Investigation of the trajectory uniformity in water dissolution ultraprecision continuous polishing of large-sized KDP crystal

Zhipeng Cheng, Hang Gao, Ziyuan Liu and Dongming Guo

Key Laboratory for Precision and Non-Traditional Machining Technology of Ministry of Education, Dalian University of Technology, Dalian 116024 People’s Republic of China

E-mail: gaohang@dlut.edu.cn

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Abstract
Large-sized potassium dihydrogen phosphate (KDP) crystals are an irreplaceable nonlinear optical component in an inertial confinement fusion project. Restricted by the size, previous studies have been aimed mainly at the removal principle and surface roughness of small-sized KDP crystals, with less research on flatness. Due to its low surface damage and high machining efficiency, water dissolution ultraprecision continuous polishing (WDUCP) has become a good technique for processing large-sized KDP crystals. In this technique, the trajectory uniformity of water droplets can directly affect the surface quality, such as flatness and roughness. Specifically, uneven trajectory distribution of water droplets on the surface of KDP crystals derived from the mode of motion obviously affects the surface quality. In this study, the material removal mechanism of WDUCP was introduced. A simulation of the trajectory of water droplets on KDP crystals under different eccentricity modes of motion was then performed. Meanwhile, the coefficient of variation (CV) was utilized to evaluate the trajectory uniformity. Furthermore, to verify the reliability of the simulation, some experimental tests were also conducted by employing a large continuous polisher. The results showed that the CV varied from 0.67 to 2.02 under the certain eccentricity mode of motion and varied from 0.48 to 0.65 under the uncertain eccentricity mode of motion. The CV of uncertain eccentricity is always smaller than that of certain eccentricity. Hence, the uniformity of trajectory was better under uncertain eccentricity. Under the mode of motion of uncertain eccentricity, the initial surface texture of the 100 mm × 100 mm × 10 mm KDP crystal did achieve uniform planarization. The surface root mean square roughness was reduced to 2.182 nm, and the flatness was reduced to 22.013 µm. Therefore, the feasibility and validity of WDUCP for large-sized KDP crystal were verified.

1 Author to whom any correspondence should be addressed.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Potassium dihydrogen phosphate (KDP) crystal is an excellent electro-optic nonlinear optical material and is the only material for electro-optic switches and laser-frequency conversion applications in high-energy laser systems for inertial confinement fusion (ICF) [1, 2]. For an inertial confinement fusion (ICF) project, the machining requirements for KDP crystals are large size, low surface roughness, and high flatness accuracy [3]. However, due to its high brittleness, soft texture, easy deliquescence, and sensitivity to temperature, KDP crystals are regarded as difficult to machine, which makes it hard to achieve defect-free machining [4]. Although the traditional processing method can obtain a surface root mean square (RMS) roughness of up to nanometer scale, these methods have inherent weaknesses such as micro-waviness and subsurface damage from single-point diamond turning (SPDT) [5, 6], plastic grinding cracks and brittle flaking pits from grinding [7, 8], and abrasive embedment and surface fogging for magnetorheological finishing (MRF) processing [9, 10].

In recent years, water dissolution polishing has been considered to be a promising technology for achieving a super-smooth, super-clean KDP crystal surface, which is based on traditional chemical mechanical polishing (CMP) and abrasive-free slurry [11–15]. Guo [16] and Zhang [17] used water dissolution polishing to conduct a test on a ZYP 280 polisher and obtained a smooth surface with a surface RMS roughness of less than 5 nm. Wang [18, 19] processed small-sized (18 mm × 18 mm × 10 mm) KDP crystals and achieved satisfactory results (a surface RMS roughness of approximately 1.7 nm) by using water-in-oil slurry and a ZYP 200 polisher. Dong [20] polished small-sized (35 mm × 35 mm × 10 mm) KDP samples with a KDP aqueous solution-in-oil microemulsion. A super-smooth surface with a surface RMS roughness of 1.5 nm was obtained.

In the previous studies, limited by their size, the investigators focused their research on the removal principle and surface roughness of small-sized KDP crystals and less research on flatness. The outcomes of these studies had little reference value to the large-sized KDP crystals needed for engineering applications. Although the surface quality of small-sized KDP crystals greatly improved with water dissolution polishing, the processing of large-sized KDP crystals has so far not been as dramatic. Continuous polishing technology is the main processing method for large-sized optical components in engineering production, which can achieve high-precision processing [21]. So, water dissolution ultraprecision continuous polishing (WDUCP) is a good choice for processing large-sized KDP crystals. The uniformity of water droplet trajectory has a significant impact on surface quality, including flatness and roughness. Furthermore, the more uniform the trajectory is distributed, the better the surface quality. Different modes of motion lead to an uneven trajectory of water droplet distribution on a KDP surface, resulting in different surface quality. Therefore, investigating the uniformity of water droplet trajectory under different modes of motion was an effective way of achieving a super-smooth, super-clean surface of large-sized KDP crystals.

In this study, WDUCP was developed to process large-sized KDP crystals. The motion trajectory equations were established based on the movement relationship between the KDP crystals and the polishing pad. The coefficient of variation (CV) was introduced as the standard for evaluating trajectory uniformity. The polishing pad with the spiral groove can achieve better processing comparing the circular groove in previous studies. Therefore, for the spiral groove of the polishing pad, the trajectory of water droplets located on the
crystal surface was simulated at certain and uncertain eccentricity modes of motion. Moreover, to verify the simulation results, some polishing tests were also conducted using a large continuous polisher. The study has reference value and guidance significant to the large-sized KDP crystals used in engineering applications.

2. Methodology

2.1. Material removal mechanism of WDUCP

Water dissolution polishing is a special CMP technology whose slurry is abrasive free. A water-in-oil microemulsion is one of the abrasive-free slurries for KDP crystals studied by our research team. The water-in-oil slurry was composed of water, oil, and surfactant; and water molecules were caged into micelles to form the water droplets [15]. The polishing pad was in direct contact with the crystal surface under a certain polishing pressure, \( F \), in the polishing zone, as shown in figure 1(b). The mechanical movement between the polishing pad and the crystal was produced by rotation. Under the effect of pressure and friction, water droplets were crushed and deformed, which led to the release of water. Then the deformed and broken water droplets dissolved materials in the dissolve layer. The dissolved product was carried away through the groove with the flow of the new slurry and the rotary motion of the polishing pad, as shown in figure 1(a). Thus, planarization polishing of KDP crystals can be achieved.

2.2. Motion trajectory of water droplets on a KDP crystal surface

At present, the motion modes of the most commonly used equipment in WDUCP are certain and uncertain eccentricity. A common certain eccentricity polishing system is shown in figure 2(a), where the center distance between the polishing pad and the KDP crystal is always the same. The polishing pad and the crystal holder rotate around their own axis. The crystal is clamped by the holder, and the processing surface is pressed against the polishing pad. The slurry is evenly dropped on the polishing pad from the near center to achieve the processing of the crystal. Most of the continuous polisher adopts the motion mode. By contrast, the polishing pad and the crystal actively rotate around their own axis for the uncertain eccentric polishing system (figure 2(b)), and the crystal swings linearly in a radial direction. The center distance between the polishing pad and the KDP crystal changes periodically. Hence, it requires a larger diameter polishing plate, which is frequently applied for processing large-sized components.

A simplified diagram of a motion model of a certain eccentricity polishing system is shown in figure 3(a). In figure 3(a), the origin \( O_1 \) is the center of the polishing pad; and \( X_1O_1Y_1 \) is the fixed coordinate system fixed on it. The origin, \( O_2 \), is the center of the KDP crystal, and \( X_2O_2Y_2 \) is the fixed coordinate system fixed on it. Also, \( R, r, e \) denotes the radius of the polishing pad and the KDP crystal, respectively; \( \omega_p \) and \( \omega_o \) are the angular velocity of the polishing pad and the KDP, respectively; and \( t \) is the polishing time. As a water droplet, whose distance apart from \( O_1 \) is \( r_o \), begins to contact the KDP at point \( P \). Then the motion trajectory, equation (1), of water droplets on the KDP crystal surface by the graphical transformation method can be shown as follows:

\[
\begin{align*}
\begin{cases}
X_{2P} &= r_o \cos(\omega_p - \omega_o) t + e \cos \omega_o t \\
Y_{2P} &= r_o \sin(\omega_p - \omega_o) t - e \sin \omega_o t
\end{cases} \quad (1)
\end{align*}
\]

A simplified motion diagram of an uncertain eccentricity polishing system is shown in figure 3(b). The crystal swings linearly on the \( X \)-axis around \( O_2 \), the swing speed is \( V \), the swing amplitude is \( A \), and the swing period is \( T \). Similarly, the motion trajectory equation (2) of initial position water droplets \( P \) on the KDP crystal surface can be shown as follows:

\[
\begin{align*}
\begin{cases}
X_{2P}' &= r_o \cos(\omega_p - \omega_o) t + e \cos \omega_o t + A \sin \frac{\pi}{T} t \\
Y_{2P}' &= r_o \sin(\omega_p - \omega_o) t - e \sin \omega_o t
\end{cases} \quad (2)
\end{align*}
\]

2.3. Simulation setup of water droplets of WDUCP

The polishing pad is in direct contact with the crystal surface, which significantly affects the removal rate and surface quality. The polishing pad grooves are one of the most elements for slurry polishing performance, and surface grooves on a polishing pad can ensure uniform slurry distribution [22]. This study used the spiral grooves of the IC1000 polishing pad (Rohm & Haas Corporation, America). According to the aspect ratio of the width and depth of grooves, it was assumed that the spiral distribution of water droplets on the polishing pad was as shown in figure 4.

When the microstructure of a work piece material, such as grain size, was comparable in size to the tool edge radius and depths of cut, the microstructure size effect occurred. The size effect was a dominant factor in the material removal mechanism used in the microcutting [23]. Similarly, the accumulation of the water droplets’ trajectory could cause the size effect in WDUCP, which affects the surface quality. So it is necessary to study the trajectory uniformity of water droplets.

In order to obtain an effective trajectory of water droplets, the model needed to be simplified; therefore, ideal uniformity hypotheses were proposed. The following assumptions were made in the trajectory uniformity simulation: the distribution of the water droplets on the polishing pad was uniform, the material removal rate of water droplets was equal in each region, the material removal amount of water droplets could linearly accumulate in each region, and the water droplets were treated as a particle.

To calculate trajectory uniformity, the crystal surface was divided into a plurality of grids, shown in figure 5. The equations of motion trajectory (equations (1) and (2)) were imported into MATLAB® for discretization analysis. The number of track points in each region, such as \( S_1 \), was counted. The number of sample points in the entire divided region was obtained by the region dividing strategy and the region statistical strategy. These sample points made up the sample
The standard deviation, \( \sigma \), and arithmetic mean, \( \mu \), were calculated.

It is noteworthy that the standard deviation and arithmetic mean have their limitations, which are easily affected by different sample data. The CV can be the assessment standard of the dispersed extent of trajectory uniformity. Liu [24] successfully used the CV to represent nonuniformity of material removal in electrochemical mechanical polishing. The CV can eliminate the influence of measurement scale and dimension. According to the equations of motion trajectory, the trajectory uniformity was affected by many factors. It is hard to see the influence law with the aid of a trajectory distribution figure. The CV can directly show the absolute value of the dispersion degree under different factors. Therefore, the CV was introduced as the evaluation standard of trajectory uniformity.

The CV is defined as the ratio of sample standard deviation, \( \sigma \), to arithmetic mean, \( \mu \), which is used to describe the degree of dispersion between two sets of samples with different expectations. It can be written as equation (3):

\[
CV = \frac{\sigma}{\mu}.
\]  

The CV is not only affected by the discrete degree but also by the average level. The smaller the CV, the better the trajectory uniformity and vice versa. The trajectory uniformity is quantified by the CV.

In this study, the trajectory uniformity of water droplets under certain and uncertain eccentricity was simulated. The specific processing parameters are shown in table 1. The simulation time was set as \( t = 10 \) s; and the speed ratio was Q.
Polishing pad
KDP crystal
Water droplets of spiral

Figure 4. Schematic of spiral distribution of water droplets.

Track point
Grid region

Figure 5. The mesh of the KDP crystal.

Table 1. Process parameters for WDUCP under the motion modes of certain and uncertain eccentricity.

| Process parameters                  | Value or value range |
|-------------------------------------|----------------------|
| Angular velocity of polishing pad, \( \omega_p \) (rad \( \cdot \) s\(^{-1} \)) | \( \pi/3 \)            |
| Radius of polishing pad, \( R \) (mm) | 540                  |
| Radius of KDP crystal, \( r \) (mm)    | 50                   |
| Eccentricity, \( e \) (mm)            | 350                  |
| Preliminary angle, \( \theta \) (\(^{\circ}\)) | 0                    |
| Swing amplitude, \( A \) (mm)          | 110                  |
| Swing speed, \( V \) (mm \( \cdot \) s\(^{-1} \)) | 200                  |
| Swing period, \( T \) (s)              | 0.55                 |
| Speed ratio, \( i \)                  | 0–1                  |

0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0. By adopting the same simulation parameters, the simulation trajectory of the water droplets under certain and uncertain eccentricity was simulated and analyzed.

For the uncertain eccentricity polishing system, the influence of the swing amplitude on the trajectory uniformity was studied further. The parameters were set as \( i = 1 \) and \( V = 50 \) mm \( s^{-1} \). The swing amplitude, \( A \), was 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, and 275. Then the trajectory of water droplets was simulated and analyzed under the different swing amplitudes.

2.4. Experiment testing setup for WDUCP under certain and uncertain eccentricity motion modes

The WDUCP tests were conducted at different speed ratios on the large continuous polisher with a 1080 mm polishing plate, which can operate the certain and uncertain eccentricity motion modes. The concrete structure is shown in figure 6. The large continuous polisher uses a hydrostatic spindle and automatic control system composed of a multimotor, multidrive, programmable logic core (PLC). The polisher can carry out steep speed changes of swing speed and automated processing. A 100 mm \( \times \) 100 mm \( \times \) 10 mm KDP crystal was chosen as the test sample.

The IC1000 polishing pad was utilized, and the water-in-oil slurry was supplied at a flow rate of 30 ml min\(^{-1}\). The polishing pressure on the KDP crystal was 10 kPa, the polishing time was 20 min, and other parameters were the same as used in the simulation. To diminish the interference factors, all of the tests were carried out in a cleanroom (grade 1000, 22 \(^{\circ}\)C). An Olympus MX40 metallurgical scope was employed (Olympus Corporation, Japan) to observe the processed surface. A ZYGO NewView™ 5022 3D surface profiler was used (ZYGO Corporation, America) to measure the surface RMS roughness. The flatness of the processed KDP crystal was measured by the Flatmaster® 200 (Corning Tropel Corporation, America).

3. Results, analysis, and discussion

3.1. The trajectory uniformity analysis under certain and uncertain eccentricity motion modes

The simulations results of certain and uncertain eccentricity are shown in figure 7. The results show that when the speed ratio was in the range of 0–1, the CV varied from 0.67 to 2.02 under the certain eccentricity motion mode and varied from 0.48 to 0.65 under the uncertain one. When the speed...
ratio was 0.1, the difference between the certain and uncertain eccentricity was the largest. A comparison of removal times is shown in figure 8. Here, the difference was the smallest at a speed ratio of 1 (figure 9). At the same speed ratio, the CV was small under uncertain eccentricity, which illustrates that trajectory uniformity was better. What is more, the material removal times were almost the same in different regions; and the fluctuation was small. Therefore, it is beneficial to achieve high-quality processing of large-sized KDP crystals for uncertain eccentricity.

Meanwhile, the CV of trajectory uniformity under certain eccentricity was relatively large; and the material removal was generated mainly in the center and on the edge of the crystal. Hence, the crystal surface tended to be boss-shaped from the center to the edge region. The material removal times were inconsistent in different regions and fluctuated severely. With the increase in the rotational speed ratio, the CV decreased gradually on the whole. The material removal uniformity of the crystal surface was continuously improved as the speed ratio increased.

Furthermore, as the speed ratio changed, the CV of the certain eccentricity changed dramatically; and the variation degree of uncertain eccentricity tended to be stable. When using a certain eccentricity motion mode, the surface accuracy can be quickly improved by changing the speed ratio. We can adopt the uncertain eccentricity motion mode to realize the ultraprecision process of large-sized KDP crystals.

3.2. The trajectory uniformity analysis of swing amplitude

Figure 10 shows that the CV decreased as the swing amplitude increased. That means an increase in the swing amplitude was beneficial to trajectory uniformity. When the swing amplitude was less than the KDP crystal diameter, the CV was larger. The CV decreased rapidly when swing amplitude, A, was greater than 100 mm. This further confirmed that a large-diameter polishing plate can significantly improve the surface quality. Therefore, the polishing plate diameter should be as large as possible in the design of a continuous polisher.

3.3. Tests results of surface quality

A comparison of surface morphology after processing under certain and uncertain eccentricity is shown in figure 11. We can see that there are fine scratches on the surface in figure 11(a). Meanwhile, there are no obvious defects on the crystal surface in figure 11(b).

A comparison of surface roughness under certain and uncertain eccentricity is shown in figure 12. The measurement results show that the surface RMS roughness after the certain and uncertain eccentricity’s processing reached 4.678 nm and 2.182 nm, respectively. The surface RMS roughness was small under the uncertain eccentricity motion mode, and a super-smooth surface was obtained.

A comparison of flatness under certain and uncertain eccentricity is shown in figure 13. The results show that flatness under the certain and uncertain eccentricity’s processing reached 32.207 µm and 22.013 µm, respectively. The surface was higher at the center than at the edge after processing. This is because the flow behavior of the polishing slurry was unequal in different locations of the polishing pad, which can affect the contact opportunities, contact area, and dissolution rate of the water droplets and KDP crystals. As a general rule, the edge of KDP crystal touches the slurry first. Then the center of KDP crystals touches the slurry with the flow of slurry. The slurry tended to accumulate at the edge due to the centrifugal effect, i.e. the slurry was not evenly distributed in the KDP crystal in the actual polishing process. The edges touched more slurry compared to the center of the KDP crystal, which means the material removal was relatively larger. The swing motion can decrease the uneven distribution under the uncertain eccentricity motion mode, which can improve the surface quality. Consequently, WDUCP can obtain a super-smooth, super-clean KDP surface under uncertain eccentricity motion mode, which is consistent with the simulation results.

4. Conclusion

The simulation and experimental tests of the trajectory uniformity of water droplets on the large-sized KDP crystal surface under certain and uncertain eccentricity motion modes obtained a super-smooth surface on the large-sized KDP crystal. The validity of the theory was tested by polishing experiments. The study verified the feasibility and effectiveness of processing large-sized KDP crystals by WDUCP. The experimental results were all in reasonable agreement with related theories. The investigation provided a theoretical guide for the polishing of large-sized, water-soluble materials. The main conclusions are:

(a) When the speed ratio was in the range of 0–1, the CV varied from 0.67 to 2.02 under the certain eccentricity motion mode and varied from 0.48 to 0.65 under the uncertain
Figure 8. The removal times at a speed ratio of 0.1: (a) certain eccentricity and (b) uncertain eccentricity.

Figure 9. The removal times at a speed ratio of 1: (a) certain eccentricity and (b) uncertain eccentricity.

Figure 10. The CV about swing amplitude under uncertain eccentricity.

Figure 11. Surface morphology after WDUCP: (a) certain eccentricity and (b) uncertain eccentricity.
eccentricity motion mode. Therefore, the trajectory uniformity was better under the condition of uncertain eccentricity.

(b) The effect of the speed ratio on certain and uncertain eccentricity was basically the same. However, the speed ratio had a greater impact on the certain eccentricity polishing system compared with uncertain eccentricity.

(c) The increase of the swing amplitude under the uncertain eccentricity motion mode was conducive to the uniform polishing. Hence, in the design of a continuous polisher, the polishing plate diameter selected should be as large as possible.

(d) By employing the WDUCP under the motion mode of uncertain eccentricity, a super-smooth surface of 100 mm × 100 mm × 10 mm was obtained without abrasive, with a surface RMS roughness of 2.182 nm and a flatness of 22.013 μm.

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ORCID iD

Zhipeng Cheng https://orcid.org/0000-0003-0230-0384

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