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The effect of rough surface on nanoscale high speed grinding by a molecular dynamics simulation

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

[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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ABSTRACT

Molecular dynamics is employed to study the nanoscale high speed grinding process of single crystal copper with rough surface. Material removal behavior of the cooper workpiece through diamond grinding is studied. The effects of texture density, texture direction, texture shape and the tool with rough or smooth surface are thoroughly investigated in terms of atomic trajectories, temperature distribution, radial distribution function, grinding temperature, grinding force, and friction coefficient. It can be found that a larger texture density results in lowering a surface smoothness of workpiece in the local area, and reduces the partial protrusion, specifically when the texture density is greater than 90%. The material removal and the smoothness of ground surface strongly depend upon the effects of texture orientation and shape. The quality of the ground surface at texture orientation parallel with the *x*-axis is the best. The texture shape that intensely influences the chip and the groove depends on the size of the contact surface, suggesting that the material removal mechanism is roughly the same under different texture shapes. The smooth prismatic tips generate a more chips than the rough prismatic tip, while the volume of the material pileups is less than that of the rough one, which means that the prismatic diamond tip with smooth surface has an absolute advantage than the rough tip to machine nanostructures and greatly improves the material removal rate. These results show that it is possible to control and tune the grinding parameters according to texture density, direction and shape during machining single crystal copper with rough surface, and provides a potential way to improve a surface integrity and a smoothness of machined surface.

1. Introduction

Machined materials with rough surface are a complex and progressive material removal process that often impacts on the surface integrity and subsurface damage [1–5]. Understanding material removal mechanism and formulating governing laws for nanoscale machining process is of great scientific and technological interest and significant economic impact. However, nanoscale machining processes that are so difficult to directly observe and understand the underlying mechanisms of material removal by in situ experiments, involve only a few nanometers or even a less length scale, and molecular dynamics (MD) provides an effective tool to gain deeper understanding to material removal mechanism of grinding on rough surface at nanoscale.

MD as a theoretical method has been a powerful tool to study the basic mechanisms of material testing and processing at the nanometer scale. Moreover, MD simulations are also widely used to solve other practical problems, such as nanoparticles [6], nanowires [7–10], and nanofilm [11]. For example, Zhang et al. [12,13] employed MD simulation to discuss the phase transformation by nanoscale indentation testing of diamond cubic silicon, and investigated the size dependent effect on friction by single asperity sliding. With the aid of MD analysis, Zhu and Fang [14] investigated the phase transition of monocrystal Ge from indentation tests, and showed that the dominant deformation mechanism is a phase transformation by a pressure rather than by dislocation mechanism. Using both MD and in situ scanning spreading resistance microscopy, Mylvaganam et al. [15] reported the evolution mechanisms of metastable phases during the nanoscale indentation on monocrystalline silicon. They suggested that the distorted diamond structure emerges at a critical size of contact between the indenter and silicon upon unloading. Subsequently, Mylvaganam

* Corresponding author at: State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, Hunan Province, 410082, PR China.
E-mail address: fangqh1327@hnu.edu.cn (Q. Fang).

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et al. [16,17] investigated the mechanisms of the frictional properties of three different forms of carbon–diamond, graphite and carbon nanotube on contact sliding against a diamond asperity using MD simulations. They found that carbon nanotube and graphene at nanoscale have low coefficients of friction due to the difference in their atomic structures. Recently, Romero et al. [18] and Lin et al. [19] discussed the temperature distribution during orthogonal nanometric machining. More recently, Li et al. [20] studied the mechanisms of material removal and subsurface damage during a nanoscale high speed grinding, and showed that the behavior of Shockley dislocations emits from the crystal orientations of (001) [100] at the angle 45° by the established analytical model. Less work involving theoretical models has been published relating to the effect of rough surfaces, and many researchers [21–23] focused on the experimental methods to study the characteristic of rough surface. However, the nanoscale surface roughness affects the components of accuracy owing to the mechanical machining process induced the adhesive and frictional forces [24–26]. In micro/nano mechanical machining, such as cutting and grinding, the adhesion contribution to friction can no longer be neglected because of large ratio of surface area to volume [27]. Although it is well known that even the best smooth surface of the real material contains a large number of peaks and valleys, in conventional MD simulation of nanoscale machining is assumed as a perfect surface. Therefore, there is a need to understand the effect of surface roughness in the workpiece on nanoscale level mechanical machining process [28,29].

We perform large scale MD simulations of nanoscale high speed grinding of single crystal copper with rough surface considering the effects of texture density, texture direction, texture shape and the tool with rough or smooth surface. We determine the dependence of the grinding surface morphology on different surface textures. In addition, we examine in detail the atomistic process of grinding single crystal copper by studying atomic trajectories, temperature distribution, number of atoms in different temperature, radial distribution function, evolution of different types of atoms, grinding temperature, grinding force, and friction coefficient.

2. Simulation method

In this study, we consider the proposed nanoscale grinding model of a diamond tool and a copper workpiece with rough surface, as shown in Fig. 1. To facilitate the description of rough surface, we use the texture surface in instead of rough surface to study the effects of texture density, texture direction, texture shape. At the nanoscale, the texture surface during the grinding process acts as a special rough surface. According to the previous literatures [30,31], the similar methods are used to simulate rough surface during nanoscale machining. The nanoscale surface roughnesses are defined as the surface roughness factors R_x and R_z in Fig. 1, where R_0 is equal to a constant value 2 nm. The texture density can be expressed as $\rho = R_x/R_0$, and reveals the surface characterization in texture cycle R_0. A face centered cubic (FCC) single crystal copper workpiece has dimensions of $30 \times 13 \times 15\ \text{nm}^3$ along x, y and z directions. This dimension is obtained based on the phonon transportation within solid materials [32] and the relevant simulation parameters of nanoscale machining [20,33]. The diamond tip/tool created from the perfect diamond atomic lattices is a spherical shape with radius 3 nm, and periodic boundary condition is applied to the y direction. The grinding is conducted along the [100] direction on the (001) surface of the workpiece, in which the three orientations are x-[100], y-[010] and z-[001]. The workpiece consists of three types of atoms: boundary atoms, thermostat atoms and Newtonian atoms. According to Ref. [33], the thicknesses of boundary layer and thermostat layer at workpiece and tool are 1 nm and 1 nm in Fig. 1, respectively. The motions of the thermostat and Newtonian atoms obey the classical second Newton's law, which are integrated using velocity-verlet algorithm with a time step of 1 fs. The bottom of workpiece is fixed to eliminate the rigid body motion of the workpiece [12,20]. Thermostat atoms during nanoscale grinding are to ensure reasonable heat dissipation, and maintain at the constant temperature of 293 K, whose velocities are adjusted at every five computational time steps using the velocity rescaling method [20].

Three different atomic interactions are adopted in the MD simulation. The interaction between copper atoms (Cu–Cu) in the workpiece is described by the embedded atom method (EAM) potential [18,20,33–36]. For the EAM potential, the total atomic potential energy of a system E is expressed as:

$$E = \frac{1}{2}\sum_{ij,i\neq j}\phi_{ij}(r_{ij}) + \sum_i F_i\left(\sum_{j\neq i}^{n}\rho_i(r_{ij})\right) \tag{1}$$

where ϕ_{ij} is the pair-interaction energy between atoms i and j, F_i the embedded energy of atom i, and ρ_i the host electron density at site i induced by all other atoms in the system. Additionally, the cutoff radius of the EAM potential is chosen as 0.495 nm to ensure that the calculations are accuracy and efficiency during the MD simulation.

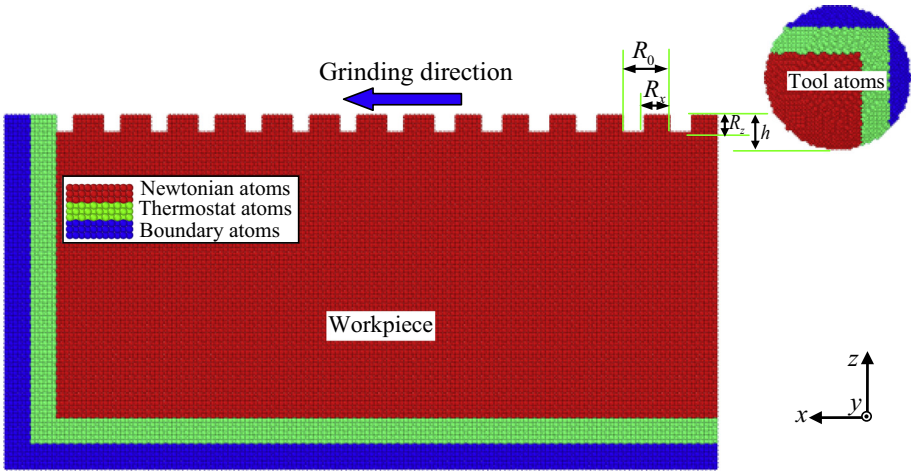

Fig. 1. MD simulation model of a nanoscale grinding a cooper with rough surface.