a larger tip radius or a larger depth of cut would result in a larger chipping volume and a greater temperature rise in the copper workpiece. A lower grinding velocity would produce more intrinsic stacking faults. It was also found that the transition of deformation mechanisms depends on the competition between the dislocations and deformation twinning. There is a critical machining angle, at which a higher velocity, a smaller tip radius, or a smaller depth of cut will reduce the subsurface damage and improve the smoothness of a ground surface. The established analytical model showed that the Shockley dislocation emission is most likely to occur with the crystal orientations of (0 0 1)[1 0 0] at 45° angle.

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1. Introduction

Nanoscale machining processes are playing an essential role in the modern manufacturing industry [1–4]. With the rapid development of the atomic and scanning probe microscopy techniques, nanoscale machining techniques have been used in the fabrication of components with nanoscale surface features and sub-micron form accuracy. This is well exemplified in the manufacturing and applications of micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS) [5–8]. Nanoscale materials due to their superior strength, strong hardness and good wear resistance represent the subject of rapidly growing research efforts [9–14]. In order to further improve the functioning properties of MEMS and NEMS, understanding the deformation mechanisms of the materials during their nanoscale machining processes has become a significant challenge. This is because a nanoscale machining process involves only a few nanometers, or even a less length scale, which makes it extremely difficult to observe the process experimentally. Therefore, molecular dynamic (MD) simulation as a theoretical method has become an important tool in studying the nanoscale machining processes [15–17].

A number of studies have used the MD simulations to analyze nanoscale machining in the past years. Komanduri et al. [18–20] investigated the material deformation and failure in single crystal copper and aluminum subjected to nanoscale machining. Zhang and his coauthors [21–23] explored the mechanisms of wear and friction on the atomic scale. Zhao et al. [24] investigated the characteristics of machining-induced subsurface damage of mono-crystalline silicon with a spherical diamond indenter by using nanoindentation simulation via MD method. Guo et al. [25] analyzed the thermal effects on a nanoscale material removal, and demonstrated the temperature distribution showing a roughly concentric shape around shear zone. Fang et al. [26] proposed a new model based on extrusion to understand how materials are removed from a workpiece in nanoscale cutting, and found that the mechanism is different from the shearing in conventional

* Corresponding author. Tel.: +86 731 89822841; fax: +86 731 88822330.
E-mail addresses: fangqh1327@hnu.edu.cn, fangqh1327@tom.com (Q. Fang).

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Table 1
Computational parameters used in the MD simulations.

Materials	Workpiece: copper	Tool: diamond
Dimensions	20 nm × 13 nm × 12 nm	Radii 1.0, 1.5, 2.0, 2.5, 3.0, 4.0 and 5.0 nm
Number of atoms	267,732	
Time step	1 fs	
Initial temperature	293 K	
Grinding velocity	50, 100, 200 and 400 m s^{-1}	
Depth of cut	0.5, 1.0, 2.0 and 3.0 nm	
Grinding distance	0–19 nm	
Grinding direction	[1 0 0] on (0 0 1) surface	

cutting. Furthermore, MD simulations have been applied to investigate the nanometric machining of various types of materials, including Si [27,28], Cu [29,30], Ni [31] and Al [32].

The previous works are helpful in understanding nanometric machining. However, they have mainly focused on clarifying the material removal mechanisms, tool wear, energy consumption, and dislocation nucleation and emission. Little has been done on improving the surface integrity of a material by nanoscale machining.

In this work, we will perform a series of large-scale MD simulations of nanoscale grinding of copper using the EAM potential. The effects of the depth of cut, grinding speed, crystal and machining angle orientation on the surface integrity of a ground surface will be investigated by analyzing the deformation and dislocation motion during grinding. To this end, our study will consist of the following key parts. Section 2 will provide a detailed description about the modeling of copper samples, the nanoscale grinding procedure and the defect analysis and visualization techniques to use. Section 3 will present the results of materials deformation and dislocation movement of copper with an emphasis on the effects of tool speed, depth of cut, tip radius, crystal orientation and machining angle. Section 4 will establish an analytical model to explore the emission of partial dislocations during nanoscale grinding. Finally, in Section 5 we summarize the results.

2. Simulation method

Fig. 1 shows the MD simulation model of nanoscale grinding of copper. The model contains a face-centered cubic (FCC) single crystal copper workpiece and a rigid diamond cutting tool. Table 1 summarizes the computational parameters used in the MD simulations. The size of the workpiece is 20 nm × 13 nm × 12 nm. The three orientations of the workpiece are in x-[1 0 0], y-[0 1 0] and z-[0 0 1]. The grinding is conducted along the [1 0 0] direction on the (0 0 1) surface of the workpiece. The workpiece includes three types of atoms: boundary atoms, thermostat atoms and Newtonian atoms. The motions of the thermostat and Newtonian atoms obey the classical second Newton's law whose equations of motion could be numerically integrated by the well-established Velocity-Verlet algorithm with the time step of 1 fs. The three layers of the boundary atoms at the left and bottom of the workpiece are kept fixed in space to eliminate the rigid body motion of the workpiece [1,7]. The next three layers of the atoms adjacent to the boundary ones at the left and bottom of the workpiece are thermostat atoms. The initial workpiece temperature is 293 K. As considerable energy adds to the thermostat atoms during grinding, heat dissipation is carried out during the MD simulation to keep the thermostat atoms at the constant temperature of 293 K, by adjusting the atom velocities at every five computational time steps using the velocity rescaling method. In addition, the temperature can be calculated from $T = \left\langle \sum_{i=1}^{N} m_i v_i^2 \right\rangle / 3Nk_B$ with k_B the Boltzmann constant, N atom number, m_i and v_i the ith atom mass and velocity, and $\langle\,\rangle$ statistical averaging over all simulation time [25]. A periodic boundary condition is maintained along the y-direction to reduce the effect of the simulation length-scale.

The diamond tip/tool created from the perfect diamond atomic lattices has a spherical shape with radius 1.0 nm, 1.5 nm, 2.0 nm, 2.5 nm, 3.0 nm, 4.0 nm and 5.0 nm, respectively. The tool is treated as a rigid body in the simulations since diamond is much harder than copper.

There are three different atomic interactions in the MD simulation: (1) the interaction between copper atoms (Cu-Cu) in the workpiece, which will be described by the embedded atom method (EAM) potential [33,34] in our study, as the EAM potential has been found reliable; (2) the interaction between diamond atoms (C-C) in the tool, which will be ignored in the present study as the tool is treated as a rigid body; and (3) the interaction between the workpiece and tool (Cu-C) atoms, which will be depicted by the Morse potential [6,7,29,35]. The parameters for Cu-C in our simulations are taken as, according to [6,7,29,35], cohesion energy D = 0.087 eV, elastic modulus α = 5.14 Å^{-1} and equilibrium distance between two atoms r_0 = 2.05 Å. The cut-off radius of the Morse potential is chosen to be 0.9025 nm [7] to ensure the computational efficiency.

All MD simulations are completed using the classical molecular dynamics package IMD with a time step of 1 fs [36]. The software OVITO is utilized to visualize the MD data and generate the MD snapshots [37]. The common neighbor analysis (CNA) [38] is adopted to identify the feature of each atom before and after deformation during nanoscale grinding. The difference between intrinsic stacking fault (ISF) and dislocation cores is distinguished.

3. Defect analysis

Our MD grinding simulation consists of two stages: the relaxation stage and the grinding stage. Following the system initialization of the workpiece and the tool with their perfect lattice configurations, atoms in the system are allowed to relax to minimum energy to accommodate any surface relaxation. After that, the grinding is performed by applying a constant velocity in the positive x-direction to the tool. Here, the objective is to elaborate the contributions of a variety of variables, such as tool speed, depth of cut, tool tip radius, crystal orientation and machining angle to the subsurface damage of the workpiece material.

3.1. Effect of tool speeds

According to different grinding speed classification, a general grinding speed is less than 45 m s^{-1}, a high speed grinding 45–150 m s^{-1}, and ultra-high speed grinding more than 150 m s^{-1}. Here, we select three of grinding speeds of 50, 100 and 200 m s^{-1} used for studying high speed and ultra-high speed grinding based on practical grinding speeds.

Fig. 2 presents the instantaneous defect structures of a few deformed single crystal copper samples, where Fig. 2(a) and (b) shows the evolution of different types of atoms, and Fig. 2(c) and (d) present the deformed atomic structures without including the FCC atoms for a clearer visualization of the damaged structures. It can be seen from Fig. 2(a) that when the tool speed is 100 m s^{-1}, the copper sample undergoes an elastic deformation at the initial stage of grinding (zone I), followed by plastic deformation via the dislocation mechanism and deformation twinning (zone II, III, IV). The decrease of the FCC atoms with the increase of ISF atoms indicates that plastic deformation is dominated by dislocation nucleation and by the length increase of the stacking fault band (zone II and IV).

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