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ARTICLE

Effect of Initial Temperature of Nano-cutting on Microstructure of Single Crystal Copper

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Abstract: Nano-cutting causes internal microscopic defects in the workpiece, and this defect structure is closely related to the initial temperature of the cutting layer. In order to reduce the defects of workpieces in nano-cutting, a nano-cutting model of single-crystal copper with a cutting layer was constructed using molecular dynamics. Firstly, the applicable initial temperature of the cutting layer was determined by analyzing the changes in the structural volume and microscopic defects of the workpiece. Secondly, the effect of the initial temperature of the cutting layer on the cutting forces, dislocations and lattice was analyzed. Finally, the simulation results were indirectly verified by experiments. The results show that the applicable initial temperature range of cutting layer for single crystal copper is 293~400 K. As the initial temperature of the cutting layer increases, the transition rate of the lattice structure increases and the magnitude of the cutting force changes significantly, but the effect on fluctuations is small. When the initial temperature of the cutting layer is set in the range of 360~390 K, the surface microscopic defects of the single crystal copper workpiece are relatively less, and thus it is predicted that the surface quality of the single crystal copper workpiece is higher when it is machined in this initial temperature range.

Key words: nano-cutting; cutting layer; initial temperature; single crystal copper; microstructure

As a common material for micro-mechanics and micro-components, single crystal copper has good signal transmission, plastic processing and fatigue resistance, and is widely used in defense precision instruments, civil communication equipment and other fields[1]. Ultra-precision single point diamond cutting is widely used in the processing and manufacturing of single crystal copper for its advantages of high machining efficiency, high precision and controllable error[2]. Nano-cutting can overcome the interaction between atoms of the workpiece and cut off the combination of atoms through the force exerted by the tool to the workpiece[3]. In this process, defects such as vacancies, cracks and dislocations are inevitable and the presence of these minor defects reduces the strength of the material and leads to low stress damage[4]. In addition, there is a very important relationship between interatomic interactions and interatomic temperatures. Guo et al[5] analyzed the temperature distribution of single-crystal copper during nanofabrication, and found that the defect structure of the workpiece is temperature dependent and that highly localized temperature fields in the shear zone and chips reduce the activation potential for dislocation nucleation and emission. Pre-heating of the cutting area before machining increases the initial temperature of the cutting layer, which will affect the interatomic temperature during the cutting process. Therefore, it is necessary to study the effect of the initial temperature of the cutting layer of the workpiece on nano-cutting in order to improve the surface quality of the workpiece.

Some research has been carried out on the effect of initial workpiece temperature on cutting. Luo et al[6] studied the effect of the cutting process of single crystal germanium at different initial temperatures and found that as the cutting temperature increases, the cutting force decreases and more atoms of the workpiece undergo deformation. Germain et al[7] found that preheating reduces the material yield strength of the workpiece during laser-assisted machining (LAM) in nickel-based alloys, and LAM significantly reduces cutting forces (up to 40%) and improves the surface quality of the

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workpiece compared to conventional machining. Chavoshi et al[8,9] studied high temperature nano-cutting of 3C-SiC and found that subsurface damages increase linearly with increasing cutting temperature, point defects occur when the thermal energy is high enough, and stacking faults grow more rapidly on the sliding surface at higher temperatures. Some scholars have obtained the optimal initial cutting temperature of some materials through experiments and simulations. For example, Rashid et al[10] found a moderate reduction in cutting forces when machining β-type Ti-6Cr-5Mo-5V-4Al titanium alloys under laser-assisted conditions in cutting temperature range of 1323~1523 K; in laser-assisted machining of Inconel 718, Attia et al[11] found that lower surface damage and lower cutting forces are obtained when the material removal temperature is set within 923~973 K. In a study on the effect of the initial temperature of the workpiece on the processing of single crystal copper, Zhang et al[12] set the maximum initial temperature to 673 K. Zhu et al[13] set the maximum initial temperature to 600 K. It was found that as the initial temperature of the workpiece increases, the chip volume in front of the tool increases and the cutting and normal forces decrease, but the effect of the initial temperature on the internal microstructure of the workpiece was not analyzed.

During the cutting process, the tool performs work on the workpiece, the workpiece undergoes plastic deformation, resulting in the breaking of metal bonds, bond energy is released, and chemical and kinetic energy is converted into heat energy[5]. Chavoshi et al[14] conducted high temperature nano-cutting processing for single crystal silicon, and found that as the initial temperature of the workpiece increases, the heat energy released during cutting decreases and the temperature rise of the workpiece decreases. A large number of studies have also been conducted on the influence the cutting temperature and thus the cutting forces, dislocations and lattice structure changes during cutting by changing the cutting parameters[15-17], but the initial temperature change of the workpiece has not been used as a separate influencing factor to analyze its effect on the internal microstructure change in the nano-cutting of single crystal copper.

In order to investigate the effect of the initial temperature of the cutting layer on the microstructure inside the workpiece during the nano-cutting process of single crystal copper, the nano-cutting process of single crystal copper at different initial temperatures of the cutting layer was simulated by molecular dynamics (MD) method. Firstly, the applicable preheating temperature range of the workpiece was determined in a wide temperature range. Subsequently, the optimal initial temperature range for nano-cutting of single-crystal copper workpieces was explored by analyzing the cutting forces, dislocations and lattice structure changes during the cutting process within this temperature range. To achieve the purpose of improving the surface quality of the workpiece by optimizing the initial temperature of the cutting layer, finally, indirect verification was performed through experiments. The specific process is shown in Fig.1.

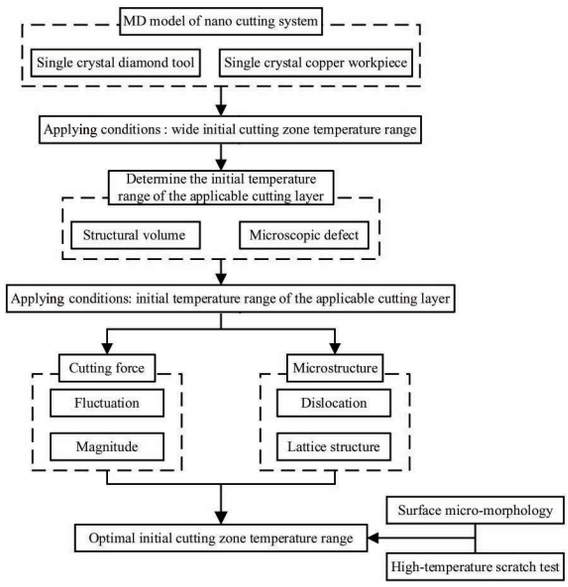

Fig.1 Research step by step thought diagram

1 Construction of the Model and Validation of the Potential Function

1.1 MD simulation model

The MD model of a single-crystal diamond tool cutting a single crystal copper workpiece at the nanoscale was established to investigate the effect of the initial temperature of the cutting layer on the nano-cutting process, as shown in Fig.2. It contains the following two main parts.

(1) Selection of tool and determination of crystal surface

Diamond tools of (100) crystalline surfaces on the front and back tool faces were selected for cutting simulation of single-crystal copper workpieces. Diamond tools have extremely high hardness and wear resistance, maintain high tip quality of nano-cutting of single-crystal copper, and have maximum microscopic strength and the lowest wear rate on their (100) crystal faces[18,19].

(2) Setting of single crystal copper workpiece

The single crystal copper workpiece and diamond tool were set in boundary layer, thermostat layer and Newtonian layer. Since the high temperature of the workpiece is mainly distributed among the cutting surface and around the tool, the workpiece model was improved by setting the cutting layer in

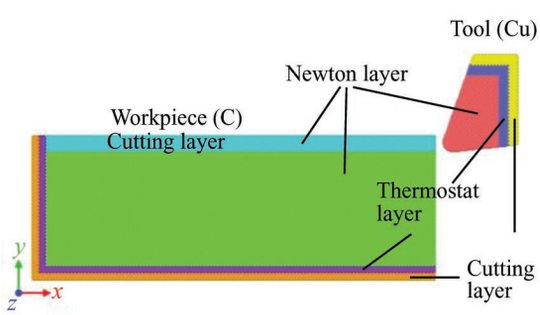

Fig.2 MD model of a single crystal diamond tool cutting a single crystal copper workpiece

the Newton layer, where the depth of the cutting layer was 1.5 nm, and different initial temperatures of the cutting layer was set by the Berendsen heat bath scale method.

The specific simulation parameters selected in this nano-cutting of single crystal copper are shown in Table 1.

1.2 Selection and verification of potential function

In the nano-cutting MD simulation of single-crystal copper, the selection of the appropriate inter-atomic potential energy function between the single-crystal copper workpiece and the diamond tool is the basis for accurate output of the workpiece and tool atomic trajectories and thermodynamics, and the specific inter-atomic potential energy function for each atom is selected as shown in Table 2, where the Morse potential parameters are selected as $D_{\text{Cu-C}}$=0.087 eV, $\alpha_{\text{Cu-C}}$=5.140 nm^{-1}, $r_{\text{Cu-C}}$=0.2050 nm[20] ($D_{\text{Cu-C}}$, $\alpha_{\text{Cu-C}}$ and $r_{\text{Cu-C}}$ are the binding energy coefficient, gradient coefficient of the potential curve, and equilibrium distance between Cu-C atoms, respectively).

The bulk modulus of the material is determined by the MD method and compared with the experimental measurements to evaluate the accuracy of the selected potential energy function. The volumetric modulus is calculated as follows:

$$B_{\text{V}} = -\frac{\mathrm{d}P}{\mathrm{d}V/V} = \frac{M}{9a_0}\frac{\mathrm{d}^2E}{\mathrm{d}a^2}\bigg|_{a_0} \quad (1)$$

where V and P are the volume of the cell and the pressure of the system, respectively; a_0 is the calculated equilibrium lattice constant; M is the number of atoms in the cell with the side length: the value of M is 4 for single-crystal copper workpieces and 8 for diamond tools.

LAMMPS programming was used to calculate the equilibrium lattice constants of diamond crystals with Tersoff potential and single-crystal copper crystals with EAM potential, and the fifth order polynomial fit curve of lattice constant versus cohesion energy was obtained, as shown in Fig. 3. The lattice structure is the most stable when the cohesion energy is the lowest, and the lattice constant at this time is the equilibrium lattice constant.

The obtained equilibrium lattice constants and the bulk modulus calculated by Eq. (1) were compared with the experimental values[22], as shown in Table 3, and the analysis shows that the simulated values match the experimental values, so the potential function selected is feasible, which provides an accuracy guarantee for the nano-cutting of single-crystal copper.

Table 1 Simulation parameters of diamond cutting single crystal copper

Parameter	Value
Workpiece size (a=0.3615 nm)	120a×40a×30a
Arc radius of tool tip/nm	1
Rake and rear corners of the cutting tool/(°)	20, 6
The boundary conditions	s s p
Relaxation steps	20 000
Time step/ps	0.001
Cutting length/nm	30
Cutting depth/nm	1.5
Cutting speed/nm·ps^{-1}	0.1

Table 2 Potential function between atoms

Atom type	Potential function
Workpiece (Cu-Cu)	EAM potential[21]
Workpiece and cutting tool (Cu-C)	Morse potential[21]
Diamond tool (C-C)	Tersoff potential[15]

2 Determination of the Applicable Range of the Initial Temperature of the Cutting Layer

The initial temperature of the cutting layer has a certain influence on the surface quality of single crystal copper. In this study, we analyzed the variation of the structural volume of the workpiece and the internal microscopic defects of the

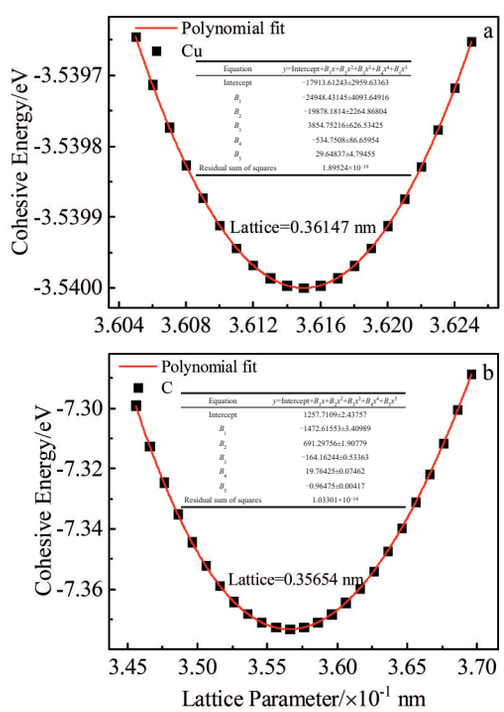

Fig.3 Fitting curves of lattice constants and cohesive energy: (a) single-crystal copper workpiece; (b) diamond tool

Table 3 Comparison of simulated and experimental values of equilibrium lattice constant and bulk modulus

Element	Potential function	Lattice constant/×10^{-1} nm		Bulk modulus/GPa		Error/%
		Experiment	Simulation	Experiment	Simulation	
Cu	EAM	3.615	3.6147	141.9	138.3821	2.479
C	Tersoff	3.567	3.5654	442	445.3005	0.747

workpiece after machining at different initial temperatures of the cutting layer. And from this, the applicable preheating temperature range of the workpiece is determined.

2.1 Volume change of workpiece structure

When determining the applicable preheating temperature range of the workpiece, the initial temperature of the cutting layer was set to 293~650 K. The applicable initial temperature range of the workpiece was initially determined by analyzing the single crystal copper lattice structure changes and volume changes.

In the atomic level, the temperature of the workpiece is expressed in the form of kinetic energy and there is a linear relationship between kinetic energy and temperature, as shown in Eq.(2)[23]. Therefore, after heating the single crystal copper workpiece, the activity of the copper atoms increases and very small displacements occur. The surface atoms of the workpiece will be disrupted due to the occurrence of displacement, leading to the destruction of the lattice structure and some changes in the volume of the workpiece.

$$T = \frac{\sum_{i=1}^{N} m_i v_i^2}{3Nk_B} \tag{2}$$

where N is the number of atoms; k_B is the Boltzmann constant; m_i is the atomic mass; v_i is the atomic velocity.

The single-crystal copper workpiece was subjected to structural optimization and relaxation at different initial temperatures, and a minor deformation of the workpiece volume was found. Fig.4 shows the distribution of the atoms of the single-crystal copper workpiece at different initial temperatures after the relaxation, where the red atoms on the surface of the workpiece are the atoms that diffuse out of the surface layer, whose y-coordinate is greater than 0 (the y-coordinate of the surface layer of the workpiece is 0); the green atoms are the atoms of the face-centered cubic (fcc) structure, and the white atoms on the surface layer are the atoms whose face-centered cubic (fcc) structure is destroyed after atom diffusion (other). Fig.5 shows a line graph of the number of atoms with y-coordinate greater than 0 and lattice structure disrupted with the initial temperature of the cutting layer.

As can be seen from Fig.4 and Fig.5, the number of atoms that diffuse out of the surface layer of the workpiece and whose lattice structure is destroyed both increase with the increase of initial temperature of the cutting layer. Particularly, the change in the number of these two atoms increases significantly when the initial temperature is above 400 K. Therefore, by setting the initial temperature of the cutting layer within 400 K, the error caused by the change in the volume of the workpiece structure to machining can be reduced.

2.2 Internal microscopic defects of the workpiece

This section further determines the applicable initial temperature range of the cutting layer for single-crystal copper workpiece by analyzing the dislocation depth and the number of vacant defects of single-crystal copper workpiece after finishing cutting at different initial temperatures of the cutting layer.

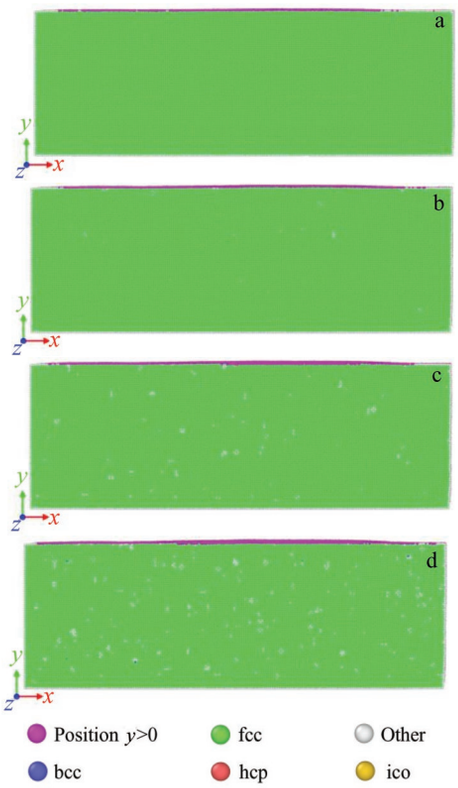

Fig.4 Distribution of workpiece atoms at different initial temperatures after the relaxation: (a) 293 K, (b) 400 K, (c) 500 K, and (d) 600 K

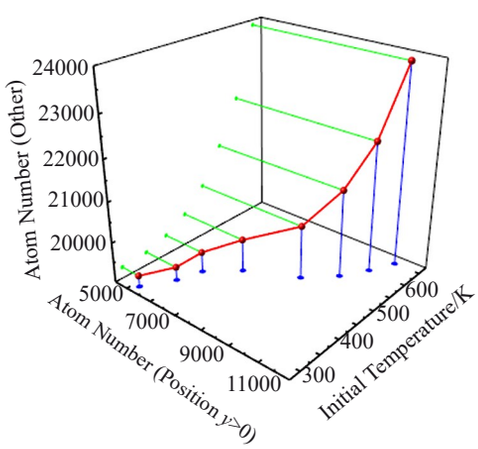

Fig.5 Variation of the atomic number with the initial temperature of the cutting layer

In the nano-cutting process of single-crystal copper, dislocation analysis was performed on the single-crystal copper workpiece at a cutting distance of 30 nm, and the atoms with a hexagonal close packed structure (hcp) were colored separately to obtain the distribution of dislocations and hexagonal close packed structure atoms, as shown in

Fig.6. It can be found that there is a significant increase in the dislocation depth of the workpiece when the initial temperature of the cutting layer exceeds 400 K. And when the initial temperature of cutting layer exceeds 500 K, there is also a significant increase in the dislocation defects of the workpiece.

Through the analysis of Fig. 4~6, we know that when the initial temperature of the cutting layer exceeds 400 K, the structural volume of the single crystal copper workpiece changes significantly and there is a significant increase in the internal microscopic defects of the workpiece, which will not only lead to a large residual stress, but also a significant reduction in surface quality. Therefore, the initial temperature of the cutting layer of single crystal copper workpiece should be set within 293~400 K.

3 Determination of the Optimal Range of the Initial Temperature of the Cutting Layer

In the nano-cutting process of single crystal copper, changing the initial temperature of the cutting layer directly affects the bonding energy between atoms and the atomic activity, which in turn affects the cutting force, dislocation and lattice structure changes during the cutting process. Within the applicable range of the initial temperature of the single crystal copper cutting layer determined, the optimum initial temperature range of the cutting layer was explored by analyzing the variation of cutting force and microstructure with the initial temperature of the cutting layer to achieve the purpose of improving the surface quality of the workpiece.

3.1 Cutting force

During the nano-cutting process of single crystal copper, the maximum value, minimum value, mean value and the difference between the two extremes of the cutting force after reaching stability with the initial temperature are shown in Fig. 7, where Fx_{max} is the maximum value of cutting force; Fx_{min} is the minimum value of cutting force; ΔFx is the difference between the maximum and minimum values of cutting force; and $Fx_{average}$ is the mean value of cutting force.

The variation of the difference between the two poles of the cutting force with the initial temperature of the cutting layer in Fig. 7 shows that the magnitude of the fluctuation of the cutting force does not change significantly with the increase of the initial temperature of the cutting layer. From the extreme and mean size changes of the cutting force, it can be found that when the initial temperature is lower than 360 K, the cutting force fluctuates more gently. After the initial temperature exceeds 360 K, together with the cutting heat, the temperature of the workpiece increases to an extent that reduces the strength of the material. The thermal softness of the workpiece increases, the energy required for atom detachment decreases, and the cutting force shows a decreasing trend with the increase of the initial temperature, which is similar to the results of Zhu et al[13]. Therefore, the change of the initial temperature of the cutting layer mainly affects the magnitude of the cutting force, and has less influence on the fluctuation of the cutting force.

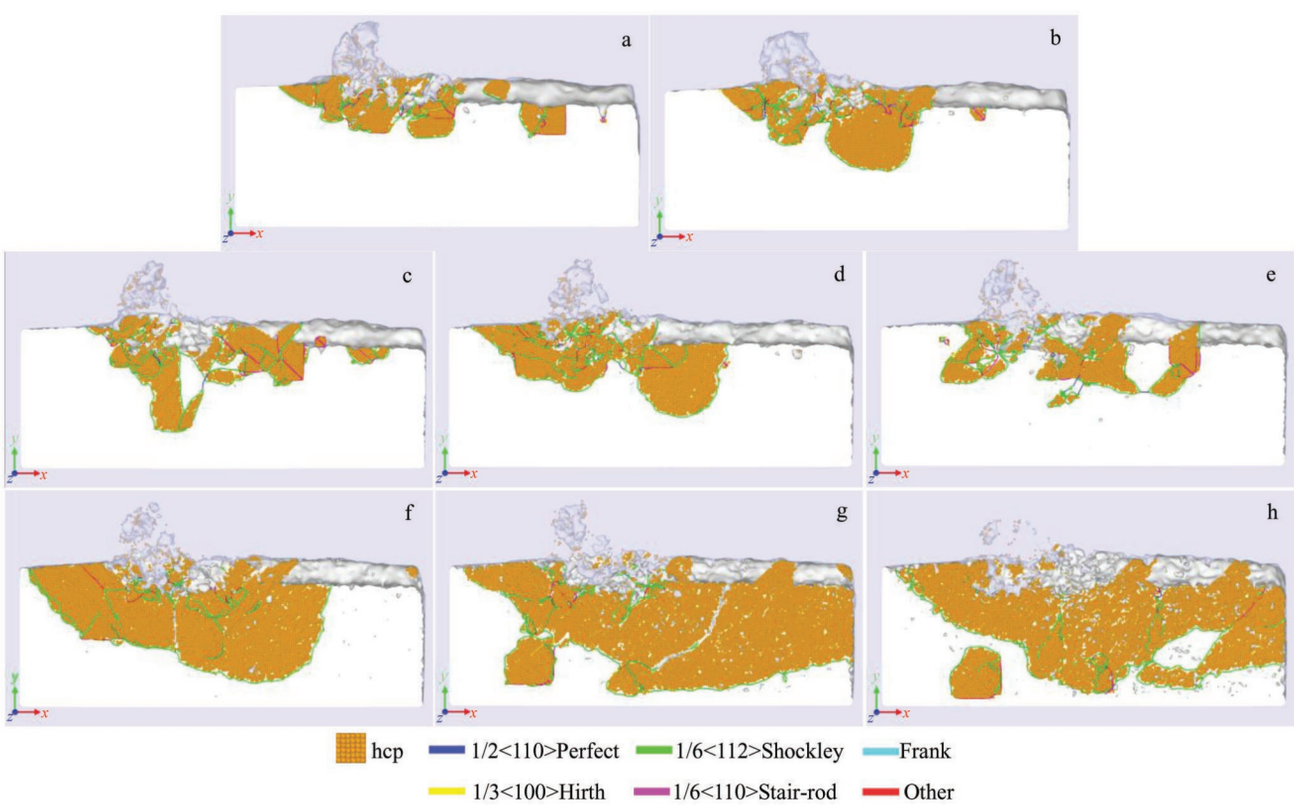

Fig.6 Distribution structure of dislocations and hcp atoms at different initial temperatures: (a) 293 K, (b) 350 K, (c) 400 K, (d) 450 K, (e) 500 K, (f) 550 K, (g) 600 K, and (h) 650 K

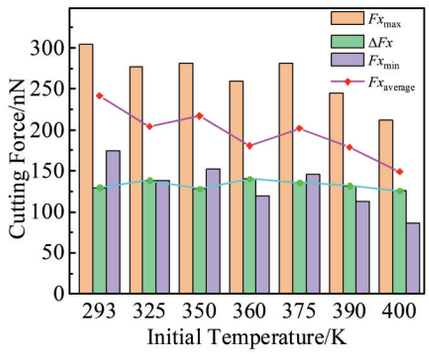

Fig.7 Graph of extreme, differential and average values of cutting force as a function of initial temperature

3.2 Internal microstructure of the workpiece

In this section, the internal microscopic defects of the workpiece at different initial temperatures of the cutting layer were analyzed from the changes of the lattice structure and dislocations of the single-crystal copper workpiece during the cutting process.

3.2.1 Lattice structure of the workpiece

The lattice structure of single-crystal copper is face-centered cubic (fcc), which is mainly transformed into the common hexagonal close packed structure (hcp) and other amorphous structures (Other) during the cutting process. The atomic distribution between the tool and the workpiece at a cutting distance of 30 nm is obtained by the centro-symmetric parameter (CSP) method, as shown in Fig. 8. Fig. 9 represents the variation of the number of atoms of each lattice structure with the cutting distance at different initial temperatures of the cutting layers, where Fig. 9b shows the fifth-order fitted curve of the number of hcp atoms.

As can be seen from Fig. 9a and Fig. 9c, the number of atoms in the face-centered cubic structure decreases and the number of atoms in the amorphous structure increases as the temperature rises at the initial position of the cut, indicating that the atoms become more active and diffuse more intensively as the temperature increases. During the cutting process, the number of atoms in the face-centered cubic lattice structure decreases and the number of atoms in the amorphous structure increases with the increase of the cutting distance, and the transition rate accelerates with the increase of the initial temperature of the cutting layer. From Fig. 9a, it can be found that when the initial temperature of the single-crystal copper cutting layer reaches 400 K, the atoms of its face-centered cubic structure have a more obvious tendency to decrease during the cutting process compared with other temperatures, indicating that the transformation of the lattice structure accelerates as the temperature rises after the strength of the material is reduced.

When analyzing the relationship between the change of hexagonal close packed structure atoms of single-crystal copper at different initial temperatures of the cutting layer, it is important to clarify the transition relationship between the face-centered cubic lattice atoms and the hexagonal close packed structure atoms. The single crystal copper atoms are displaced by the cutting force and the arrangement structure of some atoms is transformed from ABCABC..... to ABABAB....., that is, from a face-centered cubic lattice structure to a hexagonal close packed structure, as shown in Fig. 10, and the formation of such stacking layer dislocations can reduce the overall stress[24]. Since the cutting force acts in a limited range, atoms with two different lattice structures appear on both sides of the dislocation. As a result, the atoms in Fig. 6, which have been transformed from a face-centered cubic structure to a hexagonal close packed structure, are all surrounded by dislocations.

Since the production of densely arranged hexagonal structure atoms is related to dislocations, the number of

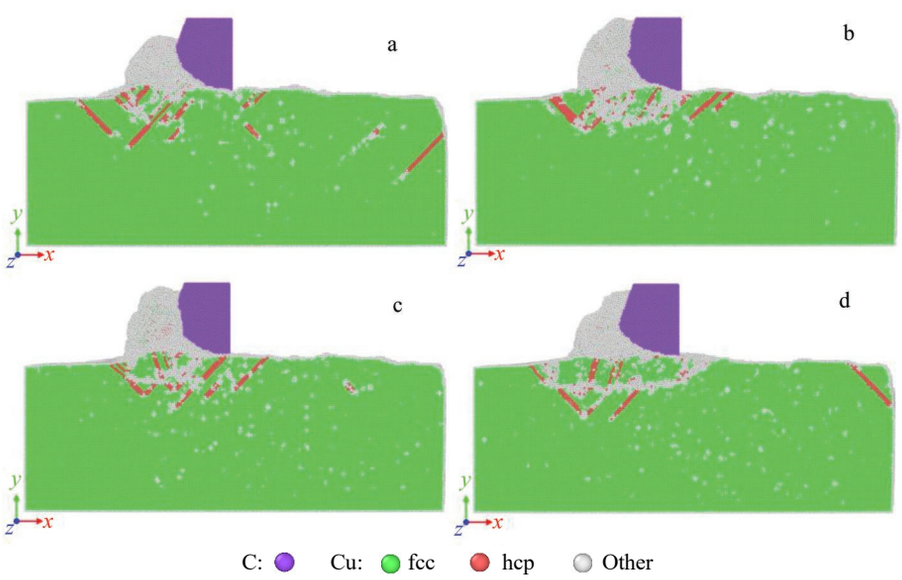

Fig.8 Distribution of atoms in the cutting process at different initial temperatures: (a) 325 K, (b) 360 K, (c) 375 K, and (d) 390 K

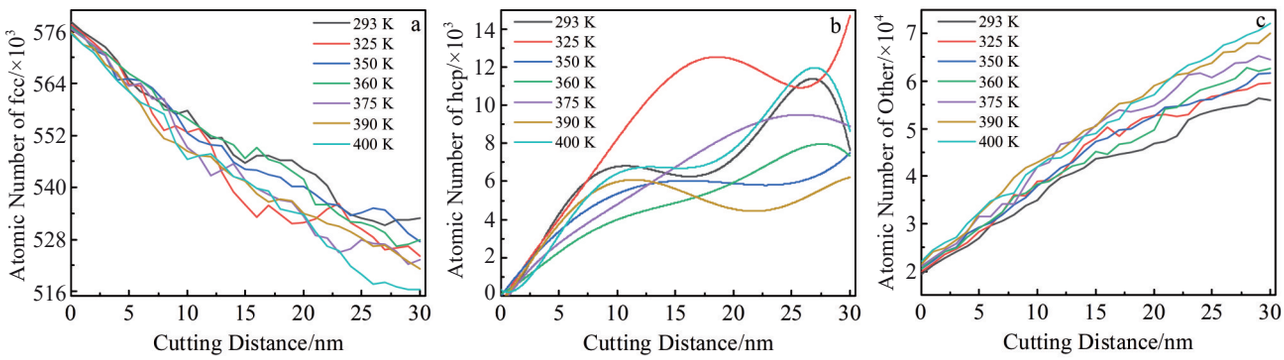

Fig.9 Curves of lattice structure changes at different initial temperatures of cutting layers: (a) fcc, (b) hcp, and (c) Other

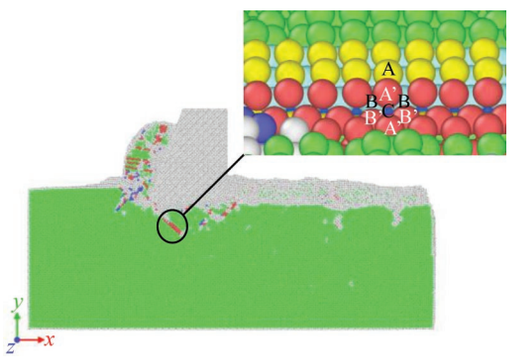

Fig.10 Diagram of the atomic structure at the junction of the fcc structure and the hcp structure

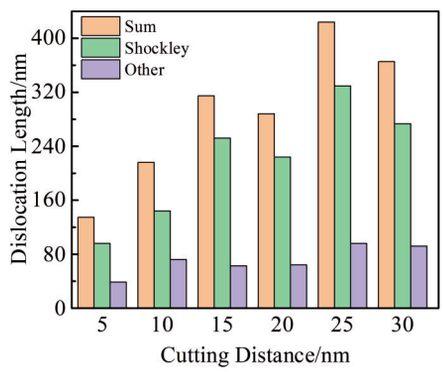

Fig.11 Histogram of dislocation type distribution

densely arranged hexagonal close packed structure atoms in Fig. 9b has a similar fluctuation variation to the dislocation length in Fig. 12b. When the initial temperature of the cutting layer is 325 K, a significant increase in the number of atoms transformed into a hexagonal close packed structure can be found in Fig. 9b, as well as a significant change in the dislocation length in Fig. 12b. When the initial temperature of the cutting layer is taken as 350 and 390 K, the number of atoms transformed from face-centered cubic structure to hexagonal close packed structure is relatively minimal and the structure of the workpiece is relatively more stable.

3.2.2 Dislocations of the workpiece

For investigating the effect of the initial temperature of the cutting layer on dislocations, dislocations in single-crystal copper workpieces were analyzed during cutting by means of a dislocation extraction algorithm (DXA). The analysis was carried out in terms of the main forms of dislocations, the length of dislocations, the number of dislocation segments and the depth of dislocations.

The dislocations at the initial cutting layer temperature of 293 K were sorted by total dislocations, Shockley dislocations and other forms of dislocations to obtain the dislocation types at different cutting distances, as shown in Fig. 11, where Sum indicates the total length of dislocations; Shockley indicates the length of Shockley form dislocations; Other indicates the length of non-Shockley form dislocations.

From Fig. 11, it can be found that the dislocations caused by the cutting process of single-crystal copper are mainly Schockley dislocations, which is the same as the main form of dislocations caused by nanoindentation of single-crystal copper[25], and from the variation of the total length of dislocations with cutting distance, it can be found that the dislocations do not show a single growth variation as the cutting proceeds. To clearly reflect the variation of dislocations during cutting, the dislocation length, the number of dislocation segments and the average dislocation length per segment were fitted to the fifth order with cutting distance at different initial temperatures of the cutting layer, as shown in Fig. 12.

As can be seen from Fig. 12, the maximum value of dislocation length after cutting appears when the initial temperature of the cutting layer is 325 K, and the minimum value of dislocation length appears when the initial temperature of the cutting layer is 390 K. During the cutting process, the number of dislocation segments and the length of dislocation do not show a single increase with the increase of cutting distance, so it can be seen that the force of the tool to the workpiece will not only lead to the generation and increase of dislocations, but also reduce part of the generated dislocations to a certain extent. The average dislocation length per segment in Fig. 12c reaches the equilibrium state when the cutting distance reaches 5 nm, then fluctuates in a certain range and has a similar fluctuation pattern at different initial temperatures, and the average dislocation length per segment reaches the maximum when the initial temperature is 400 K.

From the distribution of atoms in the hexagonal close

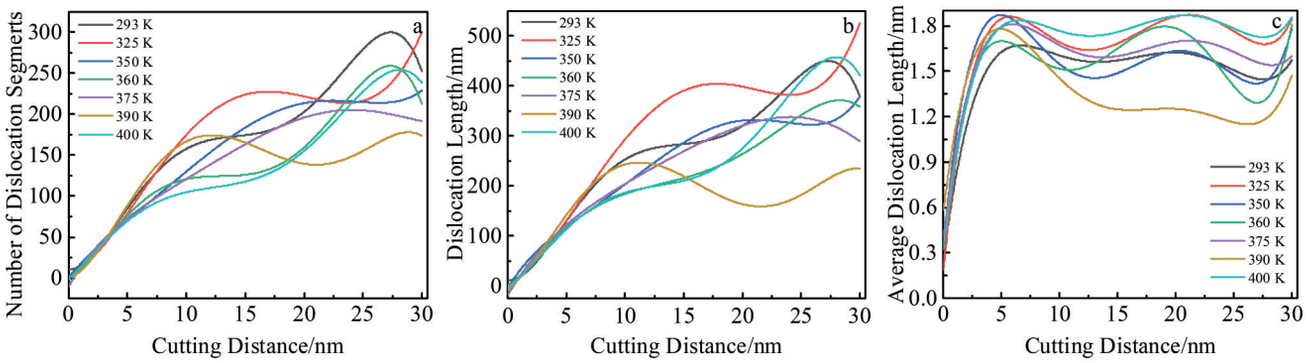

Fig.12 Plot of dislocation variation at different initial temperatures of cutting layers: (a) number of dislocation segments; (b) dislocation length; (c) averge dislocation length

packed structure in Fig. 6 and Fig. 8, the coordinate information of the lowest point of dislocation at the cutting position of 30 nm was extracted to obtain the depth of dislocation after the cutting was completed, and compared with the length of dislocation at this time to obtain the variation of dislocation depth versus length at different initial temperatures of the cutting layer, as shown in Fig.13.

From Fig.13, it can be found that both the dislocation depth and dislocation length show a trend of increasing and then decreasing with the increase of initial temperature, and then continue to increase. When the initial temperature is within 360~390 K, the dislocation depth is low and the dislocation length is also small, and the dislocation defects of the workpiece obtained under this condition are less.

To verify whether the law is still applicable under other working conditions, cutting simulations were performed on the workpiece after changing the tool structure size. Since the final application of the workpiece needs to be cooled to room temperature, the workpiece temperature was set to 293 K at room temperature by the Berendsen heat bath scale method after cutting was completed, and its internal dislocation defects were analyzed, as shown in Fig. 14, where α and R denote the tool front angle and the radius of the tool tip circle, respectively.

From Fig. 14, it can be found that at room temperature, the

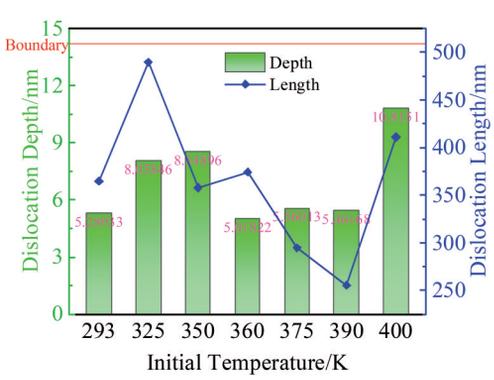

Fig.13 Histogram of dislocation depth versus length as a function of temperature

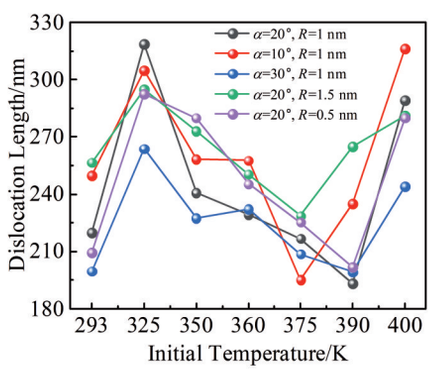

Fig.14 Plot of dislocation length with initial temperature of cutting layer under different tool parameters

dislocation length decreases with the increase of the tool front angle, while the dislocation length shows an increase with the increase of the radius of the tool tip arc, which is consistent with the existing findings[26-28]. However, the law changes when the preheating temperature is applied. Under different cutting conditions, the length of workpiece dislocations first increases, then decreases, and then begins to rise rapidly as the initial temperature of the cutting layer increases. It can be found that when the preheating temperature is between 360 and 390 K, a minimum value of dislocations occurs when the workpiece is machined under different conditions. At this time, the workpiece has fewer dislocation defects and relatively higher surface quality.

3.3 Comprehensive analysis

When the initial temperature exceeds 360 K, it can be found in Fig.7 that the magnitude of cutting force during the cutting process is lower and the variation of cutting force is smoother, which reduces the tool wear and improves its service life. When the initial temperature is between 350 and 390 K, it can be found by Fig.9 that the number of atoms transformed from fcc structure to hcp structure is less, and the workpiece structure is more stable at this time. However, when the initial temperature is taken as 350 K, it is found from Fig.13 that the dislocation depth is larger and a larger damage will be produced under this condition, while when the initial

temperature is between 360 and 390 K, it is found from Fig.14 that the dislocation length is smaller and the dislocation depth is smaller under different cutting parameters.

The cutting forces and microstructural changes of the workpiece during the nano-cutting of single-crystal copper at different initial temperatures of the cutting layer are considered comprehensively. When the cutting layer of the workpiece is preheated to the range of 360~390 K, the cutting force of the machining process is lower and there are fewer internal microscopic defects, thus triggering less residual stresses, which can effectively improve the surface quality of the workpiece.

4 Simulation and Experiment

The surface texture of the machined surface is an important measure of the surface quality of the workpiece. In this section, the surface texture of the machined surface is analyzed by analyzing the depth of cut of the machined surface of the workpiece obtained from simulation and the variation of the depth of cut obtained from experiment, and the optimal initial temperature range obtained from simulation is verified.

4.1 Simulation analysis

The depth of cut of the machined surface was analyzed when the workpiece was cooled to room temperature. The workpiece was colored according to different cutting depths to obtain the microscopic morphology of the machined surface at different initial temperatures, as shown in Fig. 15, where red indicates small cutting depths and blue indicates large cutting depths. Fig.15a shows the workpiece after coloring, the boxed part is the cutting surface, and the cutting surface obtained at different initial temperatures is enlarged. Fig. 15b~15e show the workpiece cutting surfaces obtained at initial temperatures of 293, 325, 375 and 400 K, respectively. The parts in different color from the periphery are circled to indicate a significant change in depth of cut here.

From the distribution of depth of cut at different initial temperatures shown in Fig. 15, it can be found that the color on the left side of the cutting surface, which is the initial part of the cut, is blue, indicating that the depth of cut is larger here, so the growth of dislocations is rapid at this time, and this phenomenon is the same as the change of dislocations shown in Fig.12. When the cutting reaches stability, the depth of cut at different initial temperatures has different fluctuations. Comparing the microscopic morphology of the cutting surface at different initial temperatures in Fig. 15, it can be found that when the initial temperature of the cutting layer is 375 K (Fig. 15c), there are fewer color mutations circled and the surface color of the workpiece is more uniformly distributed. This indicates that the depth of cut fluctuates less at this initial temperature and the surface is flatter.

4.2 Experimental analysis

The material used in the experiments was single crystal copper with a crystal orientation of (100), the sample size was

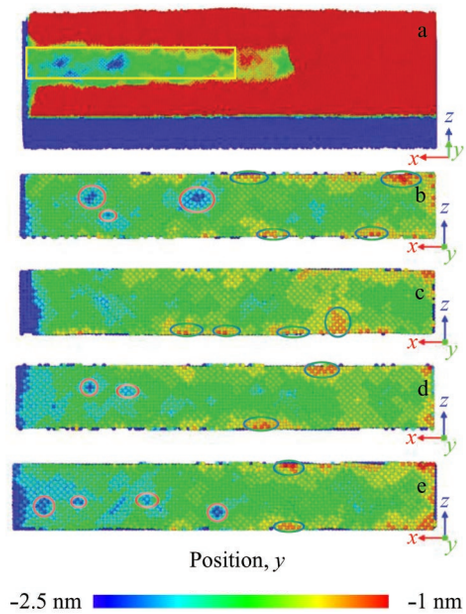

Fig.15 Microscopic morphologies of the machined surface at different initial temperatures of the cutting layer: (a) coloring of the workpiece diagram, (b) 293 K, (c) 325 K, (d) 375 K, and (e) 400 K

5 mm×5 mm×1 mm, and the surface roughness of the sample was R_a<10nm. One side of the sample was polished and the polished surface was used as the experimental surface. Before the experiments, the samples were pretreated and then soaked in acetone and ethanol for 10 min for decontamination. The tool material was diamond with a tip radius of 100 μm and a scratch length of 4 mm, and the applied load was increased from 0 to 2.5 N. Different preheating temperatures were set using the experimental bench heating. The surface morphology of the machined workpiece and the variation curve of the depth of cut were obtained by the testing system that comes with the instrument, as shown in Fig. 16. In Fig. 16a, the red line indicates the trajectory of the tested cutting depth. The depths of cut marked in green and cyan in Fig.16a are enlarged as I and II in Fig.16b.

This experiment belongs to micron cutting, which essentially uses defects in intermolecular joints for machining[3]. Therefore, if a higher degree of surface smoothness is obtained, it indirectly proves that it has fewer defects in the surface dislocations of the workpiece under this condition. From I in Fig. 16b, it can be found that in the section from 2 to 2.275 mm, the depth of cut fluctuates more significantly than that in other conditions when the initial temperature is 293 and 325 K, indicating that in this section, the surface roughness of the machining is high and the workpiece has more defects at this time. From II in Fig.16b, it can be found that in the section from 2.725 mm to 3 mm, the depth of cut fluctuates less when the initial temperature is 293 and 375 K, and the machined surface is smoother, and there are fewer defects at this time. From the plots of depth of cut of

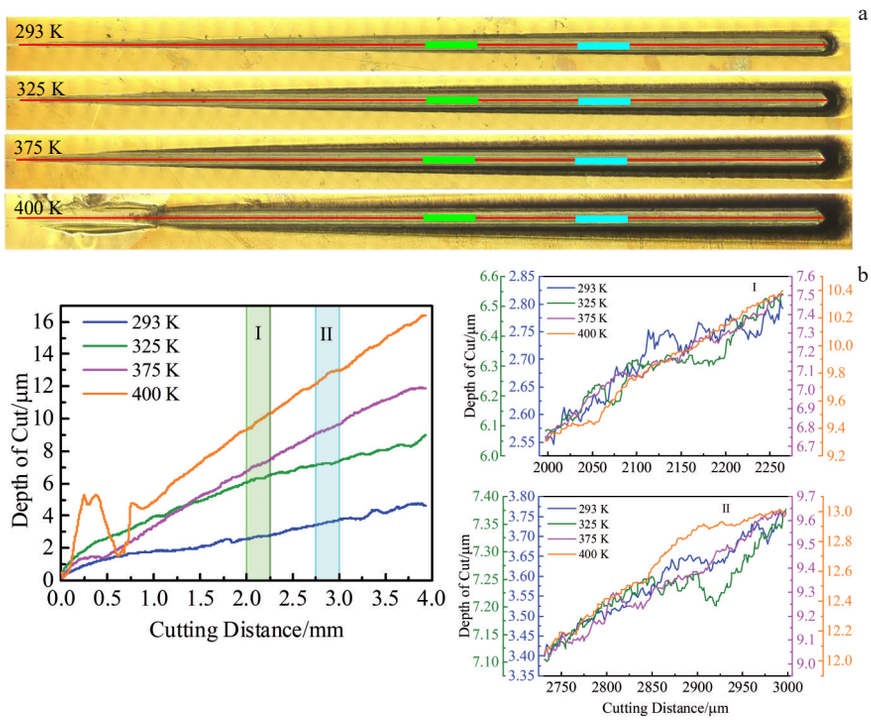

Fig.16 Microscopic images of cutting surface (a) and curves of cutting depth (b) at different initial temperatures

all cutting sections from 0 mm to 4 mm, it can be found that the depth of cut curve obtained at the initial temperature of 375 K is flatter compared with the curves in other cases, indicating that the surface of the workpiece obtained by machining in this case is smoother and has fewer defects.

By analyzing Fig.15 and Fig.16, it can be found that when the initial temperature is 375 K, the surface quality of the workpiece obtained is higher compared to under other conditions, which indicates that there are fewer defects such as dislocations in the workpiece at this time. The initial temperature of 375 K is in the range of 360~390 K, which indirectly verifies that the initial temperature in this range can obtain a higher surface quality.

5 Conclusions

1) The initial temperature of the cutting layer has a certain influence on the cutting force of single crystal copper. The variation of the initial temperature of the cutting layer has a small effect on the fluctuation of the cutting force. When the initial temperature of the cutting layer exceeds 360 K, the strength of the single crystal copper material decreases and the cutting force shows an obvious downward trend.

2) The initial temperature of the cutting layer also has an effect on the lattice structure change of single crystal copper. The higher the initial temperature of the cutting layer, the faster the lattice structure transformation of copper atoms, and the hcp structure atoms transformed from fcc structure atoms are surrounded by dislocations during the cutting process.

3) The initial temperature of the cutting layer affects the length, number and depth of cutting dislocations. The dislocations caused by single crystal copper cutting are mainly Shockley dislocations. When the initial temperature of the cutting layer is 293~400 K, the length and depth of dislocations do not show a single increasing trend with the increase of temperature, but are relatively low at 360~390 K.

4) After the initial temperature of the cutting layer exceeds 400 K, the volume deformation of the workpiece and the atomic structure transformation are large under the effect of high temperature, and the increase of internal microscopic defects during the machining process causes the reduction of the surface quality of single crystal copper. When the initial temperature is in the range of 360~390 K, the internal microscopic defects are less, the structure of the workpiece is more stable, and the cutting force is less during the machining process.

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纳米切削初始温度对单晶铜微观结构的影响

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摘　要：纳米切削会造成工件的内部微观缺陷，这种缺陷会引起残余应力的变化进而影响工件的表面质量，而这种缺陷结构与切削层初始温度有密切联系。为降低工件纳米切削加工制造中的缺陷，采用分子动力学的方法，构建了含有切削层的单晶铜纳米切削模型。首先，通过分析工件结构体积及微观缺陷的变化确定了切削层的适用初始温度；其次，分析了切削层初始温度对切削力的影响，并在不同初始温度和切削力作用下对单晶铜位错和晶格等微观结构的变化进行了分析；最后，通过实验对仿真结果进行了间接验证。结果表明：单晶铜切削层初始温度的可选范围为293~400 K；在此范围内，随着切削层初始温度的升高，切削力大小变化显著，但波动平稳，晶格结构的转变速度也随之增快；当切削层初始温度设在360~390 K范围内时，单晶铜工件的表层微观缺陷相对较少，由此可预测单晶铜工件在此初始温度范围内加工得到的表面质量较高。

关键词：纳米切削；切削层；初始温度；单晶铜；微观结构

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