Generation Mechanism and Dual Dynamic Simulations of Surface Patterns in Single-Point Diamond Turning of Single-Crystal Copper

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Title page

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ORIGINAL ARTICLE

Generation mechanism and dual dynamic simulations of surface patterns in single-point diamond turning of single-crystal copper

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Abstract: Single-crystal copper (Cu), whose atom arrangement is in the same direction and has no grain boundary, is widely used in defense technology, civil electronics and network communication. As a diamond turnable material, fan-shaped patterns appear on the machined surface, which affects the machined surface quality and the optical function it carries. Previous studies on the surface generation mechanism in single-point diamond turning (SPDT) of Cu were limited to experimental analysis, while there is a lack of fundamental understanding of the fan-shaped pattern generation mechanism and suppression method. In the present study, the different fan-shaped patterns, surface quality, cutting force and chip morphology of the typical crystal planes (100), (110) and (111) planes of Cu were studied by both theoretical and experimental analyses. A molecular dynamics (MD) simulation was conducted to present the fundamental generation mechanism of the fan-shaped patterns from atom arrangement directions and its angle change with the main cutting direction, while a cutting dynamics model was established to simulate the generation of fan-shaped patterns on the machined surface. Based on theoretical and experimental analysis, it was found that the atom density arrangement directions of Cu and its angle change with

the main cutting direction of SPDT caused fluctuations in the friction coefficient, which further caused the vibration of the cutting system and generated the fan-shaped patterns. The SPDT of crystal planes (100) can achieve the best surface quality. The present research provides a fundamental understanding of fan-shaped pattern formation on the machined surface, and provides an instruction for machining Cu to obtain better surface quality.

Keywords: Single-point diamond turning • Single-crystal copper • Anisotropy • Molecular dynamic simulation • Cutting dynamics • Surface generation

1 Introduction

In recent years, with the rapid development of semiconductors, integrated circuits and optical technology, ultra-precision machining technology has attracted increasing attention in the fields of optics, micro/nano sensors and micro/nano electromechanical systems [1-3]. With the increasing demand for high-speed, convenient and high-fidelity optical electronic components, this has placed increasing demands on the performance of conductor materials. Ordinary polycrystalline materials have been difficult to meet this requirement [4], while single-crystal materials have wide application prospects [5, 6], which eliminates the lateral grain boundary and the electrons can move without obstacles [7], so that it has good fidelity performance and high-speed propagation performance.

Some single-crystal materials have almost no ductility in traditional machining, with hard and brittle characteristics, while single-point diamond turning (SPDT) can make single-crystal materials in ductile domain machining [8, 9]. Because of the high cost of diamond tools, in the case of

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ensuring the surface quality of single-crystal workpieces in SPDT, it is also necessary to improve the wear resistance of diamond tools, which makes the research on single-crystal materials and diamond tools endless. For example, Chao et al. used different geometric dimensions of diamond tools to turn single-crystal silicon [10]. The results showed that under the same machining conditions, the use of the round nose tool could accelerate the wear of the tool and reduce the surface finish of the workpiece, while the use of the sharp tool could obtain a smooth machining surface with a roughness of approximately 5 nm, and the tool had no obvious wear. Therefore, tool wear can be reduced and workpiece surface finish can be improved by changing the tool geometry. To further investigate the wear resistance of different face diamond tools, Uddin et al. used single-crystal diamond tools to perform nanometer-scale ductile cutting of single-crystal silicon [11], and the results showed that the wear of the diamond tool mainly occurred on the flank face of the tool. When the crystal orientation of the tool rake face was $\{110\}$, the wear resistance and life of the tool were better than those of $\{100\}$ or $\{111\}$. Fang et al. proposed a new method of ion implantation surface modification for cutting single-crystal silicon [12]. This method could change the mechanical properties of the surface layer of the material, reduce the surface fracture, prolong the tool life, and improve the machining efficiency. Through theoretical analysis, Goel et al. used molecular dynamics (MD) simulations to study the plasticity mechanism of single-crystal silicon during cutting [13]. If the tool was inclined to the surface at an angle of $45^\circ - 55^\circ$, a periodic nanogroove array would be formed on the single-crystal silicon surface. Lai et al. used MD simulation and experimental methods to study the nano-cutting experiments of single-crystal germanium under different feed rates [14]. The results showed that the tool was deposited on the edge of the tool edge. The lateral flow material was the decisive factor affecting the surface topography. A defective crystal structure was observed in many areas of the machined surface rather than an amorphous germanium and the nano-cutting of partially overlapping single-crystal germanium could obtain a machining surface with little or no damage to amorphous damage. In the case of single-crystal metals, Kota et al. experimented and modeled single-crystal aluminum materials [15]. The results showed that when the single-crystal aluminum was turning, the subsurface damage layer was deep, reaching a depth equivalent to the thickness of the uncut chip. Lee et al. studied the cutting properties of single-crystal copper (Cu) under different

cutting conditions. The experimental results shown that the chip thickness and shear angle varied with the changing of crystal orientation of the cutting material, the surface roughness of the workpiece changes periodically and chose appropriate feed rate the anisotropy of surface roughness could be minimized [16]. Furthermore, Demir applied microplastic theory to predict the force and surface quality produced by the anisotropy of the mechanical properties of Cu [17]. The results show that as the milling chip pocket rotates, the shear angle changes as the crystal orientation of the cutting material changed. Lin and Shiu used MD simulations to study the slotting behavior of Cu with different crystal orientations in diamond cutting. The simulation results showed that a suitable rectangular groove could be obtained by slotting in Cu(101) along $[0\bar{1}0]$ direction, but slotting in Cu(101) along $[\bar{1}01]$ direction would result in a "V" shaped section groove [18]. Xiao et al. studied the material removal mechanism and surface formation of Cu during dynamic plowing through experiments and MD simulations, and compared it with static plowing. It has been found that dynamic plow removal was mainly due to the downward and lateral sliding of the workpiece material on the sliding surface and subsequent elastic recovery, while forward and lateral sliding were the causes of static plowing. The amount of chipping of dynamic plowing was small, while the amount of chipping of static plowing was obvious. The average machining force in dynamic plowing was significantly less than that of static plowing, which meant that the wear of the AFM tip could be reduced by using dynamic plowing because the tip wear was largely affected by the amount of machining force [19]. It can be found from the above that the research on SPDT of single-crystal materials is mainly focused on silicon, germanium and other semiconductor materials, while research on Cu and other metal materials is relatively less, and simulation is the main one, while research on SPDT of Cu is not always scarce.

Based on the experiment, this paper studies the cutting performance and surface production mechanism of Cu by SPDT, and collects the cutting force signal during the cutting process, and then uses MD simulation to imitate. The surface quality of different crystal orientations was studied using a combination of numerical and experimental methods. In addition, the friction coefficient and atomic sliding process in the process of material deformation were studied by simulation, which revealed the material removal mechanism of different crystal orientations, which provides a useful reference for its practical application in nanofabrication.

2 Experiments

In this research, the turning experiments were performed on the ultra-precision lathe (Moore Nanotechnology Systems, Swanzey, NH, USA), and the experimental setup is shown in Figure 1. SPDT experiments were performed on three Cu workpieces with typical crystal planes, (100), (110) and (111) respectively, as shown in Figure 1 (b). During the turning experiment, the workpieces were pasted to a cylindrical rod which was then fixed on spindle through a fixture and the vacuum chuck. A diamond tool with a rake angle of 0° , a clearance angle of 15° and a nose radius of 0.502 mm was used for turning. A dynamometer was employed during the turning process to capture the cutting force signal. In order to meet the rigidity requirements, the Kistler 9017C dynamometer (Kistler, Winterthur, Switzerland) was used in the force acquisition, which was preloaded to 7 kN to meet the rigidity requirement, as shown in Figure 1 (c). The cutting tool and the experimental parameters are listed in Table 1. In the experiment, Cu (100), (110) and (111) were roughed turning first and then finished, during the turning, the dynamometer collects the force signal first, and then a charge amplifier is used to amplify and output the force signals to the data collector, and then the force data is transmitted to Kistler bonded Dyno Ware software for time domain analysis and frequency domain analysis, as shown in Figure 2. The collected chips were observed by environmental scanning electron microscope (ESEM Quanta 450 FEG, Field Electron and Ion Company, Hillsboro, OR, USA). The machined surface topography and quality was observed by a white light interferometer (Contour GT-X, Bruker, Billerica, MA, USA).

Figure 1 Experimental setup

Figure 2 Capturing and processing system for cutting force signal

Table 1 Cutting parameters employed in the experiments

Tool material	Diamond
Tool rake angle	0°
Tool clearance angle	15°
Tool nose radius	0.502 mm
Workpiece material	Cu
Workpiece dimension	$10 \times 10 \times 2 \text{ mm}^3$
Crystal plane	(100), (110), (111)
Spindle rate	2000 rpm
Feed rate	5 mm/min
Cut depth	4 μm

3 Results and discussion

It could be seen that there were three or four fan-shaped patterns on the surface of the Cu after experiments. Figure 3 (a) shows the surface topography of Cu (100), which can be observed with four cloudy regions (2, 4, 6 and 8) and four clean regions (1, 3, 5, and 7). The areas of each region are equal, and the cloudy regions and clean regions are alternately distributed, eventually forming four quadruple-symmetric fan-shaped patterns on the surface. Figure 3 (b) shows the surface topography of the Cu (110), which can be observed to have four cloudy regions (1, 3, 5, and 7) and four clean regions (2, 4, 6, and 8). However, the areas of the four cloudy regions are different. There are areas of two large cloudy regions and two small cloudy regions, where the areas of the 1- and 5-region are equal, and the areas of the 3- and 7-region are equal. The areas of the cloudy regions (1 and 5) are more than twice the cloudy regions (3 and 7), while the areas of the four clean regions are equal. They are alternately distributed to form four double-symmetric fan-shaped patterns. Figure 3 (c) shows the surface topography of Cu (111), which can be observed with three cloudy regions (2, 4 and 6) and three clean regions (1, 3 and 5). The areas of each region are equal, and the cloudy regions and clean regions are alternately distributed to form three triple-symmetric fan-shaped patterns.

Figure 3 Fan-shaped patterns generated on the surface of (a) (100), (b) (110) and (c) (111) crystal planes of Cu

Fan-shaped patterns on Cu surface affect surface profile and roughness. Figure 4 shows the surface topography and roughness of the (100), (110), and (111) crystal planes of Cu, respectively. As shown in Figure 4 (a), it can be observed that the surface height at the cloudy region of Cu (100) surface is higher than that at the clean region. While it is found from Figure 4 (d), the surface roughness at the cloudy region is relatively large, whose roughness value is about 18 nm, whereas the surface roughness at the clean region is small, with a roughness value about 11 nm. Figure 4 (b) shows the surface profile of Cu (110). It can be observed that the cloudy regions with bigger fan area have the highest surface height, while the surface height on cloudy regions with smaller fan area follows, and the clean regions own the lowest surface height. From Figure 4 (e), it can be found that the surface roughness at the two big cloudy fan regions is the largest, with a value of about 40 nm, while the roughness at the two small cloudy fan regions follows, with a value of about 30 nm, the surface roughness at the four clean regions is smaller, with a value of about 20 nm. Figure 4 (c) shows the surface profile of the Cu (111), it is found that the surface height at the three cloudy fan regions is relatively high, while it is lower at the three clean fan regions. Similarly, from Figure 4 (f), the surface roughness at the three cloudy fan regions is relatively large, whose value is about 35 nm, while the surface roughness at the three clean fan regions is small, with a value of about 11 nm. Therefore from the comparison of the three crystal planes, it can be found that the surface quality of the Cu (100) is the best, with a value of 15.433 nm. The surface quality of the Cu (111) follows, its surface roughness value is 17.016 nm. The surface quality of the Cu (110) is the worst, with a surface roughness value of 20.102 nm. Figure 5 (a), (b) and (c) present the topography of the three zones (A, B and C) of the Cu (110) in Figure 4(b), respectively. It can be observed from Figure 5(a) that the surface fluctuation of the A zone is the largest, and the peak to valley height is 160 nm. The B zone follows, and the peak to valley height is 120 nm, as shown in Figure 5(b). The surface fluctuation at C zone is the smallest, and the peak to valley height is 90 nm, as shown in Figure 5(c). Comparing the surface

quality of three zones, it can be found that the surface quality at the clean fan region (C zone) is the best.

Figure 4 Surface topographies and roughness changes as turning (a, d) (100), (b, e) (110) and (c, f) (111) crystal planes

Figure 5 Surface topographies of (a) A, (b) B and (c) C zones on (110) crystal plane (as indicated in Figure 4)

The material properties can be reflected in chip morphology. By observing the chips of different crystal planes in Figure 6, it can be seen that continuous chips can be produced during the cutting process, but the chip morphology is not complete. There is a small crack structure at every interval, which indicates that the strain distribution in the chips is very uneven, and uneven distribution may be caused by the anisotropy of the mechanical properties of Cu. Therefore, cutting along the different crystal orientations of the workpiece will lead to different cutting performance, which causes a significant change in the chips in each crystal orientation, resulting in continuous and cracked chips.

Figure 6 Chip morphologies generated from turning (a) (100), (b) (110) and (c) (111) crystal planes

Cutting force analysis is a significant method to characterize the cutting mechanism of materials. Figure 7

shows the cutting force signal and its power spectrum plot in turning (100), (110) and (111) crystal planes respectively. As shown in Figure 7 (a), it is the force curve in SPDT Cu (100), it is found that the force fluctuates periodically during a turning period, wherein the force peaks 2, 4, 6 and 8 corresponds to the four cloudy regions (2, 4, 6 and 8) in Figure 3 (a), because cloudy cutting leads to the large force and therefore form the force peaks. The force valleys 1, 3, 5 and 7 corresponds to the four clean regions (1, 3, 5 and 7) in Figure 3 (a), because clean cutting generates the stable cutting force. The cutting force fluctuates periodically during a turning period, therefore the rotation frequency in the turning process is 33.3 Hz for given spindle speed 2000 rev/min, owing to the Cu (100) is four quadruple-symmetrically distributed, the force fluctuation frequency should be 133.2 Hz. From the power spectrum analysis of the captured cutting force signal, as shown in Figure 7 (d), it can be seen a power spectrum peak exists at the frequency of 133.3 Hz, which is basically consistent with the calculated value of 133.2 Hz, therefore the power spectrum analysis of cutting force can present the four quadruple-symmetrical distribution of Cu (100). Figure 7 (b) shows the force signal as turning Cu (110). It can be seen that the force fluctuates periodically during a turning period, with large peaks, valleys and small peaks alternating, which is corresponding to the surface fan patterns with 1, 2, 3, 4 in Figure3 (b). Since the frequency of a turning period is 33.3 Hz under spindle speed of 2000 rev/min, and fan patterns are distributed in four-fold and double-symmetrical distribution on Cu (110) plane, therefore the power spectrum peaks exist at the frequency of 66.6 Hz and 133.2 Hz for double-symmetrical and four-fold distribution, respectively. From Figure 7 (e) the power spectrum diagram of captured cutting force signals, two power spectrum peaks at the frequency of 66.75 Hz and 133.3 Hz exist, which are consistent with 66.6 Hz and 133.2 Hz in theoretical, proving the surface fan-patterns cause the regular fluctuation of cutting force. The cutting force signal as turning Cu (111) is shown in Figure 7 (c). It can be seen that the force curve has three peaks and valleys, which corresponds to the three-fold fan patterns 1, 2, 3, 4, 5, 6 in Figure3 (c). Since the frequency of one turning rotation is 33.3 Hz under the given spindle speed, the frequency for turning Cu (111) is 99.9 Hz. As observing the force spectrum analysis as shown in Figure 7 (f), a power spectrum peak with 100 Hz exists, which is consistent with the calculated frequency. Therefore, it is obvious that the cutting force signal and its power spectrum analysis can be used to present the surface fan-pattern of Cu.

Figure 7 Fluctuation of cutting force signals and its PSD plot as turning (a, d) (100), (b, e) (110) and (c, f) (111) crystal planes

4 Cutting dynamic and molecular dynamic simulation

It can be seen from the experiment that the surface morphology, roughness and cutting force of Cus are largely cyclical fluctuations. The main reason is the material anisotropy caused by the change in the crystallographic orientation of the single-crystal material [20]; therefore, this article will study it from macroscopic cutting dynamics and microscopic MD, respectively. A cutting dynamics model was established to predict the effect of the cutting force on the surface morphology, and a MD model was used to study the effect of different crystal orientations on the cutting performance of the workpiece material, as shown in Figure 8.

Figure 8 Flow chart of dual dynamics co-simulations for nano-surface generation

4.1 Cutting dynamic modeling

In ultra-precision cutting of Cu, due to material anisotropy, changes in cutting force, shear angle, surface roughness [21], etc. The change in the cutting force caused by material anisotropy is called material-induced vibration [22]. Because material-induced vibration cannot be eliminated by machine tool design or process control, and this vibration limits the performance of ultra-precision diamond lathes to a large extent, this paper will predict the three-dimensional surface morphology of the workpiece from the cutting force model.

4.1.1 Primary surface simulation

For ultra-precision turning of arc diamond tools, the ideal surface profile of workpiece is shown in Figure 9 (a), and its equation is as follows [23]:

$$R_{th} = \frac{f^2}{8R} \quad (1)$$

where f is the feed rate, R is the tool nose radius, a_p is the cut depth, and R_{th} is the theoretical remaining height (or theoretical surface roughness).

The surface contour within one revolution period is represented by the function $G(x)$. Because the workpiece surface has symmetry, the surface contour can be simplified to a quadratic function, given by the following [24]:

$$G(x) = Ax^2 + C \quad (2)$$

If the lowest point O of the two-dimensional shape is set to zero, the constant term C in the above formula will be omitted. The simplified surface profile function should still meet the boundary conditions, calculated as follows:

$$G\left(\pm \frac{f}{2}\right) = R_{th} \quad (3)$$

Thus, the quadratic coefficient A can be obtained by the following:

$$A = \frac{4R_{th}}{f^2} \quad (4)$$

Figure 9 Schematic of (a) the surface profile and (b) the tool path in turning

As shown in Figure 9 (b), if the center of the simulation area is set as the center of the workpiece machining surface, the coordinates of the (i, j) point in the simulation area can be calculated as follows:

$$\begin{cases} X_{i,j} = i \cdot m_x - \frac{L_x}{2} \\ Y_{i,j} = j \cdot m_y - \frac{L_y}{2} \end{cases} \quad (5)$$

where L_x and L_y represent the length and width of the simulation area, respectively, and m represents the resolution of the simulation area in the X and Y directions, respectively.

In order to facilitate the derivation of the model, the rectangular coordinate system is converted into a polar coordinate system, assuming that the coordinates of a point in the three-dimensional shape are (ρ, θ, Z) . According to the transformation relationship between the rectangular coordinate system and the polar coordinate system, the equation can be obtained as follows:

$$\begin{cases} \rho = \sqrt{X_{i,j}^2 + Y_{i,j}^2} \\ \theta = \tan^{-1}\left(\frac{X_{i,j}}{Y_{i,j}}\right) \end{cases} \quad (6)$$

Then the equivalent angle of this point is obtained by the following:

$$\theta_v = \frac{\theta}{2\pi} \quad (7)$$

The complete cycle number equation that the tool path has experienced before is as follows:

$$N_T = \left\lfloor \frac{\rho}{f} - \theta_v \right\rfloor \quad (8)$$

During the cutting process, the lowest contour line after cutting the cutting edge of the tool constitutes the final shape contour of the machined surface, so it is still

necessary to calculate the equivalent polar diameter of the corresponding point in the previous cycle, current cycle and next cycle. The equations are derived as follows:

$$\begin{cases} \rho_{v-1} = \rho - (N_T - \theta_v - 1)f \\ \rho_v = \rho - (N_T - \theta_v)f \\ \rho_{v+1} = \rho - (N_T - \theta_v + 1)f \end{cases} \quad (9)$$

Thus, the final coordinate value of the surface contour of the point can be obtained as follows:

$$Z_{th} = \min \{G(\rho_{v-1}), G(\rho_v), G(\rho_{v+1})\} \quad (10)$$

Figure 10 shows the simulation results of the two-dimensional and three-dimensional topography under ideal turning conditions.

Figure 10 (a) Two-dimensional sectional curve and (b) three-dimensional morphology of surface simulations

4.1.2 Vibration induced by material

Based on the three-dimensional surface morphology formed under ideal cutting conditions, considering the effect of material-induced vibration on the cutting morphology, a one-dimensional degree-of-freedom cutting system in which the tool is only subjected to cutting force is established. As shown in Figure 11, the cutting system consists of a diamond tool and a Cu workpiece, which can be simplified as a spring-mass-damping system. This article only studies the effect of the relative displacement of the tool by material vibration. Therefore, assuming that the workpiece is a rigid body, the tool is represented by a spring, mass and damping connected in parallel. The equations are derived as follows:

$$\begin{cases} \frac{d^2 Z(t)}{dt^2} + 2\zeta\omega_n \frac{dZ(t)}{dt} + \omega_n^2 Z(t) = \frac{F_z(t)}{M} \\ \omega_n = \sqrt{\frac{K}{M}} \\ \zeta = \frac{C}{2\sqrt{KM}} \end{cases} \quad (11)$$

where, Z is the displacement of the tool system, $F_z(t)$ is the thrust force, M is the equivalent mass of the tool system, ζ is the damping ratio of the tool system, ω_n is the natural frequency of the tool system, K is the spring constant of

the tool system, C is the dashpot constant for the tool system, and t is the machining time.

Figure 11 A lumped-parameter representation of the dynamic cutting system

Based on the fan-shaped pattern on the surface of the workpiece, the relative displacement change between the workpiece and the tool caused by the material-induced vibration can be expressed as $Z_{miv}(t)$. Because its relative displacement conforms to the change rule of the trigonometric function, $Z_{miv}(t)$ will be in the form of a trigonometric function. Because the change rules of relative displacements produced by different crystal planes are different, the expressions of relative displacements $Z_{miv}(t)$ of different crystal planes are different. The equation of Cu (100) and (111) is as follows:

$$Z_{miv}(t) = H + A_1 \cos(\omega t) + A_2 \sin(\omega t) \quad (12)$$

where H is the balance height, A_1 , A_2 is the amplitude, and ω is the angular frequency.

The relative displacement equation of Cu (110) is as follows:

$$Z_{miv}(t) = A_1 \sin(\omega t + \varphi_1) + A_2 \sin(\omega t + \varphi_2) \quad (13)$$

where, A_1 and A_2 are the amplitude, ω is the angular frequency, φ_1 and φ_2 are the initial phase difference.

Therefore, the final value of the actual contour height under the condition of material-induced vibration is as follows:

$$Z = Z_{th} + Z_{miv} \quad (14)$$

4.1.3 Simulations results

The values of the Cu (100) surface topography and thrust force values are given in Eq. (12) to fit the parameters as shown in Table 2.

Table 2 Parameters of relative displacement and thrust force on (100) crystal plane

	H	ω	A_1	A_2
Z_{miv}	1.257×10^{-3}	8.4×10^2	-1.146×10^{-2}	5.254×10^{-3}
F_z	9.18×10^{-4}	8.4×10^2	-3.035×10^{-2}	9.36×10^{-3}

Bring the Cu (110) surface topography values and thrust

force values into Eq. (13) to obtain the parameters shown in Table 3.

Table 3 Parameters of relative displacement and thrust force on (110) crystal plane

	A_1	ω_1	φ_1	A_2	ω_2	φ_2
Z_{miv}	1.876×10^{-2}	4.1×10^2	1.52	1.852×10^{-2}	8.35×10^2	1.5
F_z	2.531×10^{-3}	4.1×10^2	1.52	3.432×10^{-2}	8.35×10^2	1.5

Bring the Cu (111) surface topography values and thrust force values into Eq. (12) to obtain the parameters shown in Table 4.

Table 4 Parameters of relative displacement and thrust force on (111) crystal plane

	H	ω	A_1	A_2
Z_{miv}	-3.765×10^{-3}	4.5×10^2	-1.518×10^{-2}	-1.949×10^{-3}
F_z	2.989×10^{-3}	4.5×10^2	-7.435×10^{-2}	1.431×10^{-2}

According to the model of dynamic cutting, the surface morphology of the ideal case is superimposed on the surface morphology induced by the vibration to produce the final surface morphology, as shown in Figure 12. Figure 12 (e–g) show the simulation results of the cutting dynamics of Cu (100), (110) and (111). It can be observed that they are very consistent with the experimental results. Cu (100) has four quadruple-symmetrical fan-shaped patterns, Cu (110) has two double-symmetrical fan-shaped patterns, and the Cu (111) has three triple-symmetrical fan-shaped patterns.

Figure 12 Nano-surface simulation by overlapping (a) primary surface, and induced surface with (b, e) (100), (c, f) (110) and (d, g) (111) crystal planes

4.2 MD simulation

4.2.1 MD modeling of nano-cutting

In order to reveal the mechanism of the Cu fan-shaped pattern, this paper studied it using MD simulations. Figure 13 shows a scheme of the MD simulation model with a workpiece size of 36.15 (length) $\times$ 10.845 (height) $\times$ 3.615 (width) nm³ and a diamond tool with a radius of 3.56 nm. The workpiece consists of three kinds of atoms: boundary atoms, thermostat atoms and Newtonian atoms. The first region consists of fixed layers at the bottom and left of the workpiece to ensure the range of movement of the atomic motion during the cutting process, preventing the tool and the workpiece from being translated under the cutting force. It is a widely used boundary simplification method [25]. Next to the boundary atoms are thermostatic atoms, the temperature of the atoms in this layer is adjusted every step and kept constant at 293 K. In this way, the heat dissipation in the real experimental environment can be simply simulated to prevent the workpiece material from becoming too high in the cutting process and affecting the judgment of the machining mechanism [26]. Then there are the Newtonian atoms which are used to simulate the movement mode and trajectory of atoms in the cutting process. It is the main region to study the cutting mechanism. The periodic boundary condition (PBC) is used in the Z direction to reduce the size effect caused by the simulation scale, and the fixed boundary condition is used in the X and Y directions. In this study, a high cutting speed of 100 m/s was used to reduce the calculation demand [27]. It is worth noting that the cutting speed has a significant impact on the temperature of the cutting region, so the critical undeformed chip thickness may be affected by the thermal effect [28]. However, the cutting distance in this study was very short, and the heat generated did not have a significant impact on the critical undeformed chip thickness. The parameters used in the simulation are listed in Table 5 and the potential function parameters are listed in Table 6.

Figure 13 MD model for nano-cutting simulation

Table 5 Parameters employed in MD simulation

Workpiece material	Cu
Workpiece dimensions	$28.92 \times 10.845 \times 18.075 \text{ nm}^3$
Workpiece crystal structure	FCC
Workpiece lattice constant	$3.6149 \text{ \AA}$
Tool material	Single-crystal diamond
Cutting edge radius (tip radius)	3.56 nm
Tool rake angle	0°
Tool clearance angle	15°
Tool crystal structure	Diamond
Tool lattice constant	$3.56683 \text{ \AA}$
Equilibration temperature	293 K
Cutting speed	100 m/s
Time step	1 fs

Table 6 Potential parameters for C and Cu interaction

Atoms interaction	Potential	Parameters			
C-C	Tersoff potential [29]	A (eV)	1393.6	B (eV)	346.74
		λ ($\text{\AA}^{-1}$)	3.4879	μ ($\text{\AA}^{-1}$)	2.2119
		β	1.5724×10^{-7}	η	0.72751
		c	3.8049×10^4	d	4.3484
		h	-0.57058	R ($\text{\AA}$)	1.8
		S ($\text{\AA}$)	2.1	χ	1
C-Cu	Morse potential [30]	D (eV)	0.1	α ($\text{\AA}^{-1}$)	1.7
		r_0 ($\text{\AA}$)	2.2	/	/

Cu-Cu EAM potential [31] /

4.2.2 Calculation of crystal orientation index

During the turning process, if the workpiece is stationary, the tool will successively experience four positions of A, B, C and D in a cutting rotation period, as shown in Figure 14 (a). Because the angle between the tool and the crystal orientation of the workpiece changes during the cutting process, and the single-crystal material has anisotropic characteristics, these factors lead to different cutting mechanisms and performances of different crystal orientations of Cu, and finally lead to different fan-shaped patterns on the workpiece surface.

Figure 14 Cutting direction changes with respect to workpiece crystal orientation in turning

The determination of the relationship between cutting directions, crystal planes and crystal orientations is essential to establish the anisotropic model of Cu. When turning three typical crystal planes (100), (110), and (111) planes of Cu, the positional relationship of the cutting direction relative to the unit cell is shown in Figure 15.

Figure 15 Cutting direction ($O'Q'$) and relative position of unit cell on (a) (100), (b) (110) and (c) (111) crystal planes

The straight line O'Q' is the cutting direction, where a , b and c are the distance from the point Q' to the three coordinate axes [100], [010] and [001] respectively, L is the length of the line segment O'Q'. It is the θ between straight line O'Q and straight line O'Q'. Cu (100) is shown in Figure 15(a), and a , b , and c are derived as follows:

$$\begin{cases} a = 0 \\ b = L \cos \theta, (0^\circ \leq \theta \leq 360^\circ) \\ c = L \sin \theta \end{cases} \quad (15)$$

The cutting direction of Cu (100) is obtained by the following:

$$[uvw] = [0 \quad \cos \theta \quad \sin \theta] \quad (16)$$

The Cu (110) is shown in Figure 15(b), where a , b and c are derived as follows:

$$\begin{cases} a = -\frac{\sqrt{2}}{2} L \cos \theta \\ b = \frac{\sqrt{2}}{2} L \cos \theta, (0^\circ \leq \theta \leq 360^\circ) \\ c = L \sin \theta \end{cases} \quad (17)$$

$$[uvw] = \left[-\frac{\sqrt{2}}{2} \cos \theta - \frac{\sqrt{6}}{6} \sin \theta \quad \frac{\sqrt{2}}{2} \cos \theta - \frac{\sqrt{6}}{6} \sin \theta \quad \frac{\sqrt{6}}{3} \sin \theta \right] \quad (20)$$

4.2.3 Simulations results

The arrangement of atoms and cutting performance vary with the changing of crystal planes and crystal orientations. Figure 16 shows the arrangement of atoms in different crystal directions of Cu (100) and the material deformation during cutting. As shown in Figure 16(a), in order to visually observe the atomic arrangement, the same atomic arrangement is set to the same color. From the atomic arrangement diagram, it can be found that the arrangement of atoms on Cu(100) varies periodically in a circumferential counterclockwise direction, and the surface has four symmetrical regions, which are four symmetrical with the surface of the workpiece. As shown in Figure 16 (c), (e), (g) and (i), when cutting along [011], [0 $\bar{1}$ 1], [0 $\bar{1}\bar{1}$] and [01 $\bar{1}$] (cloudy region), shear slip occurs in the workpiece material, dislocations propagate in the cutting direction and vertical direction, and the dislocations propagate in front of and below the tool, thereby causing substantial damage to the subsurface of the workpiece. The dislocation area is mainly represented by the HCP structure, which is generated due to defects in the workpiece material during cutting [32]. As shown in Figure 16 (b), (d), (f) and (h), when cutting along [010], [001], [0 $\bar{1}$ 0] and [00 $\bar{1}$] (clean region), there is no vertical slip, but some slip was

The cutting direction of the Cu (110) is obtained by the following:

$$[uvw] = \left[-\frac{\sqrt{2}}{2} \cos \theta \quad \frac{\sqrt{2}}{2} \cos \theta \quad \sin \theta \right] \quad (18)$$

Cu (110) is shown in Figure 15(c), where a , b and c are derived as follows:

$$\begin{cases} a = -\frac{\sqrt{2}}{2} L \cos \theta - \frac{\sqrt{6}}{6} L \sin \theta \\ b = \frac{\sqrt{2}}{2} L \cos \theta - \frac{\sqrt{6}}{6} L \sin \theta, (0^\circ \leq \theta \leq 360^\circ) \\ c = \frac{\sqrt{6}}{3} L \sin \theta \end{cases} \quad (19)$$

The cutting direction of the Cu (111) is obtained by the following:

observed at an angle to the cutting direction. It can be seen that many slips caused by misalignment will interfere with each other in the cutting area in front of the tool. Because the cutting is carried out in the direction of slip, subsurface damage is lower.

Figure 16 (a) Schematic of the atomic arrangement on the (100) crystal plane and (b-i) the material deformation in MD cutting simulation

Material deformation has a close relationship with the

atomic arrangement. It can be observed from Figure 17 (a) that the arrangement of atoms on the Cu (110) changes periodically in a circumferential counterclockwise direction, and has two symmetrical regions, which are consistent with the four two-fold symmetrical fan patterns. As shown in Figure 17 (b) and (f), when cutting along $[\bar{1}10]$ and $[1\bar{1}0]$ (cloudy region). Owing to the deformation of the material in the sliding direction, the dislocations propagate in the tangential and vertical directions, so the dislocations can easily propagate downward in the material, thereby causing substantial damage to the subsurface of the workpiece. As shown in Figure 17 (d) and (h), when cutting along $[001]$ and $[00\bar{1}]$ (cloudy region), no vertical slip was found, but some were observed at an angle to the cutting direction slip. It can be seen that many slips caused by misalignment will interfere with each other in the cutting area in front of the tool. Because the cutting is performed in the sliding direction, it is observed that the deformation does not penetrate deeper into the material, which indicates that the subsurface damage in this cutting direction is less. As shown in Figure 17 (c), (e), (g) and (i), when cutting along $[\bar{1}12]$, $[1\bar{1}2]$, $[11\bar{2}]$ and $[\bar{1}\bar{1}2]$ (clean region), the slip mainly occurs at an angle to the cutting direction. It can be seen that many slips caused by misalignment will interfere with each other in the cutting area in front of the tool. Because cutting is carried out in the sliding direction, it leads to lower subsurface damage.

Figure 17 (a) Schematic of the atomic arrangement on the (110) crystal plane and (b-i) the material deformation in MD cutting simulation

The material properties in different orientations can be reflected in the evolution of structures. From Figure 18 (a), it can be observed that the arrangement of atoms on the Cu (111) changes periodically in a circumferential

counterclockwise direction, and has three symmetric regions, which is the same as the surface of the workpiece. As shown in Figure 18 (c), (e) and (g), when cutting along $[\bar{1}01]$, $[1\bar{1}0]$ and $[01\bar{1}]$ (cloudy region). First, shear slip occurs in the workpiece material, dislocations propagate in the cutting direction and the vertical direction, and the dislocations propagate in front of and below the tool, thereby causing substantial damage to the subsurface of the workpiece. As shown in Figure 18 (b), (d) and (f), when cutting along $[\bar{1}10]$, $[0\bar{1}1]$ and $[10\bar{1}]$ (clean region), no vertical slip was found, but in some slippage was observed at an angle to the cutting direction. It can be seen that many slips caused by misalignment will interfere with each other in the cutting area in front of the tool. The cutting is carried out in the sliding direction, which leads to lower subsurface damage.

Figure 18 (a) Schematic of the atomic arrangement on the (111) crystal plane and (b-g) the material deformation in MD cutting simulation

Friction coefficient is closely related to surface morphology, and the equation of friction coefficient is derived as follows:

$$\mu = \frac{F_t + F_c \tan \alpha}{F_c - F_t \tan \alpha} \quad (21)$$

where, μ is friction coefficient, F_t is axial force, F_c is tangential force.

The friction coefficient and the related atomic density are essential for the joint of micro and macro dynamic modeling. Table 7 shows the friction coefficient of experiments, friction coefficient of simulations and atomic density of different crystal planes of Cu workpieces during cutting. It can be seen from the figure that the variation trend of atomic arrangement density is similar to the variation trend of friction coefficient, which are significant representation methods of the anisotropy of Cu.

Table 7 Parameter changes in experimental cutting and MD simulations of (100), (110) and (111) crystal planes

5 Conclusions

In this study, the cutting mechanism and surface generation of single-point diamond turning (SPDT) of single-crystal copper (Cu) were studied from the perspective of chip formation and surface topography, and dual dynamic modeling and simulation were established to present nano-surface generation and fan-shaped pattern formation. The specific conclusions are as follows:

(1) When SPDT of Cu with different crystal planes, the machined surface exhibits different fan-shaped

distribution patterns. Four quadruple-symmetric fan-shaped patterns were formed on the Cu (100) crystal plane, four double-symmetric fan-shaped patterns were formed on the Cu (110) crystal plane and six triple-symmetric fan-shaped patterns were formed on the Cu (111) crystal plane.

(2) A dual dynamic model combining the MD and cutting dynamics was established to present the nano-surface generation in SPDT of Cu. The friction coefficient changes with the atom arrangement, which is the joint for cutting dynamics modeling and MD modeling.

(3) Among the three crystal planes of Cu (100), (110) and

(111), the Cu (100) crystal plane is most suitable for machining, and the surface roughness obtained is the smallest, with a value of 15.433 nm. The Cu (111) crystal plane follows, whose surface roughness value is 17.016 nm. The surface roughness obtained on the Cu (110) crystal plane are the largest, with a value of 20.102 nm.

- (4) The periodic arrangement of the atoms and the atomic density of Cu result in the periodicity of mechanical properties on crystal planes, while the atom arrangement directions and its angle change with the main cutting direction of SPDT causes the periodic fluctuation of the cutting system, and finally generates fan-shaped patterns.

6 Declaration

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Availability of data and materials

The datasets supporting the conclusions of this article are included within the article.

Authors' contributions

The author's contributions are as follows: Guoqing Zhang and Sandy To were in charge of the whole trial; Yanbin Chen wrote the manuscript; Yuqi Dai and Jiaqi Ran assisted with sampling and laboratory analyses.

Competing interests

The authors declare no competing financial interests.

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Experimental setup

Figure 2

Figure 2

Figure 3

Figure 3

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Figure 4

Figure 4

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Figure 5

Figure 5

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Figure 6

Figure 6

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Figure 7

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Figure 15

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Figure 16

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Figure 17

Figure 17

(a) Schematic of the atomic arrangement on the (110) crystal plane and (b-i) the material deformation in MD cutting simulation

Figure 18

Figure 18

(a) Schematic of the atomic arrangement on the (111) crystal plane and (b-g) the material deformation in MD cutting simulation