Simulation Analysis of Influencing Factors of High Pressure Phase Transformation in Single Crystal Germanium Ductile Cutting

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Abstract: The high-pressure phase Ge-II of germanium has similar metal cutting characteristics. In single-point diamond turning, in order to maximize the high phase transition zone of germanium, that is easily to make ductile cutting realized. The single factor test method is used to simulate the ultra-precision turning process under different machining process parameters and tool geometric parameters. Through the calculation of the area of the high-pressure phase change zone in the simulation results and the description of the cutting temperature change law, the influence law of different process parameters and tool geometry parameters on the evolution of the phase change zone is obtained, which provides a useful reference for the choice of turning test parameters.

1. Introduction

Single crystal germanium has the characteristics of high brittleness and low fracture toughness, and it is prone to chipping and cracking during processing. However, studies have shown that when the cutting thickness is less than a certain critical value, single crystal germanium can achieve ductile cutting, and the critical cutting thickness is inseparable from the high-pressure phase change of germanium. For this reason, as early as 2004, Yury Gogotsi [1] studied the HPPT of hard and brittle materials, and found that when the pressure on the contact surface between the tool and the workpiece is equal to or greater than the hardness of the material, the material will undergo HPPT. The resulting HPP has metal-like properties, thereby improving the toughness of brittle materials. Therefore, maximizing the HPP area is of profound significance for ductile cutting of hard and brittle materials. However, in the research on the HPPT of germanium in the turning process, no scholar has been found to analyze the influencing factors of the HPPT. Therefore, this article will simulate the evolution of the HPPT zone from several factors such as tool rake angle, cutting depth, cutting speed and cutting edge radius, and provide a useful reference for the experiment.

2. Modeling and simulation experiment

The simulation was completed by FEM software. The simulated workpiece was the fixed crystal orientation of the (111) crystal plane of single crystal germanium. The material model used Drucker-
Prager [2], used to adapt to pressure sensitivity and the resulting elastoplastic behavior. The model clarifies the characteristics of the material, including elastic and plastic behavior, heat transfer, thermal softening, and strain rate sensitivity. The strain hardening behavior of the D-P model is defined as:

\[ g(\varepsilon^p) = \sigma_0 f(T) \left(1 + \frac{\varepsilon^p}{\varepsilon_0^p}\right)^{\frac{1}{n}} \]  

Where \( \sigma_0 \) is the initial yield stress, \( \varepsilon^p \) is the plastic strain, \( \varepsilon_0^p \) is referring to the plastic strain, \( f(T) \) is the thermal softening function, and \( n \) is the strain hardening index. In order to reflect the influence of high-pressure phase transformation, the initial tensile stress is taken as the value after the hardness value H/2.2, and the initial compressive stress is taken as the hardness value H. The hardness range of germanium is 9-11GPa, and this paper takes 10GPa. Since temperature is also an important factor affecting processing, a fifth-order polynomial is established in the software to fit the thermal softening function. Other workpiece parameters required for simulation are shown in Table 1.

| Material parameters | Elastic Modulus | Poisson's ratio | Hardness | Density | Thermal Conductivity | Specific heat capacity |
|--------------------|----------------|----------------|----------|---------|----------------------|-----------------------|
| Value              | 103GPa         | 0.278          | 10GPa    | 5350kg/m^3 | 59.9W/m K            | 320J/kg C             |

The finite element model is shown in Figure 1, the workpiece size is set to 5μm×2μm, the tool is natural single crystal diamond material, the tool clearance angle is fixed at 10°, and the friction coefficient is set to 0.3. All cutting processes are based on the critical cutting thickness of germanium, the critical depth of cut can be obtained by Equation (2). Using a single factor test method, the cutting speed, tool rake angle, cutting depth, cutting edge radius were changed respectively, and the size and shape of the phase change area were calculated and analyzed.

\[ d_{max} = \begin{cases} a_0 & \sqrt{2Ra_0-a_0^2} \leq f \\ R - \sqrt{R^2 + f^2 - 2f\sqrt{2Ra_0-a_0^2}} & \sqrt{2Ra_0-a_0^2}>f \end{cases} \]  

Where \( a_0 \) is the depth of cut, \( R \) is cutting edge radius of tool, \( f \) is the feed.

3. Simulation results and analysis

The high-pressure phase transition of germanium is a complex process involving many intermediate phases. Reference [1] shows that the phase transition process of germanium is shown in Figure 2. It can be seen from the figure that under hydrostatic pressure, germanium transforms from the semiconductor cubic diamond phase Ge-I to the β-tin structured metal phase Ge-II. The Ge-II phase has metal-like properties and is beneficial for ductile cutting. The phase transition pressure from Ge-I to Ge-II is about 10GPa, and the presence of shear stress can reduce the pressure at the beginning of the phase transition. Therefore, this paper takes 10GPa as the limit for the completion of the Ge-II phase transition, and the initial temperature is set to 20°C, analyze the influence of process parameters and tool parameters, and the simulation results are based on steady-state output.
3.1. The influence of cutting speed

In order to study the influence of cutting speed on germanium HPPT, the cutting speed is set in the range of 1.2m/min-100m/min, and other parameters are set as: cutting depth 150nm, rake angle -35°, cutting edge radius 50nm. The simulation results are shown in Figure 3.

It can be easily seen from the figure that at a cutting speed of 1.2m/min, there is almost no phase transition zone in the workpiece, and when the cutting speed reaches 25m/min, the phase transition zone enlarged, showing an approximately triangular area. When the cutting speed reaches 100m/min, the phase transition zone further increases. It can be seen that as the cutting speed increases, the phase change area also expands, mainly concentrated below the contact area between the tool rake face and the workpiece. Then the area of the phase transition zone at different cutting speeds were calculated, and the result and cutting temperature as a function of cutting speed as shown in Figure 4 was plotted.

It can be seen from Figure 4 that the phase transition zone grows slowly when the cutting speed is 0-20m/min, and when the cutting speed is 60-100m/min, the phase transition zone expands rapidly, showing an overall upward trend. The cutting temperature also increases with the increase of the cutting speed, and the increase of the temperature will inevitably cause the thermal softening of the material, so the influence of frictional heat on the phase transition zone cannot be ruled out during high-speed turning.

3.2. The effect of cutting depth

In order to study the effect of cutting depth on germanium HPPT, the cutting depth is set in the range of 30nm-100nm, and other parameters are set as: cutting speed 20m/min, rake angle -35°, cutting edge radius 50nm, simulation results as shown in Figure 5.
Figure 5 Pressure cloud diagram at different cutting depths (tool hidden)

It can be seen from Figure 5 that when the cutting depth is 30nm, the workpiece has no phase change transition and no chips. The cutting process is mainly material extrusion. As the depth of cut increases, the phase transition zone gradually increases. When the depth of cut reaches 80nm, the phase change area reaches its maximum value. As the depth of cut further increases, the phase change area gradually decreases. The phase transition zone as a whole presents an approximately triangular shape, concentrated under the contact area between the tool rake face and the workpiece. Similarly, the area of the phase transition zone at different depths of cut is calculated, and the result and cutting temperature are plotted as a function of cutting depth as shown in Figure 6.

Figure 6 Phase transition zone and cutting temperature change curve with cutting depth

It can be seen from Figure 6 that there is no phase transition zone in the range of 30–40nm for the depth of cut. When the depth of cut exceeds 50nm, the phase transition zone increases rapidly, and when the depth of cut exceeds 80nm, the phase transition zone gradually decreases. The cutting temperature rises slightly, but the temperature rise is small. In general, the phase transition zone shows a trend of first increasing and then decreasing with the increase of the depth of cut, which is mainly related to the critical cutting thickness of germanium, which can be used to guide the selection of cutting process parameters.

3.3. The influence of tool rake angle

In order to study the influence of the tool rake angle on the germanium HPPT, the tool rake angle is set in the range of -45° to -5°, and other parameters are set as: cutting speed 80m/min, cutting depth 80nm, cutting edge radius 50nm, Figure 7 shows the result.

Figure 7 Pressure cloud diagram at different tool rake angle (tool hidden)

It can be seen from Figure 7 that when the tool rake angle is -5°, the workpiece has no phase change zone and the chip curvature is larger. As the negative rake angle of the tool increases, the pressure and shear force on the workpiece gradually increase. As a result, the phase transition zone gradually increases. When the rake angle of the tool reaches -45°, it is difficult for the workpiece to form chips. Due to the extrusion of the tool, the material accumulates near the rake face. The phase transition zone is first formed at the position close to the blunt circle in contact with the flank surface, and gradually expands to the position in contact with the rake surface. The shape also changes from an approximate
triangle to an approximate ellipse, and the larger the negative rake angle is, the larger the phase transition zone become. Similarly, the area of the phase transition zone under different negative rake angles is calculated, and the result and cutting temperature are plotted as a function curve of the rake angle as shown in Figure 8.

Figure 8 Phase transition zone and cutting temperature change curve with tool rake angle

It can be seen from the curve that the phase change zone changes little when the rake angle is between -5 and -30°, and when the current angle is less than -30°, the phase change zone expands sharply, so when processing germanium materials, the tool can be selected within a reasonable range a larger negative rake angle is beneficial to expand the size of the phase transition zone. The overall cutting temperature shows a trend of declining fluctuations. The temperature is lower at a larger negative rake angle. This is mainly due to the large negative rake angle increasing the contact area between the tool and the material, and the diamond tool has excellent thermal conductivity.

3.4. Influence of the cutting edge radius

In order to study the influence of the cutting edge radius on the HPPT of germanium, the cutting edge radius is set in the range of 10nm to 200nm, and other parameters are set as: cutting speed 80m/min, cutting depth 80nm, tool rake angle -35°, the simulation result is shown in Figure 9.

Figure 9 Pressure cloud diagram at different cutting edge radius (tool hidden)

Figure 10 Phase transition zone and cutting temperature change with cutting edge radius

It can be seen from Figures 9 and 10 that the increase of the cutting edge radius reduces the sharpness of the cutting edge, so it is relatively difficult for a large blunt round tool to form chips. When the radius of the cutting edge radius is 150nm, there is no chip generation, which is also related to the depth of cut. When the radius of the cutting edge is within 150nm, the phase transition area shows an upward trend, mainly because when the cutting depth is extremely small, the large blunt round of the cutting edge is equivalent to indirectly increasing the negative rake angle, so the pressure and shear stress Larger. When
the blunt edge of the cutting edge exceeds 150nm, it is difficult for the material to squeeze with the rake face, so there is almost no phase transition zone. The overall cutting temperature decreases as the blunt edge of the cutting edge increases, which is mainly related to the friction area between the rake face and the material.

4. Conclusion
The micro-cutting simulation of the single crystal germanium ultra-precision turning process was carried out using FEM software. Through the single factor test method, the area of the phase transition zone under different process parameters and tool geometric parameters was calculated and analyzed, and the change of cutting temperature regular curve is described. It can be known that in the process of expansion of the germanium high-pressure phase transition zone, it mainly evolves from a triangular shape to an elliptical shape; within the selected parameter range, in order to maximize the phase transition zone, the best process parameter is: cutting speed 80 to 100m/min, cutting depth 70-90nm; the best tool geometry parameters are: rake angle -35° to -45°, cutting edge obtuse radius 50-100nm, which provides a useful reference for the selection of test parameters.

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