Fluent simulation and experimental analysis of polished surface topography of single crystal germanium

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Abstract. Single crystal germanium has good physical and chemical properties but it is hard to be processed. Some researchers thought the flowing effort has no effect on the removal of test-piece surface material during the polishing process. This paper had built a flow-path simulation model and used Fluent to simulate the polishing process and designed experiment to analyse the polishing process. It was found in experimental results that, during the polishing process two-phase flow could smooth the surface of single crystal germanium, but it could also cause the edge surface material uneven removal on the test-piece, moreover, the uneven degree on both sides of polished test-piece were different, the roughness on middle part of test-piece was smaller than edge sides. Meanwhile, the residual stress was mainly caused by abrasive material properties and other conditions. The conclusion mentioned above were consisted with the simulation results, which proved the correctness of simulation model and assumptions, and the flowing effect of polishing liquid had effect on the removal of surface material. The paper provides a new research thought on two phrase flow polishing.

1. Introduction

Single crystal germanium has good physical property which makes it widely used in many fields. Meanwhile, because of the brittleness of single crystal germanium, its surface is difficult to be processed effectively by traditional polishing technology. Nowadays the two-phase flow polishing technology had been developed, by using two-phase flow polishing technology can get the surface of brittle and hard materials smoother. As in [1-4], many scholars believed it is two-body and three-body wear and uneven pressure distribution caused the remove of material on the surface of test-piece and surface defects, however, as in [5-10] there are still many scholars believed the removal of material on the surface of processed test-piece due to liquid phase flow. In order to study the material removal mechanism in polishing process, a flow-path model had been established based on the relative location, motion relationship and abrasive theory. This paper used Fluent finite element software to simulate the polishing process and designed experiments to verify the correctness of simulation, provided a new research idea on single crystal germanium two-phase flow polishing.

2. Two-phase flow polishing theory

2.1 Impact theory of abrasive
Hrosovsky advanced: The grains suffer vertical and horizontal force which cause micro-cut and impact wear on the surface of test-piece. However, impact removal effect could not only be informed by grains cutting action, to make up this deficiency, researcher proposed the theory of rigid grains impact wear on plastic material. The expression of wear rate in unit time and area is:

$$W = \sum_{i=1}^{n} E / A$$  \hspace{1cm} (1)

Where: $W$- the wear rate in unit time and area (unit: kg/m$^2\cdot$s), $E$- wear loss, $n$- the number of grains impact on the wall of test-piece in unit time, $A$- the wear area. The expression of wear loss $E$ is:

$$E = c \cdot f(\gamma) m v^2 / \psi \sigma_f K$$  \hspace{1cm} (2)

Where: $c$- rate of effective impact grains, $m$- particle mass, $v$- speed of grains, $\psi$-ratio of cutting length and depth, $\sigma_f$- flow stress of plastic material; $K$-grain shape parameter; $f(\gamma)$ - effect of impact angel. The expression of impact angle $f(\gamma)$ is:

$$f(\gamma) = \begin{cases} 
(\sin 2\alpha - 6 \sin^2 \alpha) \rho, & (\alpha < \alpha_0) \\
\cos^2 \alpha \rho, & (\alpha > \alpha_0) 
\end{cases}$$  \hspace{1cm} (3)

Where: $\alpha$ -angel of impaction; $\alpha_0$ - critical angle of incidence; $\rho$ -density of test-piece material.

This model can explain the wear law of polygonal grains on plastic materials under the condition of small impact angel. However, the erosion error of non-polygonal grains, the error of large angle impaction and error of non-typical plastic materials are large.

2.2 Particle dynamics theory in solid-liquid two-phase flow

The interaction between particles are affected by fluid and fluid motion, if the influence of abrasives on abrasive flow is neglected, the research on solid-liquid flow motion is changed into the research on abrasive dynamic. According to the Newton’s Second Law, the simplified single abrasive motion equation is:

$$m(dv / dt) = \sum F$$  \hspace{1cm} (4)

Where the $m$ is the abrasive quality, $m(dv / dt)$ is abrasive inertia force, $\sum F$ is resultant forces on abrasives, the resultant efforts are as follows:

$$\sum F = F_d + F_b + F_a + F_m + F_B + F_P + F_M + F_S + ...$$  \hspace{1cm} (5)

3. Simulation and analysis of impact effect of abrasive flow

3.1 Establishment of simulation model and simulate

Rotary polishing machine is widely used in the polishing process. This kind of polishing machine consists of polishing disk, carrier disk, polishing pad and polishing liquid delivery system, the simplified polishing process is shown as figure 1(a). In this paper, the material removal effect on the surface of test-piece in polishing process is studied. Therefore, we assume that the carrier disk and polishing disk are relatively stationary, only the polishing liquid flows in a single direction. To simplify the abstract model, the surfaces of single crystal germanium, carrier disk and polishing disk are taken as the boundary of the flow-path model. During the simulation process, the boundary of flow-path is thought to be static, only polishing liquid flows in the flow-path, so the constraint condition of each edge of flow-path and simulation model is shown as figure 1(b).
3.2 Simulation of different abrasive materials

During the polishing process, the material of abrasive would have effect on the surface quality of test-piece. According to this conclusion, the paper selected silicon dioxide, diamond, alumina and cerium dioxide four common abrasive materials for the simulation, the size of abrasives were set in 0.5μm, the speed of polishing liquid flow was 90m/s, the simulation results were shown as figure 2.

![Figure 2. Simulation results](image)

It can be seen from figure 2(a) to figure 2(d) that, during the polishing process, the pressure decreases sharply at the abrupt change of flow-path shape in the inlet and outlet side. From figure 2(e) we can see that, the pressure difference drives abrasives in polishing fluid to move along the direction of pressure change, at this moment, the speed vector significantly changed, which causes the surface material removal more serious on the inlet and outlet sides of the flow-path than the narrow part of flow-path. Meanwhile, because of the negative pressure area at the outlet side is larger, which may increase the disorder of abrasives moving direction and make the surface material removal on the outlet side is more serious than that of inlet side. The pressure difference between two sides of test-piece makes abrasive move alone the flow-path, and had little effect on the moving direction of flowing abrasives, which caused material removal on the middle part on the surface of test-piece, made the middle part on the surface is smoother than that of two edge sides of test-piece. From the results above we can conclude that, the change of pressure caused by the shape change of flow-path has effect on the direction of abrasive motion. The abrasive motion causes the removal of surface material and has effect on the surface roughness of test-piece.
From figure 2(b) and figure 2(c) we can see that by using diamond and cerium dioxide abrasives, the negative pressure area near the outlet is relatively large. It can be inferred that, by using those two materials of abrasive could cause relatively obvious material removal and surface undulation on the edge of test-piece. The pressure difference caused by using diamond abrasive is larger than that caused by using cerium dioxide, the simulation result shows that the negative pressure area caused by those two abrasives are extended to narrower flow-path area. The pressure difference and the negative pressure caused by using diamond and cerium dioxide are relatively large, which could make abrasives have more kinetic energy, the removal effect of surface material could relative large and surface roughness of middle part of test-piece surface could be relative small, especially by using diamond abrasive may have the smallest surface roughness, meanwhile, using silica abrasives could not get a better surface quality because of the low pressure difference.

The residual stress may mainly cause by the impaction of flowing abrasives, which means the abrasive motion irregularity could have effect on the residual stress on the surface of processed test-piece. The negative pressure area caused by using abrasives of diamond and cerium dioxide materials are relatively large, which means the motion disorder caused by using those two abrasive materials are large. So using abrasives of those two materials could cause larger residual stress, and using silica abrasives could get lower residual stress.

By analysing the simulation results we could make following assumptions: 1) After processing, the degree of material removal and surface undulation on both edge sides of the test-piece will be different, 2) Using diamond and cerium dioxide abrasive would cause the most serious surface material removal and surface undulation on both edge sides of test-piece, 3) The roughness of middle part of test-pieces surface are smaller than the edge sides, 4) The residual stress caused by using diamond and cerium dioxide abrasives may larger than caused by using abrasives of other two materials, 5) The larger pressure difference could cause the smaller surface roughness, 6) By using diamond abrasive could get the minimum Roughness and the max residual stress.

4. Experimental design and results analysis

4.1 The design of experiment

In order to verify the effectiveness of simulation, the polishing experiments were carried out with polishing machine. The size and material of abrasives used in experiment were: 0.1μm diamond, 0.1μm silicon, 0.5μm alumina and 0.5μm cerium dioxide. After processed the test-pieces were cleaned and tested.

(a) 0.1μm diamond abrasive
(b) 0.5μm alumina abrasive
4.2 Analysis of the experimental results

The tested surface topographies of polished test-piece are shown as figure 3. From the experimental results we can conclude that, the surface accuracy had been improved after polished, meanwhile by using 0.1μm diamond abrasive could get the minimum roughness. However, it can be seen that, the planeness of test-piece is uneven, on the both edge sides of test-piece this phenomenon is much obvious. From figure 3(a) and (b) we can see, the surface topography of both edge sides are rougher than the middle part, and the roughness on one edge side of test-piece is rougher than that of the other side, the roughness of both sides is larger than that of the middle part of test-piece. The conclusions mentioned above are consistent with the assumption 1), assumption 2), assumption 3) and assumption 5).

By using diamond and alumina abrasives could get smaller roughness in the middle part of test-piece surface, from simulation results we can see that, the pressure difference on both sides of test-piece caused by these two abrasives are relative large, makes abrasive have higher kinetic energy, which strengthened the impaction of abrasive on the surface of test-piece, and makes surface material removal more effective, this experimental result is also consisted with the simulation result and assumption 4), proving the effective of simulation model. However, the surface roughness obtained by using cerium dioxide abrasive is not consistent with the simulation result, this is mainly because the polishing liquid used in the experiment has large viscosity, caused the larger disorder of abrasive motion made the roughness of test-piece larger. In order to get more obtain more accurate simulation results, the viscosity of polishing liquid should be considered during the process of simulation.

Figure 4. The residual stress

The residual stress value of polished test-pieces is shown as Figure 4. From figure 4 we can conclude that, by using silica abrasive could get the largest residual stress, and using cerium dioxide abrasive could get smallest residual stress. Using diamond abrasive, we get larger residual stress, but it is relatively smaller than that of using silica abrasive. The conclusions based on figure 4 prove that the
disorder of abrasive motion and flowing of polishing liquid may cause the residual stress, but those two conditions are not the main reasons of causing residual stress, the material properties such as the size and the modulus of elastic are the main conditions for producing residual stress, which means the assumption 4) and 5) are not correct. In order to research the factors affecting residual stress, the simulation of abrasive impaction should be done.

5. Conclusion
1) A flow-path simulation model had been built. By analysing the results of simulation and experiment, we can conclude that, during the process the liquid effect have effect on the removal of surface material, which verified the correctness of simulation.

2) The removal degree of surface material on the surface and the both edges of test-piece are different, the roughness of middle part of surface is relatively smaller than that of both sides, this phenomenon mainly caused by the pressure difference of flowing polishing liquid.

3) The residual stress has no effect with the pressure difference caused by using different materials of abrasive. In order to study the relation between abrasive materials and residual stress, the impaction simulation should be done.

4) Processing with existing conditions and polishing liquid, using 0.1μm diamond abrasive could get small surface roughness.

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