Applied Surface Science 317 (2014) 432–442

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Molecular dynamics simulations of nanometric cutting mechanisms of amorphous alloy

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ARTICLE INFO

Article history:
Received 31 May 2014
Received in revised form 6 August 2014
Accepted 7 August 2014
Available online 19 August 2014

Keywords:
Amorphous alloy
nanometric cutting
molecular dynamics

ABSTRACT

Molecular dynamics simulations are employed to study the nanometric cutting process of $Cu_{50}Zr_{50}$ amorphous alloy. The effects of cutting depth, cutting speed and tool edge radius on the cutting force, workpiece pile-up and temperature of the cutting region are studied to investigate the mechanisms of the material removal and surface formation in the nanometric cutting process. It is found that the material removal of amorphous alloy workpiece is mainly based on extrusion at the nanoscale instead of shearing at the macroscale. The plastic deformation of amorphous alloy is mainly due to the formation of shear transformation zones during the nanometric cutting process. The results also suggest that bigger cutting depth and cutting speed will lead to larger tangential force and normal force. However, the tool edge radius has a negligible effect on the tangential force although the normal force increases with the increase of tool edge radius. The workpiece pile-up increases with an increase of the cutting depth, but decreases with an increase of the edge radius of the tool. The workpiece pile-up is not significantly affected by the cutting speed. It is also found that larger cutting depth and cutting speed will result in higher temperature in the cutting region of workpiece and the average Newtonian layer temperature of the tool. Tool edge radius has no significant effect on the temperature distribution of the workpiece and the average Newtonian layer temperature of the tool.

1. Introduction

Amorphous alloy, also called metallic glass has excellent mechanical, thermal and magnetic properties due to its unique amorphous structures [1,2]. The great prospects in the application of amorphous alloy, especially in nanotechnology and micro electro-mechanical systems, make the study of nanoscale machining of amorphous alloy even more important. Therefore, nanometric cutting of amorphous alloy has attracted more and more attention since nanometric cutting is an excellent nanoscale manufacturing method to fabricate components with nanometric surface finish, complicated shape and submicron geometry accuracy [3]. Cutting involves a large plastic deformation of workpiece. It is widely accepted that localized shear bands that evolve from "shear transformation zones (STZs)" are responsible for the inhomogeneous plastic deformation of amorphous alloy [4]. However, homogenous plastic deformation is also observed in the nanoscale amorphous alloy [5,6]. Therefore, the deformation mechanism of amorphous alloy has not been fully understood yet. In addition, during the cutting process of amorphous alloy, what has bothered most scholars is the poor machinability [7], e.g., much heat production, poor thermal conductivity and serious tool wear, etc. Therefore, at present the study of material deformation mechanism of amorphous alloy at the nanoscale has been a hotspot. Hodge and Nieh [8] studied the wear resistance of several kinds of amorphous alloy through nanoscratching experiments and stated the relationship between the wear resistance and hardness. Rahaman *et al.* [9] studied the friction and wear mechanism of $Ti_{40}Zr_{25}Ni_3Cu_{12}Be_{20}$ amorphous alloy under contact sliding and expounded the effect of the frictional heating on the change of material friction characteristics. Huang *et al.* [10] studied mechanical properties of several kinds of amorphous alloy through nanoscratching experiments, the results of which show the nanoscratching resistance is related to the nanohardness of the material. Noritakat *et al.* [11] conducted nanomachining experiments of the $Zr_{55}Cu_{30}Al_{10}Ni_5$ amorphous alloy by atomic force microscopy and analyzed the deformation of the material, chip formation and tool wear during the cutting process. In addition to the experiments, Zhao et al. [12] used the molecular dynamics (MD) to conduct the nanometric cutting simulations of $Cu_{50}Zr_{50}$ amorphous alloy and analyzed the chip

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http://dx.doi.org/10.1016/j.apsusc.2014.08.031
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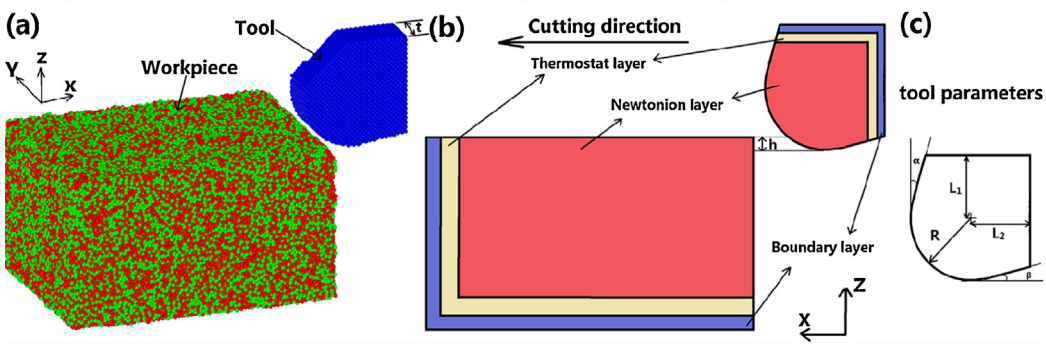

Fig. 1. The model of the MD simulation (Cu atoms are green, Zr atoms are red and C atoms are blue).

formation process. Zhu and Fang [13] adopted a virtual spherical tool for the molecular dynamics simulations of nanometric cutting $Cu_{50}Zr_{50}$ amorphous alloy. Since at the nanoscale, cutting involves only a few nanometers or less on the workpiece surface, the nanoscale cutting process cannot be accurately described by the macroscale cutting theory. So far, the fully understanding of cutting mechanisms of amorphous alloy at the nanoscale has been lacking.

Since binary alloys are easier to model than alloys with more elements and $Cu_{50}Zr_{50}$ can reveal the typical characteristics of amorphous alloy [2], $Cu_{50}Zr_{50}$ become an attractive amorphous alloy to study theoretically [14]. $Cu_{50}Zr_{50}$ is the most classic one of CuZr binary systems [15] and can be processed into high precision parts for aerospace and micro electro-mechanical systems [1]. Moreover, because it is rather difficult to directly observe the deformation process of amorphous alloy by in-situ experiments with atomic-scale resolution, molecular dynamics (MD) provides a powerful tool to gain deeper insights into the deformation mechanism of amorphous alloy during nanometric cutting process. Therefore, to further reveal nanometric cutting mechanisms of amorphous alloy, this paper employs molecular dynamics simulations to study the nanometric cutting process of $Cu_{50}Zr_{50}$ amorphous alloy. The effects of cutting depth, cutting speed and tool edge radius on the material removal mechanisms will be thoroughly investigated.

2. Simulation method and model

Fig. 1 shows the MD simulation model. The amorphous alloy sample is prepared from a melting and quenching simulation [13,16,17]. A crystalline mixture of $Cu_{50}Zr_{50}$ is initially relaxed under periodic boundary conditions at 293 K for 200 ps within NPT (constant pressure and constant temperature) ensemble. Then the sample is heated gradually to 2500 K for 44ps, allowing the solid to melt. After that the sample is kept at 2500 K for 40ps and quenched to 293 K at a constant rate over 25ps. The pressure was maintained at zero during the whole process. Table 1 shows the MD simulation parameters. Both the workpiece and cutting tool consist of three kinds of atoms: boundary layer atoms, thermostat layer atoms and Newtonian layer atoms [13,18–21]. As shown in Fig. 1 (b), the boundary atoms with a thickness of 1.0 nm at the left and bottom of the workpiece and a thickness of 0.5 nm at the right and top of the tool are kept fixed to form fixed boundary conditions. The thermostat atoms with a thickness of 1.5 nm of the workpiece and a thickness of 0.5 nm of the tool adjacent to the boundary atoms are kept at a constant temperature of 293 K by the velocity scaling method to imitate the heat dissipation in real cutting process. It is well-known that in macroscale traditional machining process, the cutting heat generated due to the plastic deformation of workpiece and friction at the tool-chip interface is carried away by chips and lubricant and by conduction into the tool and workpiece. However, the nanometric cutting model is not capable of dissipating the cutting heat itself, so the thermostat layer atoms are employed to dissipate the cutting heat [21]. The rest of atoms are Newtonian atoms, whose motions obey classic Newton's second law [22,23]. Periodic boundary conditions are imposed in the y direction. The cutting process is simulated by moving a tool at a constant speed along the x direction with a fixed cutting depth as shown in Fig. 1 (b). The cutting depth h is defined as the distance from the top surface of the workpiece to the bottom of the tool along z direction. Both the relaxation and nanometric cutting simulations are conducted in microcanonical ensemble (NVE). After a fully relaxation, the cutting begins and the tool moves along the cutting direction at a constant cutting speed.

Atomic interactions in the workpiece are modeled by embedded atom method (EAM) potential with parameters given by Mendelev et al. [24,25]. The total energy E_i of every atom i satisfies:

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_{\alpha\beta}\left(r_{ij}\right)\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}\left(r_{ij}\right) \quad (1)$$

Embedding energy F is function of the atom's electron density ρ. Φ is a pair potential interaction parameter. α and β are the element type parameters of atom i and atom j.

$$F_\alpha = -A\sum_i \sqrt{\rho_i} \quad (2)$$

$$\rho_i = \sum_{j\neq i} V(r_{ij}) \quad (3)$$

Table 1
The MD simulation parameters.

Properties	Parameters
Workpiece material	$Cu_{50}Zr_{50}$ amorphous alloy
Tool material	Diamond(C)
Workpiece dimensions	21nm × 15nm × 12 nm
Tool dimensions	Thickness t = 3 nm
	Rake angle α = 12°
	Clearance angle β = 8°
	L_1 = 4 nm, L_2 = 4 nm
Simulation system	microcanonical ensemble(NVE)
Algorithm	velocity-Verlet
Potential for workpiece	EAM potential
Potential for tool	Tersoff potential
Potential between workpiece and tool	Lennard-Jones(L-J) potential
Timestep	1 fs
Initial temperature	293 K
The edge radius of tool(R)	3,4 and 5 nm
Cutting speed(v)	50,100,200 and 400 m/s
Cutting depth(h)	0.5, 1, 2, 3 and 4 nm
Cutting distance(l)	14 nm