



The effects of pore and second-phase particle on the mechanical properties of machining copper matrix from molecular dynamic simulation



Jia Li ^{a,b}, Qihong Fang ^{a,*}, Bin Liu ^{c,*}, Youwen Liu ^a

^a State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, Hunan Province 410082, PR China

^b Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

^c State Key Laboratory for Powder Metallurgy, Central South University, Changsha 410083, PR China

ARTICLE INFO

Article history:

Received 16 March 2016

Accepted 11 May 2016

Available online 19 May 2016

Keywords:

Nanomachining

Porous metals

Metal matrix composites

Molecular dynamics

Second-phase particle

Pore healing

ABSTRACT

The subsurface damage and surface integrity of a spherical diamond indenter sliding against a face-centred cubic copper (100) surface considering the pore and second-phase particle effects is investigated by means of molecular dynamic simulations of nanoindentation followed by nanomachining. In this investigation, we establish an analytical model for pore healing, and provide a criteria to determine whether or not pore can be healed. The results show that with increase of machining distance pore becomes smaller and then closes due to machining-induced compressive stress, resulting in low material damage and strong structure stability. Compared to free pore workpiece, machining force slightly relies upon the existence of pore and second-phase particle while friction coefficient strongly depends on the existence of that. In addition, particle induces work hardening due to Lomere-Cottrell lock and dislocation slip during machining metal matrix composites. It is helpful to understand the relation of machining performance and material parameter for obtaining higher surface integrity and lower subsurface damage during machining porous metals and particle reinforced metal matrix composites.

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1. Introduction

Particle reinforced metal matrix composites (MMCs) and porous metals are extensively used as raw material in the automotive, railway industry and aerospace industries [1,2]. Particle reinforced MMCs have high specific modulus, strength, and thermal stability [1]; porous metals possess low density, large specific surface area and excellent energy absorption [2]. However, the full potential of particle reinforced MMCs and porous metals is hindered by the high manufacturing costs associated with the difficulties experienced in machining these materials. In order to achieve a deeper understanding of machining these materials in the nanoscale level, the deformation behaviors as important performance indicators are analyzed in detail [1–4]. Due to the experimental observation at the nanoscale constrained by long time, high costs and large uncertainty of measurements [3,4], therefore, molecular dynamic (MD) simulations as an important complementary tool may appro-

priately help to reveal the deformation mechanism of particle reinforced MMCs and porous metals.

In the past years, MD simulations and microscopic experiments have been used widely to analyze scratching mechanism [5–7], nanoindentation mechanism [8–10], and nanomachining mechanism such as cutting [11–13], nanomilling [14], turning [15], grinding [16,17], nanoforming [18,19], polishing [20,21], and nanolithography [22,23]. For example, Zhang et al. [24–26] explored in detail the mechanisms of wear and friction as well as phase transformation using the models of the nanoindentation of silicon. Using MD simulations, Zhang et al. [27,28] investigated the deformation mechanisms of nanotwinned copper (Cu) during nanoscratching, and obtained the relationship between twin boundary spacing and friction coefficient. Recently, Li et al. [7,29] employed MD simulations to study the nanoscale high speed grinding process of a single crystal Cu considering the effect of rough surface. Their results show that it is possible to control and tune grinding parameters to improve the surface integrity and subsurface damage. However, many scholars mainly focus on the homogeneous metal materials in the absence of pore and second-phase particle, which exist in particle reinforced MMCs and porous metals. The void and crack effects on [30–34] were explored during machining and loading.

* Corresponding authors.

E-mail addresses: fangqh1327@hnu.edu.cn (Q. Fang), binliu@csu.edu.cn (B. Liu).

Table 1
Computational parameters used in the MD simulations.

Materials	Workpiece: Copper	Tool: Diamond
Dimensions	300 Å × 177 Å × 100 Å	Radius 50 Å
Number of atoms	About 455, 500	92, 286
Time step	1 fs	
Initial temperature	293 K	
Machining velocity	100 m s ⁻¹	
Depth of cut	10 Å	
Machining distance	0–120 Å	
Machining direction	[1 0 0] on (0 0 1) surface	
Hole radii	10, 15, 20 and 25 Å	
Inclusion radii	10, 15, 20 and 25 Å	

For example, Hosseini et al. [35] studied the nanometric cutting of a single crystal Cu considering the void effects using MD simulations. Zhu and Fang [36] used MD simulations to study the void effects during the cutting process of metallic glass, and found that the large deformation zones appear from the machining surface to the void surface. For second-phase particle, finite element modeling and experiment for the machining of particle reinforced MMCs predict cutting forces, chip morphology, stresses, and temperature distributions [37]. A number of recent studies have been published in this area but they are mainly focused on the evolution of machining-induced-microstructure due to the effects of pore and second-phase particle, which are considered one important contribution to the mechanical properties of machining metal matrix [1,2].

In this study, we employ MD simulations of machining single crystal Cu with second-phase particle or pore. Considering the second-phase particle and pore effects, surface integrity and subsurface damage are investigated in terms of particle evolution, pore evolution, dislocation evolution, shear strain, surface morphology, atomic displacement, machining force, and friction coefficient. This study contributes to a better understanding of the pore and second-phase particle effects on surface integrity and subsurface damage during machining porous metals and MMCs.

2. Simulation method

The MD simulation system of nanomachining comprises a diamond tool and a Cu workpiece with particle or pore, as shown in Fig. 1a. In order to a reasonable study, a single pore (second-phase particle) is introduced MD simulation, because the distribution and density of many pores or second-phase particles affect the surface integrity and subsurface damage during machining porous metals and MMCs. A more detailed analysis of distribution and density of pores or second-phase particles on machining performance however exceeds the scope of this study and is left for future work. Here, this paper is focused on the effect of single pore or single second-phase particle during machining. To create a single pore, the atoms in a spherical region are removed from Cu matrix. To create a single particle, the atoms in a spherical region are removed, and then this blank region fill another kind atoms. The distance of pore (second-phase particle) upper surface to matrix upper surface is defined as pore height (particle height) h , and the radius of second-phase particle or pore is r , demonstrated in Fig. 1b. The orientations of Cu workpiece are x -[1 0 0], y -[0 1 0] and z -[0 0 1], and machining direction is along the [1 0 0] direction on (0 0 1) surface. Table 1 gives simulation parameters of workpiece and tool used in the present study. The size of Cu workpiece comprising about 455, 500 atoms is $30 \times 17.7 \times 10 \text{ nm}^3$. A diamond particle of radius 5 nm is employed as a tool/tip [5,8–10,30]. The Cu workpiece is divided into three different zones: Newton layer, thermostat layer and boundary layer. The motion of atoms in Newtonian and thermostats layers obeys Newton's second law of motion. The thermostats layer maintains at

a constant temperature of 293 K to ensure a reasonable heat dissipation away from the machined zone. The boundary layer is fixed to eliminate the unexpected rigid body motion of Cu workpiece during machining. The periodic boundary conditions are set in x and z directions.

When workpiece contains pore, we have used the embedded atom method (EAM) potential for the Cu–Cu atom interactions [6–9,16,17]. When workpiece contains particle, the workpiece and particle interactions are to describe EAM/alloy potential which is used to construct an interatomic potential for (1) Cu–Cu, Cu–Ag, and Ag–Ag in workpiece with Ag particle [38]; (2) Cu–Cu, Cu–Al, and Al–Al in workpiece with Al particle [39]; (3) Cu–Cu, Cu–Fe, and Fe–Fe in workpiece with Fe particle [40]; (4) Cu–Cu, Cu–Ni, and Ni–Ni in workpiece with Ni particle [40]. For the C–C atom interactions, this effect is ignored since diamond is much harder than Cu [6–9,16,17]. Usually, the Cu–C atom interactions is described by the Morse potential [6–9,16,17].

3. Simulation results and discussion

In this study, the three dimensional MD simulations are performed to study the pore or second-phase particle effect during machining porous metals and MMCs. All MD simulations are completed using the classical molecular dynamics package IMD [41], and the software OVITO is utilized to visualize MD data and generate MD snapshots [42]. The common neighbor analysis (CNA) [43] is adopted to identify the crystal structure before and after machining. Firstly, the energy minimization using the conjugate gradient method is carried out to avoid overlaps in the positions of the atoms. Secondly, workpiece temperature is equilibrated to 293 K under microcanonical ensemble dynamics for 100 ps. After a fully relaxation, pore and second-phase particle are stable. The tool presses down at the velocity of 100 m s^{-1} along the negative z -direction until the indentation depth is 1.0 nm. And then the tool has a constant velocity of 100 m s^{-1} along the positive x -direction [32,36].

3.1. The pore effect

Fig. 2 shows pore evolution at different machining distances during machining. As the tool moves forward, a number of intrinsic stacking faults (ISFs) and dislocations take place in the subsurface of workpiece [17,28], interact with pore, and reduce pore size (See Fig. 2 a–d). When the tool approaches pore, pore breaks down due to the high shear strain around pore (See Fig. 2e), and eventually evolves into the vacancy, as shown in Fig. 2d. This machining process leads to pore-healing and lowers subsurface damage. Here, subsurface damage specifically means a large scale defect (pore), and we ignore the zero-dimensional defect (vacancy) and the one-dimensional defect (dislocation) during machining. The pore plays a critical role in material failure compared to zero-dimensional and one-dimensional defect. In summary, a transition from pore dissociation to pore annihilation is induced by machining process, and it is beneficial to reducing the extent of subsurface damage and improving the machined workpiece stability. This similar phenomenon can be found in previous work, such as, hole-healing in a nickel thin film during nanoindentation [32], and fatigue crack closure in an aluminum alloy during constant amplitude loading [33], as well as roughness induced crack closure at higher stress region [34].

Fig. 2(f) shows evolution of number of reducing atom with the increase of machining distance. From Fig. 2(f), there are significant differences in various kinds of atom number for the perfect and defective workpiece because of machining induced pore-healing. As a result, the number of reducing HCP and FCC atoms

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