Computational Materials Science 126 (2017) 418-425

Contents lists available at ScienceDirect

Computational Materials Science

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



Molecular dynamics simulation on formation mechanism of grain boundary steps in micro-cutting of polycrystalline copper



Dehao Liu^{a,b}, Gang Wang^{a,b,*}, Jianchao Yu^{a,b}, Yiming (Kevin) Rong^{a,c}

^a State Key Laboratory of Tribology & Institute of Manufacturing Engineering, Department of Mechanical Engineering, Tsinghua University, Beijing 100084, China
^b Beijing Key Lab of Precision/Ultra-precision Manufacturing Equipments and Control, Tsinghua University, Beijing 100084, China
^c Mechanical and Energy Engineering Department, South University of Science and Technology of China, Shenzhen 518055, China

ARTICLE INFO

Article history: Received 24 June 2016 Received in revised form 27 September 2016 Accepted 1 October 2016 Available online 22 October 2016

Keywords: Molecular dynamics Micro-cutting Grain boundary steps Sub-grain Polycrystalline copper

ABSTRACT

Three-dimensional molecular dynamics (MD) simulations were performed to investigate the formation mechanism of grain boundary (GB) steps in the micro-cutting of polycrystalline copper. The effects of the GB and misorientation angle on the surface quality were studied. Based on the simulation results, the surface maximum peak-to-valley height of polycrystalline copper was greater than that of single crystal copper owing to the formation of grain boundary steps. The dislocations continuously nucleated on the tool-workpiece interface were stopped and piled up at the GB. As the dislocations piled up at the GB, the dislocations became aligned and formed the sub-grain boundary to minimize the total system energy. Sub-grains with transitional crystal orientations formed at the GB during the micro-cutting of polycrystalline copper for the plowing of the cutting edge and crystal rotation. The misalignment in the slip directions between sub-grains and original grain resulted in the grain boundary step. A peak cutting force appeared at the GB in the cutting of polycrystalline owing to the geometrical hardening effects. It is revealed that the GB has a strong effect on the surface quality of a workpiece during the micro-cutting process.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

In recent years, a highly efficient machining method called micro-cutting has been developed to produce high-accuracy miniaturized components, which are widely used in various industries, including electronics, aerospace, automotive, biomedical engineering and communications [1]. The cutting mechanism of micro-cutting is very different from that of conventional cutting because of size effects [2]. The schematic diagram of micro-cutting is shown in Fig. 1. Many materials cannot be regarded as homogeneous and isotropic in machining when the depth of cut is on the same order as the tool edge radius [3]. In addition, unlike single crystals, polycrystalline materials are composed of grains with different crystallographic orientations and grain boundaries, and the microstructure of a workpiece containing interstitial atoms, voids and dislocations has a strong effect on the cutting mechanism [4,5].

E-mail address: gwang@tsinghua.edu.cn (G. Wang).

The properties of grain boundaries have been extensively researched because of their significant effects on the mechanical behavior of materials [6,7]. The classical Hall-Petch relationship is commonly used to describe the hardening effect of grain boundaries in single-phase polycrystalline materials. At the micrometer scale, it is a challenge to research the mechanical behavior of grain boundaries. It was found that the nanohardness in the vicinity of grain boundaries increased by a factor of 1.5 compared with nanohardness inside the grains via nanoindentation tests of annealed and electropolished high-purity copper [8]. Therefore, the elasticity modulus of grain boundaries could be higher than that of the grain. The frictional coefficient at grain boundaries is higher than that inside the grains based on molecular dynamics (MD) simulations of nanoscratching of bi-crystal copper [9].

The difference in mechanical properties between grain boundaries and grains has a significant influence on the mechanical behavior of materials during micro-cutting. The formation of grain boundary (GB) steps in micro-cutting of polycrystalline materials has been found by a few researchers. In the micro-orthogonal fly cutting of annealed polycrystalline oxygen-free copper with single-crystal diamond tools, grain boundaries became increasingly obvious on the free surface with increasing depth of cut. However, grain boundaries disappeared when the depth of cut



^{*} Corresponding author at: State Key Laboratory of Tribology & Institute of Manufacturing Engineering, Department of Mechanical Engineering, Tsinghua University, Beijing 100084, China.



Fig. 1. Schematic diagram of micro-cutting.

was reduced to the order of 0.1 μ m [10]. It was observed that the grain boundary step was approximately 20 nm high during the micro-cutting of polycrystalline germanium, which was attributed to the elastic deformation [11]. It was found that the height of grain boundary steps increased with increasing cutting speed in the ultra-precise cutting of beta titanium alloy [12]. Annealing treatment can magnify the difference in mechanical properties between grain boundary steps. During the micro-cutting of original polycrystalline oxygen-free copper and annealed copper with single-crystal diamond tools, the grain boundary step appeared on the machined surface of annealed copper, whereas it was absent on that of original copper, as shown in Fig. 2(a) and (b) [13]. It is notable that the twin boundary step was observed in partial enlarged view Fig. 2(c) using white light interferometer.

However, few efforts have been made to reveal the formation mechanism of the grain boundary step. Because it is difficult to observe the dynamic formation process of grain boundary steps in micro-cutting in situ using current experimental methods, simulations provide insights into the potential cutting mechanism and

formation of grain boundary steps. Komanduri made a review of the MD simulations of machining at the atomic scale [14]. Ye et al. has performed MD simulations of the nanometric cutting of single-crystal copper were performed with the embedded atom method (EAM) potential [15]. Pei et al. performed large-scale MD simulations with the model size up to 10 million atoms to study materials deformation in nanometric cutting of single crystal copper [16]. The mechanics of nanometric cutting were investigated with the aid of MD modelling and simulations, which were compared with the results of cutting trials of single crystal silicon on an AFM [17,18]. During cutting of single crystal and polycrystalline copper with a rigid diamond tool through MD simulations, smaller cutting forces were required to machine the polycrystalline structure than the single crystal structure [19]. Based on MD simulations results of scratching polycrystalline Cu for investigating plastic deformation mechanism, both dislocations and GB play a significant role in affecting plastic deformation [20]. Stressinduced crystallization of amorphous was observed in nanocutting process of crystalline copper through MD simulations [21]. The effects of pore and second phase particle on the subsurface damage and surface integrity during machining pore copper materials were also investigated using MD simulations [22]. However, no obvious grain boundary steps were found in the simulation on cutting of polycrystalline copper. Shimada used MD simulations to study the ultimate surface quality of a workpiece in diamond micro-cutting of copper. In the cutting of polycrystalline copper, the dislocations were stopped and piled up at the GB; meanwhile, a sub-grain was generated by the rotation of the grain plane. A tiny grain boundary step was observed on the surface of polycrystalline copper; however, the height of the step was at the same level as that of single crystal copper [23]. MD simulations of micro-cutting of polycrystalline silicon carbide were performed to investigate the microstructure effects on cutting forces. The grain boundary step and variations of cutting forces were observed in the simulation, which could be attributed to



(a) original pure copper

(b) annealed pure copper



(c) twin boundary step

Fig. 2. Machined surface of polycrystalline in white light interferometer.

elastic deformation [24]. However, elastic deformation cannot account for the peak at the GB as shown in Fig. 2(b). The real formation mechanism of the grain boundary step has not been fully revealed.

In this work, MD simulations were used to probe into the formation mechanism of the grain boundary step in micro-cutting of polycrystalline copper. This study will help explain the mechanical behavior and accommodation of grain and grain boundaries in microscale plastic deformation, especially the change of surface integrity in micro-cutting.

2. Methodology

Compared with other simulation techniques, such as the finite element method (FEM), MD simulation is an effective and promising tool to address many machining problems at the atomic scale [14]. MD simulations are performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Plimpton [25]. Fig. 3 presents the MD simulation model of micro-cutting of polycrystalline copper. The model comprises a face-centered cubic (FCC) pure copper workpiece and a rigid diamond tool. Table 1 shows the computational parameters used in the MD simulations. The workpiece contains three types of atoms: boundary atoms, thermostat atoms and Newtonian atoms. The velocity Verlet algorithm is used to integrate Newton's equations of motion with a time step of 1 fs. The eight layers of boundary atoms at the left and the bottom of the workpiece are kept fixed in space to reduce the edge effect. The next eight layers of atoms close to the boundary atoms are thermostat atoms. In these layers, the velocities of atoms are reset by explicitly rescaling their velocities for every specific time step using isokinetic thermostat to stabilize the temperature and dissipate the heat produced by plastic deformation in cutting. The bulk temperature of the workpiece is maintained at room temperature (293 K). Periodic boundary conditions are applied in the Z-direction to reduce the effects of simulation scale.

The crystal setup of the workpiece is described with combinations of the cutting plane and cutting direction in the form of (hkl)[uvw] [26]. In this work, the model including two grains of different orientations is used to simulate the micro-cutting of polycrystalline copper. For bi-crystal copper, the microstructure of a symmetrical tilt grain boundary (STGB) existing between grain *A* and grain *B* is set up with the Coincidence Site Lattice (CSL) model [27]. According to the CSL model, the grain boundary is expressed



Fig. 3. Model of micro-cutting of polycrystalline copper for MD simulation.

Table 1

Computational parameters used in the MD simulations.

Configuration	3-D ortho	3-D orthogonal cutting	
Work material	Single-cry	Single-crystal copper, bi-crystal	
	copper	copper	
Workpiece dimension	200a × 12	200a $ imes$ 120a $ imes$ 3a (a = 3.615 Å, lattice	
	constant o	constant of Cu)	
Crystal setup of workpiece	No. of	Corresponding grain	
	atoms	boundary	
$(\overline{1}30)[\overline{3}\overline{1}0]$ (single crystal)	287,871	N/A	
$(\bar{1}40)[\bar{4}\bar{1}0]-(140)[\bar{4}10]$	288,267	$\sum 17(410)28.07^{\circ}/[001]$ STGB	
$(\bar{1}30)[\bar{3}\bar{1}0]-(130)[\bar{3}10]$	287,922	$\sum 5(310)36.87^{\circ}/[001]$ STGB	
$(\bar{2}50)[\bar{5}\bar{2}0]-(250)[\bar{5}20]$	287,820	$\sum 29(520)43.60^{\circ}/[001]$ STGB	
The distance of GB from the left end of workpiece	37 nm		
Tool material	Diamond		
Number of atoms in tool	4479		
Tool edge radius	3.615 nm		
Tool rake angle	0 °		
Tool clearance angle	5°		
Depth of cut	14.46 nm		
Cutting length	54 nm		
Cutting speed	20 m/s		
Time step	1 fs		
Bulk temperature	293 K		
Potential used	EAM pote	EAM potential, Morse potential	

 $(D = 0.087 \text{ eV}, \alpha = 5.14 \text{ Å}^{-1}, r_0 = 2.\overline{05 \text{ Å})}$

in the form of $\sum n(hkl)\theta/[uvw]$, where $\sum n$ represents the density of coincidence sites, (hkl) is the crystal orientation, θ is the misorientation angle, and [uvw] is the rotation axis. For instance, if the z orientation of the workpiece is [001] and the x orientation of grain A is [310], then the STGB of bi-crystal copper can be expressed as $\sum 5(310)36.87^{\circ}/[001]$, and the crystal set-up of the workpiece is $(\bar{1}30)[\bar{3}\bar{1}0] - (130)[\bar{3}10]$.

There are three types of atomic interactions in the MD simulations. The embedded atom method (EAM) potential is used to describe the Cu-Cu interaction between copper atoms in the workpiece because the EAM potential is the most widely used interatomic potential for metals and alloys [28]. For EAM potential, the total energy E_i of an atom i is given by

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

where *F* is the embedding energy, which is a function of the atomic electron density ρ , ϕ is the potential interaction of a pair, and α and β are the element types of atoms *i* and *j*, respectively.

The tool is regarded as a rigid body in the simulations because the diamond is much harder than the copper. Therefore, the C-C interactions between carbon atoms in the tool are ignored.

Since there are not available EAM potential for Cu-C interaction, Morse potential was adopted, which has been widely used in cutting simulations of copper [20,21,29–31]. The Morse potential is expressed as

$$\phi(r_{ij}) = D(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)})$$
(2)

where $\phi(r_{ij})$ is the potential energy function of a pair, *D* is the cohesive energy, α is the elastic modulus, and r_{ij} and r_0 are the instantaneous and equilibrium distances between atoms *i* and *j*, respectively.

At the beginning of each simulation, random velocities are initially assigned to the atoms, and then the system is relaxed for 60 ps using the Nose-Hoover thermostat in a constant NPT ensemble. After the relaxation, the cutting simulation is conducted in a constant NVE ensemble, meaning that the moles N, the volume V, and the energy E of the system, remain constant in the cutting process. The total simulation time of the cutting is 3000 ps with a time step of 1 fs and a cutting speed of 20 m/s. At the end of cutting, the tool retracts and leaves the surface of the workpiece, which allows the stress to be relieved.

The open source software called OVITO is adopted to visualize the atomic configuration [32]. The Adaptive Common Neighbor Analysis (a-CNA) method developed by Stukowski is used to identify the crystal structure and lattice defects [33]. The a-CNA method provides efficient and unambiguous classification of local atomic arrangements, allowing it to effectively distinguish lattice defects from undisturbed atoms.

3. Results and discussions

3.1. Micro-cutting of polycrystalline copper

A MD simulation of polycrystalline copper was performed to investigate the effects of grain boundaries on the surface quality and cutting forces. The model of the workpiece contained two grains and a symmetrical tilt grain boundary (STGB) of $\sum 29(520)43.60^{\circ}/[001]$. Because $\sum 29(520)$ STGB has a bigger misorientation angle, it helps to illustrate the effect of GB on micro-cutting of polycrystalline copper. The GB was far from the left end of the workpiece to reduce the interference of the fixed boundary layer.

Fig. 4 presents the deformation behavior of polycrystalline copper during the cutting process. The discussions of the results are based on the MD simulation snapshots and the observation of the animations of the cutting process. Because copper is a face-centered cubic (FCC) crystal, the dislocations in the deformed layer of grain *B* were propagated along the $\langle 1 1 0 \rangle$ direction (close-packed direction) on the $\{111\}$ planes (close-packed direction) as shown in Fig. 4(a). Meanwhile, some dislocations were generated and emitted from the GB. The dislocations continuously nucleated on the tool-workpiece interface in grain *B* were stopped and piled up at the GB as shown in Fig. 4(b). As the dislocations piled up at

the GB, the dislocations became aligned and formed the subgrain boundary to minimize the total system energy [34]. Meanwhile, slippage of material in grain A contributed to the formation of the sub-grain boundary. Therefore, the cessation of dislocations and slippage of material resulted in the formation of sub-grains. It was observed that sub-grain C rotated around the z-axis in an anticlockwise direction owing to the plowing of the cutting edge. With the progress of the cutting edge, the orientation of sub-grain C approached that of grain A. It should be noted that the misalignment between the slip directions of sub-grains C and D resulted in the grain boundary step. After the cutting edge passed the GB, new dislocations were generated in grain A and penetrated into the workpiece. Finally, when the cutting edge left the workpiece, as Fig. 4(d) shows, most dislocations annihilated when moving toward the surface, contributing to the grain boundary step.

After the stress relief of the workpiece, an obvious grain boundary step was observed on the machined surface of polycrystalline copper. The height of the grain boundary step was approximately 20 Å. Most defects were stored in the vicinity of the GB, whereas the other parts of the workpiece were nearly a perfect lattice structure.

Fig. 5 shows the variations of cutting forces during the cutting of polycrystalline copper. The first peak cutting force was caused by the resistance to nucleation and propagation of dislocations. After dislocations began to propagate, the cutting forces decreased rapidly. The blocking effect of the fixed boundary layer to the left of the workpiece accounted for the final peak in the cutting forces. A peak cutting force appeared at the GB, which could be caused by the geometrical hardening effect. Because the crystal orientation of sub-grain C approached that of grain A during the cutting process, the Schmid factor of sub-grain C changed as well, which determines the stress applied to the material when slippage occurs in the primary slip system. Therefore, slipping in the workpiece became more difficult, and cutting forces increased. The peak cutting force at the GB correspond to the experimental discovery in the micro-cutting of polycrystalline Al-alloy [4]. The peak cutting force at the GB can magnify the vibration of the tool during the cutting process, contributing to the grain boundary step.



Fig. 4. Deformation behavior of polycrystalline copper during the micro-cutting process at cutting distances of (a) 2 nm, (b) 19 nm, (c) 37 nm and (d) 54 nm.



Fig. 5. Variations of cutting forces during cutting of polycrystalline copper.

3.2. Micro-cutting of single crystal copper

A MD simulation of single crystal copper was performed for comparison with polycrystalline copper. Fig. 6 shows the representative MD simulation snapshots of single crystal copper cut in the direction of $[\bar{3}\bar{1}0]$ on the $(\bar{1}30)$ plane.

As shown in Fig. 6, with the advancement of the tool, complicated deformation of the workpiece occurred around the cutting edge. Some lattice defects were produced during the microcutting process, including point defects, dislocations and stacking faults. Many dislocations nucleated on the surface moved downward and penetrated into the workpiece as shown in Fig. 6(c). In Fig. 6(d), after the passing of the cutting tool, most of penetrated dislocations annihilated when moving toward the surface because of the relaxation in the workpiece. Most of penetrated dislocations will annihilate after enough time to relax. Because of the stress relief, atomistic steps formed on the surface of the workpiece. It should be noted that some small parts of the workpiece rotated around the z-axis and formed sub-grains on the surface of workpiece edge owing to the severe plastic deformation of the workpiece.

The machined surface of single crystal copper is rather smooth with a maximum peak-to-valley height of 10 Å. There are small lattice defects that remain on the surface of single crystal copper, making it a near-perfect lattice structure. Compared with single crystal copper, the maximum peak-to-valley height of the machined surface of polycrystalline copper is larger. The grain boundary step appears on the surface of the polycrystalline copper, whereas it was absent on that of single crystal copper.

There were some fluctuations in the cutting forces during the cutting process as shown in Fig. 7(a), which was quite different from that of polycrystalline copper. The periodic fluctuations of cutting forces could be caused by the cycles of formation and disappearance of dislocations, which is known as the stick-slip phenomenon in tribology as shown in Fig. 7(b) [35]. Atomic-scale stick-slip was associated with dislocation nucleation and propagation. The cutting forces increased during the elastic deformation until dislocations began to form, and then they decreased abruptly after the formation and movement of dislocations because of plastic yielding. When dislocations moved toward the surface and annihilated, a new cycle of movement of dislocations began.

3.3. Effects of misorientation angle

MD simulations of polycrystalline coppers with different grain boundaries were performed to investigate the effects of the misorientation angle on the surface quality and cutting forces as shown in Fig. 8. It was common that dislocations were stopped and piled up at grain boundaries. Sub-grains were formed in the vicinity of grain boundaries with different transitional crystal orientations. The lattice defects were stored close to the GB. The grain boundary step can be identified on the surfaces of the workpiece.

Table 2 summarizes the results of single crystal and polycrystalline copper, including maximum peak-to-valley height, averaged cutting force.

The results show that the surface maximum peak-to-valley height of polycrystalline copper was greater than that of single crystal copper owing to the formation of the grain boundary step.



Fig. 6. Deformation behavior of single crystal copper during the micro-cutting process at cutting distances of (a) 2 nm, (b) 19 nm, (c) 37 nm and (d) 54 nm.



Fig. 7. Variations of cutting forces caused by stick-slip during machining of single crystal copper.



Fig. 8. Machined surface of polycrystalline copper with grain boundaries of (a) $\sum 17(410)28.07^{\circ}/[001]$, (b) $\sum 5(310)36.87^{\circ}/[001]$ and (c) $\sum 29(520)43.60^{\circ}/[001]$.

Table 2	
Comparison of results of single crystal and polycrystalline copper.	

Work material	Maximum peak-to- valley height (Å)	Averaged cutting force (nN)
Single crystal copper (310) Polycrystalline copper $\sum 17(410)$ Polycrystalline copper $\sum 5(310)$ Polycrystalline copper $\sum 29(520)$	10 16 19 20	63 69 61 57

The misorientation angle had an obvious effect on the maximum peak-to-valley height of polycrystalline copper. The averaged cutting force of polycrystalline copper $\sum 5(310)$ was smaller than that of single crystal copper (310) because single crystal copper has less lattice defects and higher mechanical strength. The averaged cutting force changed little with increasing misorientation angle.

3.4. Formation of grain boundary steps

Based on the MD simulation results of micro-cutting of polycrystalline copper, the formation mechanism of grain boundary steps was investigated, which can be illustrated in Fig. 9. With the advancement of the tool, in Fig. 9(a), the dislocations continuously nucleated on the tool-workpiece interface in grain *B* are stopped and piled up at the GB because of the geometrical discontinuity between grain *A* and grain *B*. As the dislocations piled up at the GB, the dislocations become aligned and form the sub-grain boundary for reaching the minimization of energy. Owing to the plowing of the cutting edge, sub-grain *C* rotates around the z-axis in an anti-clockwise direction, allowing the orientation of sub-grain *C* to approximate that of grain *A*. The misalignment in the slip directions between sub-grains *C* and *D* results in the grain boundary step as shown in Fig. 9(b). After the cutting edge passed the GB, new dislocations were generated in grain *A* and penetrated into the



Fig. 9. Schematic diagram of formation of the grain boundary step: (a) generation of dislocations, (b) formation of sub-grain, and (c) stress relief.

workpiece. Finally, when the cutting edge left the workpiece, as Fig. 9(c) shows, sub-grain *C* rotated slightly in a clockwise direction because of the stress relief. Most dislocations annihilated when moving toward the surface, contributing to the grain boundary step.

4. Discussions

The experiments adopted Single Point Diamond Turning (SPDT) technique while the depth of cut was at the micrometer scale. However, due to the limitation of high computational cost, the model in this work is not as realistic as actual experiments. The depth of cut in simulations is at the nanometer scale (\sim nm) rather than the micrometer scale ($\sim \mu m$). The size of the workpiece in simulations was enlarged to approach the actual conditions in experiments. The formation of grain boundary steps is assumed to be a kind of local phenomenon, which is more related with the property of grain boundary and movement of dislocations. The size of grains or workpiece is not the predominant reason for the formation of grain boundary steps. Due to the high computational cost, the width of workpiece is small (~nm). However, the grain boundary steps are about 40-60 nm high based on the experimental observation, which is much smaller than grain size and the length of grain boundary ($\sim \mu m$). Therefore, the formation of grain boundary steps is assumed to be a local phenomenon in a twodimensional way, and more related with depth of cut and cutting length. The width of workpiece has less to do with the formation of grain boundary steps. Periodic boundary conditions are applied in the direction of width (Z-direction) to reduce the effect of simulation scale. The cutting speed (20 m/s) is much higher than the real one, which is several meters per second. Therefore, the height of the grain boundary step (\sim Å) is difficult to verify with the actual one $(\sim nm)$ in the experiment.

When the cutting edge was cutting in the interior of the left grain, boundary layer on the left side did affect cutting forces, which was difficult to avoid. The blocking effect of the fixed boundary layer on the left side accounted for the final peak of cutting forces. This is not corresponded with actual experimental results. However, when the cutting edge was passing the grain boundary, boundary layer on the left side had little effects on the formation of grain boundary steps. The formation of grain boundary steps is the focus, which was related with the property of grain boundary and movement of dislocations. It can be seen in Fig. 5 that the cutting force fluctuates when the cutting edge crosses the grain boundary even there is some effect from fixed boundary layer.

5. Conclusions

In this paper, Molecular Dynamics (MD) simulations were conducted to investigate the formation process of grain boundary steps in micro-cutting of annealed polycrystalline copper. This study provides insights into the formation mechanism of grain boundary steps in micro-cutting of polycrystalline material. It also helps explain the mechanical behavior and accommodation of grains and grain boundaries in microscale plastic deformation, especially the change in surface integrity in micro-cutting. It was found that sub-grains with transitional crystal orientations formed at the grain boundary owing to the plowing of the cutting edge and crystal rotation. The effects of the GB and misorientation angle on the surface quality are investigated. Based on the simulation results, conclusions are given as follows.

- (1) The dislocations continuously nucleated on the toolworkpiece interface were stopped and piled up at the GB. As the dislocations piled up at the GB, the dislocations became aligned and formed the sub-grain boundary to minimize the system energy. Sub-grains with transitional crystal orientations formed at the GB owing to the plowing of the cutting edge and crystal rotation. The misalignment in the slip directions between sub-grains and original grain resulted in the grain boundary step.
- (2) A peak cutting force appeared at the GB in cutting of polycrystalline copper because of the geometrical hardening effects. The variations in cutting forces at the GB could increase the vibration of the tool and contribute to the formation of grain boundary steps. The periodic fluctuations of cutting forces in the cutting of single crystal copper could be caused by the cycles of formation and disappearance of dislocations, which is known as the stick-slip phenomenon.
- (3) The surface maximum peak-to-valley height of polycrystalline copper is greater than that of single crystal copper. The misorientation angle had an obvious effect on the maximum peak-to-valley height of polycrystalline copper. When the misorientation angle increases from 28.07° to 43.06°, the range of maximum peak-to-valley height is 16–20 Å.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Project 51575305) and Beijing Natural Science Foundation (Project 3152013).

References

- [1] J. Chae, S.S. Park, T. Freiheit, Int. J. Mach. Tools Manuf. 46 (2006) 313-332.
- [2] D. Dornfeld, S. Min, Y. Takeuchi, CIRP Ann. Manuf. Technol. 55 (2006) 745-768.
- [3] K. Nakayama, K. Tamura, J. Eng. Ind. 90 (1968) 119–126.
- [4] Y. Furukawa, N. Moronuki, CIRP Ann. Manuf. Technol. 37 (1988) 113–116.

- [5] M. Sato, Y. Kato, K. Tsutiya, Trans. Jpn. Inst. Met. 20 (1979) 414–422.
- [6] J.P. Hirth, Metall. Trans. 3 (1972) 3047-3067.
- [7] R.Z. Valiev, V.Y. Gertsman, O.A. Kaibyshev, Phys. Status Solidi 97 (1986) 11–56.
- [8] Y. Soifer, A. Verdyan, M. Kazakevich, E. Rabkin, Scr. Mater. 47 (2002) 799-804.
- [9] K. Sun, L. Fang, Z. Yan, J. Sun, Wear 303 (2013) 191–201.
 [10] T. Moriwaki, CIRP Ann. Manuf. Technol. 38 (1989) 115–118.
- [11] J. Yan, Y. Takahashi, J. Tamaki, A. Kubo, T. Kuriyagawa, Y. Sato, JSME Int. J. Ser. C 49 (2006) 63-69.
- [12] H. Yasui, A. Shinozaki, A. Toyama, S. Sakamoto, Y. Kajiwara, in: 21st Annu. Meet. Am. Soc. Precis. Eng, 2006, pp. 1-4.
- [13] J. Yu, G. Wang, Y. Rong, Procedia Manuf. 1 (2015) 655–662.
- [14] R. Komanduri, L.M. Raff, Proc. Inst. Mech. Eng. Part B J. Eng. Manuf. 215 (2001) 1639-1672.
- [15] Y.Y. Ye, R. Biswas, J.R. Morris, A. Bastawros, A. Chandra, Nanotechnology 14 (2003) 390-396.
- [16] Q.X. Pei, C. Lu, H.P. Lee, Y.W. Zhang, Nanoscale Res. Lett. 4 (2009) 444-451.
- [17] K. Cheng, X. Luo, R. Ward, R. Holt, Wear 255 (2003) 1427–1432.
- [18] X. Luo, K. Cheng, X.J. Guo, R. Holt, 41 (2007) 1449-1465, http://dx.doi.org/10. 1080/0020754031000069607.
- [19] J. Shi, M. Verma, Mater. Manuf. Process. 26 (2011) 1004-1010.
- [20] J. Li, B. Liu, H. Luo, Q. Fang, Y. Liu, Y. Liu, Comput. Mater. Sci. 118 (2016) 66-76.

- [21] Y. Zhao, X. Wei, Y. Zhang, J. Wang, D. Huo, J. Non. Cryst. Solids 439 (2016) 21-29
- [22] J. Li, Q. Fang, B. Liu, Y. Liu, Appl. Surf. Sci. 384 (2016) 419-431.
- [23] S. Shimada, N. Ikawa, H. Tanaka, J. Uchikoshi, CIRP Ann. Manuf. Technol. 43 (1994) 51-54.
- [24] S. Venkatachalam, O. Fergani, X. Li, J. Guo Yang, K.-N. Chiang, S.Y. Liang, J. Manuf. Sci. Eng. 137 (2015) 21020.
- [25] S. Plimpton, J. Comput. Phys. 117 (1995) 1-42.
- [26] R. Komanduri, N. Chandrasekaran, L.M. Raff, Wear 242 (2000) 60-88.
- [27] D. Brandon, Acta Metall. 14 (1966) 1479-1484.
- [28] M.I. Mendelev, A.H. King, Philos. Mag. 93 (2013) 1268-1278.
- [29] J. Zhang, T. Sun, Y. Yan, Y. Liang, S. Dong, Appl. Phys. A Mater. Sci. Process. 94 (2009) 593-600.
- [30] Q.X. Pei, C. Lu, H.P. Lee, Comput. Mater. Sci. 41 (2007) 177-185.
- [31] Q.X. Pei, C. Lu, F.Z. Fang, H. Wu, Comput. Mater. Sci. 37 (2006) 434-441.
- [32] A. Stukowski, Model. Simul. Mater. Sci. Eng. 18 (2009) 15012.
- [33] A. Stukowski, Model. Simul. Mater. Sci. Eng. 20 (2012) 45021.
- [34] N.R. Tao, Z.B. Wang, W.P. Tong, M.L. Sui, J. Lu, K. Lu, Acta Mater. 50 (2002) 4603-4616.
- [35] M.H. Cho, S.J. Kim, D.S. Lim, H. Jang, Wear 259 (2005) 1392-1399.