Investigation of the Optical Effects of Single Point Diamond Machined Surfaces and the Applications of Micro Machining

Dissertation

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ABSTRACT

The ultraprecision Single Point Diamond Turning (SPDT) technology has been developed for over 40 years and has been successfully applied to numerous fields. At present, the ultraprecision single point diamond turning technology already expanded to Single Point Diamond Machining (SPDM) technology, which includes several related processes in addition to the more conventional single point diamond turning. The other related processes are Fast Tool Servo (FTS), Slow Tool Servo (STS), broaching, and fly cutting.

Though this technology has many notable merits, for example it can achieve micro meter or even sub micron form accuracy and nano meter surface roughness, there still has some drawbacks. One of the objectives of this research is to investigate one of these drawbacks, the diffraction and scattering of the ultraprecision single point diamond machined surfaces. Another objective is to extend the application of the SPDM by developing new design and new machining processes for freeform micro devices used in optical, mechanical, electronic, and biomedical fields.

The mechanism and model of the ultraprecision single point diamond turning and micro cutting were first reviewed and discussed. The related subjects to the SPDT and micro cutting were also involved. The optical effects of diamond machined
surfaces were studied. The diffraction and scattering generated from the diamond machined surfaces was analytically and experimentally studied. The influences from machining parameters, such as tool mark spacing, feedrate, spindle speed, tool radius, tool condition and different diamond machining process were considered. An empirical relationship between the machining conditions and the first order diffraction from the diamond machined surfaces was setup. This model can be used to select optimal machining conditions for diamond machining process.

The design, machining and testing of microlens arrays by using SPDM process were introduced. Two microlens array examples were given. One is a 5 by 5 matrix arranged concave microlens array on flat brass substrate. The other one is a circular arranged 3D microlens array, which has 341 plano-convex micro lenslets, on a thin spherical PMMA substrate. Using the fabricated 3D microlens array, a 3D micro projection system was developed. The formed micro pattern dimension was 340 μm by 460 μm, giving an overall projection ratio of 34:1. It has been demonstrated that a low cost and simple manufacturing process for true 3D micro scale structures on non-planar substrates based on microlenses can be realized.

Last but not least, an affordable polymer SAR micromixer was developed based on a high accuracy, low cost, and flexible micro machining process. Specifically both the mixing performance and the fabrication process were carefully studied. An improved design of the SAR micromixer was also given, the mixing efficiency of the two designs were 0.11 and 0.065 respectively.
The present research work was carried out at Department of Integrated Systems Engineering and under the support of Center for Affordable Nanoengineering of Polymeric Biomedical Devices (CANPBD) at the Ohio State University since 2004. It has been much appreciated to have such an opportunity.

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CHAPTER 1: INTRODUCTION

1.1 Ultraprecision Single Point Diamond Machining and Micro Machining

Ultraprecision single point diamond turning (SPDT) is one of the most important and successful technologies in the field of precision engineering in the past several decades. This is not only because the SPDT integrates numerous state-of-the-art technologies of precision engineering, such as ultraprecision machine tool design, high speed and ultraprecision air spindle, high stiffness and ultraprecision hydrostatic slideways, multi axis servo computer numerical control (CNC), fine polished monocrystalline diamond cutting tool, precision metrology, just to name a few, it is also because the SPDT technology has already been applied in a broad range of fields from advanced science and technology for defense, energy, electronics applications to commercial and consumer products.

Ultraprecision single point diamond turning is a technology that uses monocrystalline diamond tools and ultraprecision machine tools to fabricate components with sub micrometer form accuracy and less than a few tens of nanometers surface roughness [1].

The earliest work of diamond turning can be traced back to as early as the beginning of 20th century and later in World War II by Frank Cooke of Cooke Optical
and several others companies [2; 3; 4] . An important time for the development of diamond turning was the 1960s’ with the increasing demands for high accuracy parts used for energy, computer, electronics and defense application [3; 5; 1]. The work was mainly completed by Y-12 (Union Carbide Nuclear Division, Oak Ridge, Tennessee) and Lawrence Livermore National Laboratory (L.L.N.L.) and these studies have become the foundation of the ultraprecision single point diamond turning technology of today. From 1960's to 1970's, the ultraprecision single point diamond turning technology was mostly developed in national laboratories and a few companies and the products were used for advanced science and technology such as the optical components for NASA grazing-incidence x-ray space telescopes [6]. In this period, the key technology had been used in the diamond turning machine tool included air spindle, laser interferometer position feedback, capacitance gage, numerical control, three-axis or two-axis machining, brushless DC motor, pneumatic vibration isolators, and temperature control [7].

In the 1980's, with the commercial diamond turning machine tool became available and more and more sophisticated technology had been used in diamond turning, the SPDT technology began to be widely used in industrial and commercial products. The new technologies used included hydrostatic slideways and second rotary axis [8; 9]. With additional demand for non-rotationally symmetric parts, such as toric lenses, a special device, which was later named fast tool servo (FTS), that was capable of small and high frequency synchronized movement with the main spindle was developed. Though the theoretical design of this device first appeared in 1976 [10], the
first report of the realization of this device was in 1983 by Douglass [11] and later the
device was also built by Patterson that was used on a diamond turning machine [12]. In
this era the well known products fabricated by SPDT included computer memory disk,
scanner parts in photo copying machines, as well as many other early complex
components.

In recent 20 years, the SPDT technology has been rapidly developed. The
related technologies have undergone significant renovations with features such as high
resolution glass scales, high speed CNC controls, high speed spindle, DC linear motor,
and high precision on-machine measurement technique. The SPDT technology was
quickly adopted in both industry and academia. The SPDT was an expensive process at
the beginning of its appearance and was suitable for single piece or small volume
production. When combining with mass production process such as injection molding
and compression molding, the SPDT became appropriate for high quality low cost
consumer products and quickly popularized among related industries. To extend the
ability of SPDT, many different technologies have also been added to the diamond
turning machine, i.e. ultrasonic vibration turning [13], micromilling, raster fly cutting
and grinding.

At present, the complicated multi-axis control system provides SPDT the
ability to machining freeform device rather than just spherical and aspherical surfaces,
both of which are axisymmetric. SPDT process has been expanded to single point
diamond machining (SPDM) process, which includes several related processes as well
as the more conventional single point diamond turning. The other related processes are fly cutting, fast tool servo, slow tool servo (STS)/ slow slide servo, and broaching.

Figure 1.1 [14; 15; 16] shows the time line for the achievable 'machining' accuracy including major mechanical machining processes and major microelectronic machining process. The achievable precision for ultraprecision machining technology (including the ultraprecision single point diamond turning) can reach as precise as nanometer.

![Achievable 'Machining' Accuracy Chart](chart.png)

Figure 1.1 Achievable machining accuracy of last sixty years[14]

### 1.2 Research Motivation and Objectives

The ultraprecision SPDM has been widely used and very well developed, but in reality the surface of these optics still contain defects from variations in the associated
machining process. Undoubtedly, these defects will affect the optical performance of the devices. To understand how these defects affect the quality of the machined devices and the relationship between the defects and the machining parameters is important.

The research included two areas; the first area was focused on studying the diffraction and scattering caused by the residual tool marks of the diamond machined surfaces, the second area was the applications of SPDM and micro machining.

For the first area, both the analytical analysis and experimental study were applied. The overall objective was to develop a model for the SPDM machined surface characteristics and the machining process and ultimately optimize the machining conditions based on this model.

The specific objectives of this research were:

- Analytically and experimentally study the scattering and diffraction from the SPDM machined surface.
- Quantify the optical performance of the SPDM machined surfaces by optical indicators such as specular reflectivity and imaging quality.
- Relate the surface optical quality and machining conditions, and develop a model based on the research. Optimize the SPDM process based on the developed model.
- Compare the characteristics and the optical quality of the several SPDM processes, such as diamond turning, slow tool servo and broaching process.
• Study the characteristics and the optical quality of SPDM process where very small size tools are used for micro machining.

For the second area, the main goal is to develop and study new processes of SPDM and micro machining, to extend the applications of SPDM and micro machining, and to develop advanced optical, microelectronic, and biomedical devices.

The content of this dissertation is arranged as follow:

Chapter 2 is a review and discussion of the mechanism and model of the ultraprecision single point diamond machining and micro cutting.

Chapter 3 is the research on optical performance of the single point diamond machined surfaces.

Chapter 4 is an application example of SPDM for one type of freeform optics: the microlens array, and the application of microlens array in 3D micro machining.

Chapter 5 is another application example of SPDM and micro machining for a biomedical micro device: an affordable split-and-recombination (SAR) micromixer.

Chapter 6 is the conclusions and future work.

The relation of these research topics is shown in Figure 1.2. The optical effects of the SPDM machined surfaces are related to both fundamental and process research. The two application examples are both related to process research and application research.
Figure 1.2 Structure of the research topics

SPDM: diamond turning, slow tool servo and broaching.

SPDM mechanism and model (chapter 2)

Optical effects of SPDM machined surfaces (chapter 3)

Fundamental Research

Process research

Applications

Optics

Electronics

Biomedical

Microlens array (chapter 4)

Micromixer (chapter 5)

...
CHAPTER 2: THEORETICAL MODEL FOR ULTRAPRECISION DIAMOND MACHINING AND MICRO MACHINING

For conventional macro scale cutting processes, a commonly accepted basic orthogonal cutting model (Figure 2.1) was constructed on several assumptions [17]:

1. The tool is perfectly sharp and there is no contact along the clearance face.

2. The shear surface is a plane extending upward from the cutting edge.

3. The cutting edge is a straight line extending perpendicular to the direction of motion and generates a plane surface as the work moves past it.

4. The chip does not flow to either side (plane strain).

5. The depth of cut is constant.

6. The width of the tool is greater than that of the workpiece.

7. The work moves relative to the tool with uniform velocity.

8. A continuous chip is produced with no built-up edge.

9. The shear and normal stresses along shear plane and tool are uniform.
For macro scale turning model research, the cutting force model is principally based on these assumptions. While for ultraprecision diamond turning and micromachining, many of these assumptions become invalid. The cutting mechanisms of micromachining is different with that of macro scale machining and a widely accept model has not been set up until now. After more than 30 years research on micro cutting, many models have been developed base on theoretical analysis, experimental observation, Finite Element Modeling (FEM) simulations, Molecular Dynamics (MD) simulations, and the combination of these approaches.

Although the mechanisms for micro cutting has not been set up, there are many common findings about micro cutting, for example the size effect of specific energy, the effect of tool cutting edge radius, the effects of workpiece materials etc. The following section summarizes the mechanism and model of the ultraprecision single point diamond machining and micro cutting. This is a review and discussion of the
state-of-the-art research work of related work of SPDM and micro cutting. The contents were organized in several aspects that are important to the physics of SPDM and micro machining. Because the machining principle for these SPDM processes is similar and the diamond turning process was mostly well studied, we will mainly introduce the theory of diamond turning.

2.1 Micro Cutting Mechanisms and Micro Cutting Force

The size effect of the specific energy was one of the most noticeable phenomena of micro cutting. The size effect of the specific energy is the fact that the energy used to remove unit volume of material increases as the depth of cut decreases. This size effect was related to the micro cutting mechanism.

According to Shaw's research, for micro cutting at very small depth of cut (around microns and sub micron level), normally ductile metals behave like brittle materials, the chip-forming model shifts from concentrated shear to microextrusion[17].

The reason for the size effect of the specific energy is still unknown. According to Liu and Melkote's review [18] many hypotheses have been introduced and tested by experiments or FEM simulation. These theories include: (1) Shaw and Backer attributed the size effect to the decrease in the probability of encountering a stress-reducing dislocation or a defect capable of inducing dislocations as described previously; (2) Kopalinsky and Oxley and Marusich attributed the size effect to an increase in the shear strength of the workpiece material; (3) Larsen-Basse and Oxley
attributed the size effect to material strengthening due the increase in the strain rate in the primary shear zone; (4) Fang attributed the size effect to the material constitutive behavior of varying shear flow stress; (5) Dinesh et al. attribute the material strengthening effect to the intense localized inhomogeneous plastic deformation within the primary and second deformation zones; (6) Nakayama and Tamura attributed the size effect to a decrease in the shear plane angle and greater energy dissipation associated with plastic flow in the workpiece subsurface; (7) Armarego and Brown attributed the size effect to greater relative contribution of ploughing forces arising from frictional rubbing and ploughing associated with material removal by a blunt tool; (8) Atkins attributed the size effect to the energy required for new surface creation via ductile fracture; (9) Liu and Melkote use a strain-gradient-based FE model for the micro-cutting and predict the size effect; (10) The affect by cutting tool edge radius suggested by many researcher and this will be discussed in next section.

The cutting force model of the ultraprecision diamond turning and micro machining is very important for understanding the mechanism of the machining process. Due to the very small cutting force, which is normally smaller than 1 Newton and can be as small as tens of micron Newtons [19; 20; 21; 22], the measurement of the cutting force is difficult and require high signal-to-noise ratio force sensor. Because the cutting force of diamond turning and micro machining is small, the effect of other factors, such as material spring back force which can be neglected in macro size machining, cannot be ignored any more.
Dow's group has developed several tool force model for precision diamond turning [19; 20]. In their model, they took some minor factors, such as material spring back force and material work hardening, for normal machining into account.

Drescher and Dow developed a tool force model which considered material work hardening [19]. According to the research at the National Institute of Standards and Technology (NIST), material exhibit an exponentially increasing hardness near surfaces [19] and can be expressed as \( H(d) = H_0 + ke^{-md} \). There exists a depth \( \rho = re^{(\alpha - 0.5)} \), which depends on the tool cutting edge radius \( r \), below surface where work hardening can be negligible. Due to work hardening, the normal stress of the material greatly increased as well as the cutting force. Unlike other cutting force model, Drescher considered the cross-sectional area of the undeformed chip (Figure 2.2). In this section it can be seen that the depth of cut \( t(\theta) \) is a function of feedrate \( f \) and angular position \( \theta \). The depth of cut of the left side is smaller than the minimal work hardening depth \( \rho \) and the hardness significantly increased for this part. Thus, the total cutting force of the tool is the integral of the forces at each sub area \( dA \), which can be seen has a uniform hardness. According to their results, their empirical model was fitted well with the measured data and both feedrate and tool edge radius had great influence on the cutting force while the cutting speed had no obvious affect on cutting force [19].
Arcona and Dow developed another empirical tool force model based on their observed segments like chip shape [20]. In this model, the material spring back force, which is a small amount compare to the cutting force, was considered in both cutting force direction and thrust force direction.

Both these two models took into account only one additional factor and also based on some assumptions. Both these models are appropriate for some specific conditions and they have given some reasonable explanations for the practical cutting force model.

2.2 Tool Cutting Edge Geometry

For micro machining especially ultraprecision single point diamond turning, one of the biggest differences to normal cutting process is the radius of the tool's cutting edge or in other words the sharpness of the cutting tool. The cutting edge radius of a regular monocrystalline diamond tool is around 0.5 μm to 0.05 μm and a well
prepared tool can have a cutting edge radius as small as 0.02 μm or even smaller [23; 24; 25; 19]. Compare to a tungsten carbide tool, the radius of which is decided by the particle size, sintering technique and the preparation process for the rake face. The edges radius of a carbide insert can vary from 50 μm to less than 5 μm [26] which is more than 10 to 100 times larger than that of a monocrystalline diamond tool.

In an ultraprecision micro cutting process, not only the radius of the cutting edge $r$ is small, the depth of cut $d$ is also very small (from around tens of micrometers to tens of nanometers or smaller) and is at about the same order of $r$. By contrast, the depth of cut $d$ in conventional cutting is much larger than cutting edge radius $r$, by at least three orders of magnitude [27].

Lucca et al. studied the effect of tool cutting edge radius to cutting force and the depth of the plastically deformed layer [28]. They found out that the tool cutting edge radius will significantly affect the thrust forces at low uncut chip thickness ($\leq 1\mu m$ for 105nm radius tool) but the tool cutting edge radius will not affect the cutting force as well as the depth of the plastic layer. They also found that the uncut chip thickness had not affected the depth of plastic layer.

Z.J. Yuan et al. studied the effect of diamond tool sharpness theoretically and experimentally [23]. In their model (as shown in Figure 2.3), there exists a critical point A. During cutting, materials above point A will become chips and below point A will form the machined surface. They found a expression for the minimum depth of cut $a_{c_{\text{min}}}$ by considering the relationship between the normal force and tangential force at
point A. Finally he gave an estimated number for the minimum depth of cut for diamond turning of Al-alloys, that is $a_{c_{mn}} = (0.322 \sim 0.249)\rho$. Besides the relationship between minimum depth of cut and tool cutting edge radius, Yuan’s group also experimentally studied the influence of tool sharpness on surface roughness, microhardness of the machined surface, residual stresses, and dislocations. The larger tool cutting edge radius tends to generate larger surface roughness, higher surface microhardness, higher residual stress, and higher dislocation density in machined surface. They also noticed the size effect when the depth of cut is at the same order of the cutting edge radius.

![Figure 2.3 relationship between the minimum cutting thickness and the cutting edge radius](image)

Komanduri et al. utilized molecular dynamics (MD) simulations for nanometric cutting. In his studies, the depths of cut $d$ were very small (0.362 nm - 2.172 nm), and the ratio to tool cutting edge radius $r$ was also very small ($d/r = 0.1, 0.2$, and $0.3$). He
propose a general material removal mechanism based on two tool parameters: the cutting edge radius and rake angle [29]. In his model (Figure 2.4), according to the relationship of cutting edge radius and depth of cut and tool rake angle, all the material removal processes can be classified into four different styles: 1) conventional cutting, the depth of cut is much larger than cutting edge radius and rake angle is positive, zero, or slightly negative. In this case, the cutting force is about twice the thrust force, and the chip is mainly formed by shear deformation in the first shear zone. 2) grinding of ductile material, the depth of cut is much larger than abrasive cutting edge radius and the abrasive has a very large negative rake angle (about -60°). In this case, the cutting force is about half of the thrust force. 3) ultraprecision machining and micro machining, the depth of cut is about the same order or smaller than cutting edge radius, and the rake angle equivalent to a large negative value. In this case the cutting force is smaller than half of thrust force. 4) indentation-sliding, the depth of cut is smaller than the tool radius and has a very large negative rake angle (close to -90°). In this case the cutting force is much smaller than thrust force and the material has a very large plastic deformation due to the high pressure. This case can also be used to explain grinding of brittle materials.

From this model, it can be seen that when the depth of cut becomes very small and the rake angle becomes a large negative value, more energy is used to generate material plastic deformation. The material in front of the tool is pushed by the tool underneath and to the other sides to form the machined surface and residual tool
marks. For the same depth of cut, the blunter the tool, the higher the pressure and larger the deformation of the materials.

Figure 2.4 material removal mechanism proposed by Komanduri to cover a wide range of process[29]: (a) conventional cutting, (b) grinding, (c) ultraprecision machining, and (d) indentation-sliding.

There are also several other groups studied the effects of tool cutting edge geometry to the residual stress, cutting force, and temperature by means of Finite Element Analysis (FEA) [30; 31; 27]. These research activities may not restricted to ultraprecision diamond turning, but they have got similar results that with the change of the ratio $d/r$ and negative rake angle many consequences such as the plastic deformation of the material, residual stresses of the machined surface, hydrostatic pressure et al. also greatly affected.
Due to the complexity of ultraprecision diamond turning, all the prescribed work especially the finite element analysis were 2D orthogonal cutting and the effect of tool cutting edge sharpness to the residual tool mark height was seldom analyzed.

2.3 Workpiece Material

The diamond machinable materials cover a very large range from metal to semiconductor to polymers. The details on the diamond machinable materials can be found in Paul's work [32]. For ultraprecision diamond machining, the depth of cut is usually a few micrometers or even sub micron, thus the materials which are considered homogeneous and isotropic in conventional macro scale machining are actually heterogeneous and anisotropic now. The diamond machinable materials can be divided into monocrystalline materials, polycrystalline materials, and amorphous materials based on their crystalline state. They can also be divided into ductile materials and brittle materials based on their cutting property. In this section, the effect of material property to the ultraprecision diamond machining will be reviewed.

The effect of material crystalline state to the diamond machining process has been studied by many groups [33; 34; 35; 36] and it is well known that in micro cutting (depth of cut down to a few micrometers) the crystallographic orientation and micro defects of the materials contribute to the cutting force fluctuation and the resultant surface finish.

Moronuki et al. carried out a series of experiments on the material properties on microcutting processes. They observed that for polycrystalline materials, such as
aluminum alloys, the fluctuation of cutting force was mainly due to the crystal grain boundaries and the influence of anisotropy of the aluminum alloy on cutting force can result in cutting force change as much as three times. They also observed that for single crystalline materials, such as single crystal silicon and pure aluminum, the cutting force and surface finish were different for different cutting direction while for amorphous materials, like PMMA, the cutting properties do not change [33].

Zhou et al. studied the effects of crystallographic orientation on cutting force and surface finish experimentally on single crystal aluminum, brass and copper [35]. They also tried to analyze the effects based on a model that used by Lee et al. [34]. In their explanations, the variance of the cutting force and the variance of surface roughness at different crystallographic orientation is mainly caused by shear angle change. Komanduri’s group also studied the effects of crystallographic orientation using molecular dynamics (MD) simulation [36]. They found the force and cutting mechanism difference for different crystallographic orientation and also related the difference to the shear angle. However, the conclusions of these two research results about the maximum and minimum cutting force direction seemed to be opposite to each other.

Lee's group studied the deformation behavior of different crystallographic orientation of aluminum single crystal material [37] and they used a microplasticity analysis to connect the crystallographic orientation of aluminum to the cutting force variation [38]. They also studied the surface texture affected by the orientation of the grains in aluminum material and the grain orientation was thought to be connected to
both crystallographic orientation and metal prepare methods like cold-working and annealing [39].

Besides the crystallographic orientation effect, the size of the material grains, the purity of the material, and the micro structures of the material all greatly affect the machining process and the machined surface finish [40].

2.4 Surface Finish

One of the most important attractions of single point diamond machining is the optical surface finish and for decades the major research endeavor is to further improve the surface quality. Besides the prescribed factors like cutting force variation, tool cutting edge, and material properties, there are other causes that may affect the surface finish. In this section, the surface roughness related topics will be discussed.

Figure 2.5 shows the set up of the ultraprecision diamond turning, and the other SPDM processes have the similar set up as that of diamond turning. Workpiece was mounted on the main spindle, which rotates at speed \(n_s\) (rpm). The diamond tool will move along the radial direction at a speed \(V_r\) (mm/min) to turn the surface of the workpiece. This process will leave residual tool marks on the workpiece surface. Ideally, the cross section of the residual tool marks can be roughly considered consisting of continuous circular arcs (Figure 2.6), the arcs are the replicas of the tool nose radius. The ideal residual tool mark peak height can be approximated using the following equation:
\[ h = r - \sqrt{r^2 - \left(\frac{f}{2}\right)^2} \approx \frac{f^2}{8r} \quad \text{(3.1)} \]

where \( f \) is the distance between two adjacent tool traces (for diamond turning \( f = \frac{V_t}{n_s} \) is the tool feed per workpiece revolution), and \( r \) is the tool nose radius. For an ideal machining process, the surface roughness is consisted of periodic residual tool trace, and the theoretical average surface roughness of a single point tool turned surface can be estimated as [41]:

\[ R_a = 0.0321 \frac{f^2}{r} \quad \text{(3.2)} \]

Figure 2.5 Set up of ultraprecision diamond turning
Using spectrum analysis method [42; 43; 44], the ideal periodic tool marks on the diamond turned surface can be transformed into several spatial harmonic components (figure 3). The amplitude and the shape of the harmonic components are decided by the tool nose size and shape, the tool-workpiece interaction, the turning parameters, and the degree of swelling and recovery etc. Using the spectrum analysis method, the factors that contribute to the surface finish can be obtained [42; 43; 44]. The surface roughness caused by the period tool marks can be partially controlled by adjusting machining parameters. Hocheng and Hsieh [44] used the spectrum method to analyze the surface characteristics and gave some critical values for feedrate under certain spindle rotational speed and tool nose radius to reduce $R_a$ and maximize productivity.

Figure 2.6 Idea cross section the ultra precision diamond turned surface
As described in equation 3.2, the surface roughness is related to feedrate and tool nose radius. In reality the surface roughness may be much larger than the calculated value especially in diamond turning due to other process variation.

Due to swelling and recovery [42; 43; 44; 45; 46], both the actual residual tool mark depth and the actual surface roughness are much higher than the estimated value using the analytic equation. The actual residual tool mark period is also slightly different from the ideal one. The swelling and recovery of the material after cutting can be illustrated in Figure 2.8 [46].
Liu and Melkote [47] gave an explanation for the mechanics of material swelling during micro turning and developed a model. Liu and melkote made an analogous cutting model to the case of indentation (Figure 2.9) and developed an expression for the material pile up (or swelling). In their model, the material plastic flow caused material pile up, this pile up is characterized as $R_p$ and it can be expressed as [47]:

$$R_p = k_1 \ln x + k_2$$  \hspace{1cm} (3.3)

where

$$x = \frac{Ec \cot \theta}{\bar{\sigma}_y e}$$  \hspace{1cm} (3.4)
is a rheological factor. \( E \) is the material elastic modulus, \( \theta \) is the semi-apical angle of the tool, \( \bar{\sigma}_y \) is the average flow stress, \( e \) is the ratio of the average flow stress with strain gradient strengthening to the average stress without strain gradient strengthening, \( k_1, k_2 \) are coefficients that need to be calibrated in experiments. This is the only model can be found related to the material swelling during micro cutting. Liu and Melkote experimentally validate this model but for ultraprecision diamond turning and for other SPDM process this model has not been verified. It can be seen from equation 3.3 and 3.4 that the swelling is related to the material property, tool shape, and machining conditions.

Figure 2.9 Material pile up during a scratch test by using an indenter[47]

Besides the residual periodic tool marks, there are some periodic variation as well as random roughness on the machined surface [44; 48; 49; 50; 51; 52]. These
surface characters are caused by tool-workpiece vibration, material variation, temperature variation and cutting chips.

### 2.5 Temperature and Heat

During the cutting process, most of the mechanical energy associated with chip formation will convert to thermal energy [17] and part of these thermal energy will cause the temperature rise in the workpiece and the tool. This temperature rise is important to the machining process for it will change the material properties of both the workpiece and the tool. For conventional cutting, the temperature at the rake face of the tool can be as high as 1200 °C [17].

For ultraprecision diamond turning, the temperature at the rake face of the tool is much lower due to the small cutting depth, small cutting force, and quick heat dispersion. Udea et al. measured the temperature at the rake face of a diamond tool while turning Aluminum and copper at a cutting speed range 400-900 m/min. An infrared detector, a two-color detector were used as the detector and an optical fiber was used to transmit the temperature related infrared light. The measured maximum temperature was 190 °C for aluminum and 220 °C for copper at a cutting speed of 620m/min [53]. Their measured data showed that the temperature increases with the increase of cutting speed and the value agreed with their FEM simulation results.

Zong et al. studied the relationship between the temperature and cutting velocity [54]. They found that the temperature rises incrementally with the enlargement of the cutting velocity and the maximum temperature is around 650 °C.
The thermal induced problem is important toultraprecision diamond machining. The high temperature at the rake face of the diamond tool was thought to be an important reason for the wear of the diamond tool [1; 55]. In addition to the wear of the tool, the temperature also causes errors to the accuracy of the dimensions and the surface quality (both waviness and surface roughness). Rakuff et al. studied the temperature change and the thermally induced dimension change during the diamond turning process [56].

2.6 Chips

In the ultraprecision diamond machining the chips formation and flow mechanisms are very important to the quality of the machined surfaces [1]. The chips will easily cause scratches and other types of damages to the optical surfaces without careful control of the chips flow. Very few studies were done on the chips formation and flow [57; 58; 59; 60]. Tow's group carried out a study to predict the shape and flow direction of the chips [57; 58; 59]. In Jared's research [58], he experimentally found the qualitative relationship between the shape (curvature) of the chips and the cutting parameters and developed an expression for the curvature of the chips based on experiment data. He also qualitatively found the relationship between the cutting parameters and the chip flow direction and experimentally investigate the methods to control the chip flow.
2.7 Cutting Fluid

In conventional machining, the cutting fluid has two main functions. One is lubrication at relatively low cutting speeds and the other is cooling at relatively high cutting speeds because at high cutting speeds there is no time for fluid to penetrate the chip-tool interface [17]. For ultraprecision diamond machining, the cutting fluid has a third important function besides the above described two functions. The third function is to control the formation and flow of the chips [58], because in ultraprecision diamond machining the chips are always very small and the controlling of the chip flow is significant to surface quality. In ultraprecision diamond turning, the cutting fluid has an important role on reduce the wear of diamond tool [61; 62].

2.8 Summary

In this chapter, the mechanism and model of the ultraprecision single point diamond turning and micro cutting were reviewed and discussed. The related subjects of SPDT and micro cutting were also involved. From the analysis, it can be seen that SPDT and micro cutting have big different with the conventional macro scale cutting. Due to the small cutting depth, numerous factors that can be ignored in macro scale become ineligible or even significant. Due to the lacking of proper testing and analysis methods, many aspects of the SPDT and micro cutting are still unknown or uncertain.

To briefly summarize, the major features of the ultraprecision SPDT and micro cutting are:
1. Cutting mechanism of SPDT and micro cutting is different. In conventional macro scale cutting, the main cutting mechanism is shear deformation while in SPDT and micro cutting the material plastic deformation, extrusion, and ploughing become important or even dominant.

2. There is common observed size effect in SPDT and micro cutting due to factors such as cutting force, specific energy, material property, abnormally change at small cutting depth.

3. The cutting forces is much smaller than that of macro scale cutting and several other forces such as thrust force, friction force become important in SPDT and micro cutting.

4. The tool cutting edge radius is an important factor that can affect the cutting mechanism and surface quality.

5. Some of the material properties such as crystallographic orientation, grain boundary, grain size, micro particles, micro hardness are critical to the cutting process.

6. Besides the machine tool vibration, the material properties such as material swelling and recovery are also important to the surface roughness.

7. The chips movement becomes important because the chips can damage the machined optical surface finish.
8. Temperature variation is very important to the accuracy and surface finish and the heat is very important to tool wear.

9. Cutting fluid is important for control the movement of the chips and the temperature of the machining process.
CHAPTER 3: THEORETICAL AND EXPERIMENTAL STUDY ON THE RELATIONSHIP BETWEEN THE SPDM MACHINED SURFACE AND THE OPTICAL PERFORMANCE

One of the major application fields of the ultraprecision single point diamond machining process is precision optics. Having nanometers surface finish, ideally the ultraprecision single point diamond machined devices can be directly used for optical application without polish. In reality, the surface of these optics still contain defects from variations in the associated machining process, as discussed in the previous chapter. Undoubtedly, these defects will affect the optical performance of the devices. Among these defects, the most dominant one is the periodic residual tool marks and this is also the most typical features on a diamond machined surface. In many applications, the effect of the periodic residual tool marks is too severe to use the device directly and additional post machining polish is required [63]. However the polish process will undoubtedly increase the cycle time and cost of the products.

The previous studies about the surface roughness of diamond turned surfaces were mainly focused on the causes of the surface texture and their relationship with the machining mechanism. As a result, one of the main goals of these studies was to reduce the surface roughness ($R_a$). However, for many of the diamond machined
surfaces used in optical applications, surface roughness ($R_a$) analysis alone is not always adequate.

Besides the studies on surface roughness from a mechanical machining point of view, there were also numerous investigations on the relationship between the surface roughness and the scattering or diffraction off the optical surfaces [64; 65; 66; 67; 68; 69; 70; 71; 72]. These studies have resulted in several methods that are capable of predicting and measuring optical scattering. However, since the analyses in these studies were often based on simplified surface models, they were not necessarily a full representation of actual machined surfaces and the relationship between the diamond machining process and the optical performance was unknown.

It is important to understand the diffraction caused by the periodic tool marks and its relationship with the SPDM process so high quality optics can be made without polishing. Many of the optics fabricated by SPDM are apt to be used in applications requiring low quality optics or applications in the infrared range due to the diffraction from the surfaces. For high quality optical applications and improperly machined surfaces, post machining polish is frequently required, thus greatly increases the machining cost. Moreover, since polishing is a divergent process, it is difficult to polish freeform surfaces, microlens arrays, and micro optics with less than 2-3 mm features.

The object of this chapter is to present a preliminary study of light diffracted by surfaces created with ultraprecision single point diamond machining process in order
to understand the specific process conditions under which diffraction occurs. Beyond that the ultimate goal of this research is to provide a methodology for the optical industry on how to minimize diffraction effects consistent with efficient processing by changing process conditions. We will present data from our measurements and indicate areas where further study maybe needed.

To study the quality of diamond machined surfaces, four different indicators, normalized first order diffraction ratio, normalized specular reflectivity, surface roughness ($R_a$) and periodic tool mark depth, are used from different points of view. For the actual device which one of these indicators is more helpful depends on the application of the device.

In this chapter the methods to describe the characteristics of the diamond machined surfaces are first introduced in Section 3.1, and then the analytical approach to analyze the optical behavior of the diffracted light are presented in Section 3.2. In Section 3.3, six sets of diamond machining tests and the measurement methods for the machined samples are described. In Section 3.4 the data from the six sets of tests are discussed and an empirical mathematical model is presented. Section 3.5 contains a summary of results and conclusions.

3.1 Methods for Describing the Surface Characteristics

The surface characteristics can be described from two different ways, namely, the mechanical method and the optical method. There are numerous paper and books
describing the definition, metrology, calculation of these methods and also the relationship between the mechanical and the optical method.

For mechanical method, there are two most important values about the surface characteristics: the surface roughness and the power spectral density of the surface roughness.

The surface roughness measurement directly measures the texture of a surface and represents the surface texture in the form of profile graph. The surface roughness can be obtained from a 2D line measurement or a 3D surface measurement. The commonly used parameters for characterizing the surface roughness are amplitude parameters such as the root mean square (RMS) roughness $R_q$ and average roughness $R_a$, which are defined as [73]:

\[
R_q = \sqrt{\frac{1}{L} \int_0^L z^2 \, dx} \tag{3.1}
\]

\[
R_a = \frac{1}{L} \int_0^L |z| \, dx \tag{3.2}
\]

where $z = f(x)$ is the one dimensional surface profile that can be obtained by several methods, $L$ is the length of the profile being assessed.

The power spectral density (PSD) function of the surface roughness can be derived from the measured surface roughness data.
There are a number of different methods for the measurement of the surface roughness and these methods can be divided into two different types: contact and non-contact. The contact method typically uses a small stylus to move across the sample surface to measure the surface vertical deviations. No matter how small is the contact force between the stylus and the sample surface, dragging trace will be left on the sample surface by this method. For stylus profiler, the measurement accuracy is limited by the size of the stylus. The non-contact method includes several different technology, including interferometry and methods based on electrical capacitance. Since it is non-contact, the surface will not be scratched by the measurement and it is considered more proper for optical surface evaluation.

The optical methods for sample surface characteristic describing are generally indirectly using some parameters reflecting the scattering or diffraction caused by surface roughness. The commonly used optical scattering methods used for surface roughness measurement are Total Integrated Scattering (TIS), Angle Resolved Scattering (ARS), Bidirectional Reflective Distribution Factor (BRDF), and Bidirectional Scatter Distribution Function (BSDF), among which TIS is scalar method while ARS, BRDF and BSDF are vector methods.

TIS is based on the Kirchhoff scalar diffraction theory and is defined as the ratio of the sum of all scattering light within a hemisphere (not including the specular reflection light) to the total reflect light and can be expressed as

\[ PSD = \frac{1}{L} \left| \int_{-\infty}^{\infty} z(x) e^{-j2\pi z} dx \right|^2 \]  

(3.3)
\[ TIS = \frac{R_d}{R_0} = 1 - \frac{R_S}{R_0} = 1 - e^{-\frac{4\pi\delta}{\cos \theta \lambda}} \approx \left( \frac{4\pi\delta}{\lambda} \right)^2 \]  \hspace{1cm} (3.4)

Where \( R_d \) is the summation of all the scattering light, \( R_s \) is the specular reflection, \( R_0 \) is the total reflectance of the incident light, and \( \delta \) is the RMS height of the surface roughness. The ARS, BRDF and BSDF method all based on vector theory and take the light polarization into consideration. The expressions for these three methods are similar and can be expressed as a function of light incident angle, light scattering angle, and surface PSD function. The definition of these methods can be found in reference [64]. The measurement of these factors includes some special optical instruments.

3.2 Calculation of the Diffraction and Scattering off Diamond Machined Surface

As described in chapter 2 and at the beginning of this chapter, the diamond machined optical surface has some specific texture and is unfavorable for optical application. In this section, the calculation of the diffraction and scattering caused by these textures will be discussed. In this section only flat device and uniform incident light was considered.
The simplified model of the diffraction from diamond machined surfaces is sketched in Figure 3.1. Assume the diamond machined surface is on object plane $X_0$-$Y_0$, plane $X_1$-$Y_1$ is the observation plane. Here, the observation plane is a spherical surface. point $A$ and point $B$ are two points on object plane and observation plane respectively. $\vec{r}$ is a vector point from $A$ to $B$. $\theta$ is the angle between vector $\vec{r}$ and $Z$ axis. According to diffraction theory, diffraction on the plane $X_1$-$Y_1$ from plane $X_0$-$Y_0$ is [74]:

\[ E_i(x_i, y_i, z_i) = \frac{jk}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E_0(x_0, y_0, z_0) \cos \theta \frac{e^{-jkr}}{r} \, dx_0 \, dy_0 \]  

(3.5)

Where $r = \sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2}$ and $\cos \theta = \frac{|z_1 - z_0|}{r}$. 

If \( z_i \gg x_0, y_0 \) and \( r_i^2 = x_i^2 + y_i^2 + z_i^2 \gg x_0x_i + y_0y_i \) then with \( z_0 = 0 \), \( r \) and \( \cos \theta \) can be approximated as:

\[
\begin{align*}
    r &= \sqrt{(x_i - x_0)^2 + (y_i - y_0)^2 + (z_i - z_0)^2} \\
    &\approx \sqrt{x_i^2 + y_i^2 + z_i^2} \left(1 - \frac{x_i x_0 + x_i y_0}{x_i^2 + y_i^2 + z_i^2}\right) \\
    &= r_i - \frac{x_i x_0 + x_i y_0}{r_i}
\end{align*}
\]

\[
\cos \theta = \frac{z_i}{r_i} = \cos \theta_i.
\]

Then Eq. 3.5 can be expressed as:

\[
E_i(x_1, y_1, z_1) = \frac{jk}{2\pi r_i} \cos \theta_i e^{-\frac{r_i}{r_i}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E_0(x_0, y_0, z_0) e^{\frac{jk(x_0 x_1 + y_0 y_1)}{r_i}} dx_0 dy_0 \quad (3.6)
\]

Eq. 3.6 can be further simplified as (the simplifying process is in Appendix A1):

\[
E_i(u_1, v_1, z_1) = A_i \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (1 + j\kappa z_2 \sum_{n=-L}^{L} d_n e^{j2\pi u_n} + j\kappa \cdot d_r(u_0, v_0)) e^{j2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 \quad (3.7)
\]

where \( A_i = \frac{jk}{2\pi} \frac{z_i a b}{r_i^2} e^{-\frac{r_i}{r_i}} E_0 \), \( u_0 = \frac{x_0}{a}, \quad v_0 = \frac{y_0}{b}, \quad u_1 = \frac{x_1}{r_i \lambda}, \quad v_1 = \frac{y_1}{r_i \lambda} \), \( \kappa = \frac{a}{2\pi}, \quad \kappa = \frac{b}{2\pi} \).

Eq. 3.7 includes three parts:

1. The specular reflection,
\[ E_{\text{spec}}(u, v, z) = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i2\pi(u\mu_1 + v\nu_1)} du_0 dv_0 \]  

(3.7a)

2. The periodic tool marks caused high order diffraction,

\[ E_{\text{per}}(u, v, z) = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} jK_2 \sum_{n=-L}^{L} d_n e^{i2\pi\mu_0} \cdot e^{i2\pi(u\mu_1 + v\nu_1)} du_0 dv_0 \]  

(3.7b)

3. The random background scattering caused by the surface roughness;

\[ E_{\text{random}}(u, v, z) = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} jK_2 d_0 (u_0, v_0) \cdot e^{i2\pi(u\mu_1 + v\nu_1)} du_0 dv_0 \]  

(3.7c)

Each part can be calculated as follow:

a). In Eq.3.7, \( E_{\text{spec}}(u, v, z) \) is the specular reflection from the surface, this expression can be evaluated and simplified.

\[ E_{\text{spec}}(u, v, z) = A \int_{0}^{1} e^{i2\pi(u\mu_1 + v\nu_1)} du_0 dv_0 = A \frac{\sin \mu_1}{\mu_1} e^{i\pi_1} \frac{\sin \nu_1}{\nu_1} e^{i\pi_1} \]  

(3.8)

Figure 3.2 shows the detector’s position for measuring the diffraction light by using a photo detector. The upper part of figure 3.2 is the 2D plot in X-Z plane, and the lower part of figure 3.2 is the 2D plot in Y-Z plane. The detector rotates about the \( y_0 \) axis, and the center of the detector move along the semicircle \( T \) in plane X-Z. The detector center position is \( \theta_{td} \) in X-Z plane and is 0 in Y-Z plane. The position of the
zero order diffraction along the semicircle \( T \) is \( \theta_{10} \) in \( X-Z \) plane and is 0 in \( Y-Z \) plane. \( \theta_1 \) is the position in of point \( B \) in \( X-Z \) plane and is \( \phi_1 \) in \( Y-Z \) plane. \( \delta \theta_1 \) is the angle between point \( B \) and the \( n^{th} \) order diffraction center in \( X-Z \) plane and \( \delta \phi_1 \) is the angle between point \( B \) and the zero order diffraction center in \( Y-Z \) plane.

Then, the total irradiance measured by detector at position \( \theta_{id} \) is (the analysis process is in Appendix A2):

\[
I_{1d}(\theta_{id}, \theta_{10}, \alpha, \beta, r_1)
\]

\[
= \frac{1}{2Z_0} r^2_1 \sin \theta_0 \int_{-\beta/2}^{\beta/2} \int_{-\alpha/2}^{\alpha/2} \sin \left( \frac{\pi}{\lambda} \cos \theta_0 \delta \theta_1 \right) e^{i \frac{\pi}{\lambda} \cos \theta_0 \sin \theta_0 \delta \phi_1} \sin \left( \frac{\pi}{\lambda} \sin \theta_0 \delta \phi_1 \right) e^{i \frac{\pi}{\lambda} \sin \theta_0 \delta \theta_1} d \delta \theta_1 d \delta \phi_1
\]

\[
= \frac{|A|^2}{2Z_0} r^2_1 \sin \theta_0 \int_{-\beta/2}^{\beta/2} \sin^2 \left( \frac{\pi}{\lambda} \sin \theta_0 \delta \phi_1 \right) d \delta \phi_1 \cdot \int_{-\alpha/2}^{\alpha/2} \sin^2 \left( \frac{\pi}{\lambda} \cos \theta_0 \delta \theta_1 \right) d \delta \theta_1
\]

\[ (3.9) \]
Figure 3.2 Setup of the detector

b). The second part of Eq. 3.7 is the high order diffraction caused by periodic tool marks. The expression for the light diffracted by the periodic tool marks can be similarly evaluated and simplified.

\[ E_{\text{nd}}(u_t, v_t, z_t) = A \left( \int_{-\infty}^{\infty} j2\kappa \delta(u_t, v_t) e^{i\pi n u_t + i\pi n v_t} \, du_t \, dv_t \right) = j2\kappa A \frac{\sin \pi z_t}{\pi} e^{i\pi z_t} \sum_{n=1}^{L} \left( d_n \frac{\sin \pi (u_t + f_n)}{\pi (u_t + f_n)} e^{i\pi n z_t} \right) \] (3.10)

For the detector at any position \( \theta_{id} \) around the \( n^{th} \) order diffraction beam, the total light irradiance entering the detector is the integration of Eq. 3.10 at the detector’s surface (the derivation process is in Appendix A3):
\[ I_{in}(\theta_{id}, \theta_{in}, r_1, \alpha, \beta) \]

\[
\approx r_1^2 \sin \theta_{as} \beta \int_{-\beta/2}^{\beta/2} \frac{1}{j2\kappa d_s} \frac{1}{\pi \lambda} e^{j2\pi \cos \theta_{as} \sin \theta_{as} \delta \phi_1} \sin \left( \frac{\pi \sin \theta_{as} \delta \phi_1}{\lambda} \right) e^{j\pi \cos \theta_{as} \sin \theta_{as} \delta \phi_1} d\delta \phi_1 d\delta \phi_2 \]

\[
= \frac{2\kappa d_s A}{2Z_0} \int_{-\beta/2}^{\beta/2} \frac{1}{\pi \lambda} e^{j2\pi \cos \theta_{as} \sin \theta_{as} \delta \phi_1} \sin \left( \frac{\pi \sin \theta_{as} \delta \phi_1}{\lambda} \right) d\delta \phi_1 d\delta \phi_2 \] (3.11)

\[
E_{ir}(u_1, v_1, z_1) = A \int_0^1 j2\kappa d_s (u_0, v_0) e^{j2\pi (u_0u_1 + v_0v_1)} du_0 dv_0 \] (3.12)

Because the scattering light is random, we use the ensemble average for the scattering light intensity. The ensemble is assumed to be a set of identical configuration which differs only by the random contribution to the tool marks. In practice, several traces from the same sample might be used.

We are interested in the ensemble average of the irradiance.

\[
\langle I_{ir}(u_1, v_1, z_1) \rangle = \left\langle \frac{1}{2Z_0} |E_{ir}(u_1, v_1, z_1)|^2 \right\rangle
\]

By calculation, the scattering irradiance at point \((u_1, v_1, z_1)\) is (the derivation process is in Appendix A4):
\[ I_r(\theta_d, \alpha, \beta, r_1) = \int_{-\beta/2}^{\beta/2} \int_{-\alpha/2}^{\alpha/2} \langle I_r(\theta_1, \phi_1, z_1) \rangle r_1^2 \sin \theta_1 d\theta_1 d\phi_1 \]  \hspace{1cm} (3.13)

where

\[ \langle I_r(u_1, v_1, z_1) \rangle = \frac{1}{2Z_0} 2\kappa \Phi(u_1, v_1) \]

and

\[ \Phi(u_1, v_1) = \left| \int_0^1 \int_0^1 d_r(u_0, v_0) e^{i2\pi(u_0u_1+v_0v_1)} du_0 dv_0 \right|^2 \]

is the estimated power spectrum density of the random surface roughness.

d). Total light field:

Combine Eq. 3.8, 3.10, and 3.12

\[ E_1(\delta \theta, \delta \phi, \theta_1, r_1) \]

\[ = A \frac{\sin \left( \frac{\pi \cos \theta_1 \delta \theta a}{\lambda} \right) e^{j \pi \cos \theta_1 \delta \phi a / \lambda} \sin \left( \frac{\pi \sin \theta_1 \delta \phi b}{\lambda} \right) e^{j \pi \sin \theta_1 \delta \phi b / \lambda}}{\pi \cos \theta_1 \delta \theta a / \lambda} \frac{\pi \sin \theta_1 \delta \phi b / \lambda}{\pi \cos \theta_1 \delta \phi b / \lambda} \]

\[ + A \frac{\sin \left( \frac{\pi \cos \theta_1 \delta \theta a}{\lambda} \right) e^{j \pi \cos \theta_1 \delta \phi a / \lambda} j2\kappa \sum_{n=0}^{L} \left( \frac{\sin \left( \frac{\pi a \cos \theta_1 (\delta \theta_d + \delta \theta)}{\lambda} \right) e^{j \pi \alpha \cos \theta_1 (\delta \theta_d + \delta \theta)}}{\pi \alpha \cos \theta_1 (\delta \theta_d + \delta \theta)} \right) }{\pi \cos \theta_1 \delta \theta a / \lambda} \]

\[ + E_{1r}(u_1, v_1, z_1) \]

Combine Eq. A.9, A.11, and A.13 is the total light intensity measured by detector at any position \( \theta_1 \):

43
\[ I_1(\delta \theta, \delta \varphi, \theta_1, \varphi_1) \]

\[
= \frac{|A|^2}{2Z_0} r_1^2 \sin \theta_{i0} \int_{-\beta/2}^{\beta/2} \sin^2 \left( \frac{\pi b}{\lambda} \sin \theta_{in} \delta \varphi_1 \right) d\delta \varphi_1 \cdot \int_{\theta_{in} - \alpha/2}^{\theta_{in} + \alpha/2} \sin^2 \left( \frac{\pi a}{\lambda} \cos \theta_{i0} \delta \theta_1 \right) d\delta \theta_1 \\
+ \frac{2\kappa d_n |A|^2}{2Z_0} r_1^2 \sin \theta_{iin} \int_{-\beta/2}^{\beta/2} \sin^2 \left( \frac{\pi b}{\lambda} \sin \theta_{in} \delta \varphi_1 \right) d\delta \varphi_1 \cdot \int_{\theta_{iin} - \alpha/2}^{\theta_{iin} + \alpha/2} \sin^2 \left( \frac{\pi a}{\lambda} \cos \theta_{iin} \delta \theta_1 \right) d\delta \theta_1 \\
+ \sum_{-\beta/2}^{\beta/2} \sum_{\theta_{iin} - \alpha/2}^{\theta_{iin} + \alpha/2} \left( I_{1r}(\theta_1, \varphi_1, Z_1) \right) r_1^2 \sin \theta_1 d\theta_1 d\varphi_1 \tag{3.15} 
\]

Through the analytical investigation, the diffraction effects are related to the sample surface characteristics and both the diffraction and scattering field and irradiation of these components can be calculated as long as some parameters are known. In next sections, the relationship between the diffraction effects and the machining process will be studied.

3.3 Experiments for Studying the Diffraction from Diamond Machined Surface

To establish the relationship between machining process parameters and optical performance of a single point diamond machined surface, a number of tests were designed and performed. Each test consisted in preparing a set of diamond machined samples, examining each sample optically with laser light and then with a Veeco Profilometer. The data thus obtained were manipulated, plotted and compared.
3.3.1 Machining Experiments

All machining were performed on the 350FG Freeform Generator (Figure 3.3a), an ultraprecision diamond turning machine which has three linear axes that are equipped with linear laserscales capable of resolving 8.6 nm at a maximum speed of 1800 mm/min. The straightness on all slides is less than 250 nm. The work spindle is capable of reaching 6,000 rpm while maintaining axial and radial error motion of less than 100 nm. The work spindle can also maintain angular position to less than 0.5 arcs second in a modulated mode. The diamond turning machine is also capable of performing slow tool servo and slow tool broaching by controlling various motions of the axes and spindle as will be described shortly (as in Figure 3.3b).

Figure 3.3 Experiment setup:(a) Nanotech 350FG Freeform Generator, (b) Axis configuration and motion direction of the diamond turning machine.
The sample material used in this research was Al 6061. All the samples were in disc shape, 44 mm diameter and 15 mm thick. For simplification, in this research only flat surfaces were machined on the top surface.

Five different kinds of test were performed. These tests included variable spacing turning (VST) test, constant spacing turning (CST) test, diffractive tool turning (DTT) test, slow tool servo cutting (STSC) test, and broaching cutting (BC) test.

The first (VST) and second (CST) tests were designed to study the conventional diamond turning process with a normal size diamond tool (tool nose radius around several millimeters, rake angle is 0°, and clearance angle is 8°). To study reproducibility, variable spacing turning test includes two sets of test (VST_1 and VST_2, as shown in Table 1 and Table 2). In the VST test, the spindle speed was kept constant (1,000 rpm) while the feedrate were varied. As a result, the tool mark spacing was reduced from 15 μm to 0.8 μm and the relationship between the tool mark spacing...
and surface quality can be investigated. Eight samples were machined in the VST_1 test and nine samples in the VST_2 test. In the constant spacing turning test (CST, Table 3), the spindle speed and feed rate were both changed so that the tool mark spacing remained unchanged. From CST test, the affect of spindle speed and feedrate can be studied. For both VST and CST test, the tool moved in the x direction as shown in Figure 3.3b.

Table 3.1 Variable spacing turning tests (VST_1)

<table>
<thead>
<tr>
<th>No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedrate (mm/min)</td>
<td>0.8</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>10</td>
<td>15</td>
</tr>
<tr>
<td>Spindle speed (rpm)</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Tool radius (mm)</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
<td>3.048</td>
</tr>
<tr>
<td>Depth of cut (μm)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Tool mark spacing(μm)</td>
<td>0.8</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>10</td>
<td>15</td>
</tr>
</tbody>
</table>

Table 3.2 Variable spacing turning tests (VST_2)

<table>
<thead>
<tr>
<th>No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedrate (mm/min)</td>
<td>0.8</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>10</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>Spindle speed (rpm)</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Tool radius (mm)</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
<td>2.54</td>
</tr>
<tr>
<td>Depth of cut (μm)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Tool mark spacing(μm)</td>
<td>0.8</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>10</td>
<td>15</td>
<td>20</td>
</tr>
</tbody>
</table>
The third test, the diffractive tool turning test (DTT, Table 4), was designed to study the efficiency and quality of the optical surfaces that were fabricated with a very small tool, a type which is widely used in diffractive optics and micro structures fabrication. The tool nose radius is 2.5 μm, rake angle is 0° and clearance angle is 8°. The depth of cut was 1 μm, and the spindle speed was kept constant at 1,000 rpm while the feedrate was decreased from 2 mm/min to 0.3 mm/min. Only four samples were machined, all with small tool mark spacing, consistent with the small tool size.
The fourth and fifth test, the slow tool servo cutting test (STSC, Table 5) and broaching cutting test (BC, Table 6), were particularly aimed at investigating the slow tool servo (STS) process and the slow tool broaching process. During the STS process, the rotation of main spindle (C axis) was under precise control and the rotational speed
is much lower than that of turning. In general, for STS the diamond tool moves along the $X$ axis while $C$ axis rotates and $Z$ axis feeds synchronously (Figure 4b). For this study, the $Z$ axis was fixed to the depth of cut. During the slow tool broaching process, the main spindle ($C$ axis) is stationary while for the general case the machine moves in the vertical direction ($Y$ axis) and $Z$ direction (depth) to contour the surface. Tool feed direction in broaching process is also along the $X$ axis. Both the STS process and broaching processes are very useful in freeform surface machining and creating of complicated structures with optimal surface finish. For simplification, only flat surfaces were machined in STSC and BC tests. To compare STS and broaching processes with the conventional diamond turning process, some samples were also machined by diamond turning using the same tool. The diamond turning process was carried out at 1,000 rpm and at several different feedrates. Table 5 shows five STS samples and three turning samples. Similarly Table 6 shows 5 broaching samples and three turning samples.

### 3.3.2 Measurement

For each of the 42 samples, both surface profile and direct optical scattering measurements were made on the machined surface.

The surface profiles of the samples were measured on NT 3300 Veeco White Light Profilometer (www.veeco.com), which is capable of non-contact 3D surface profile measurement with nanometer resolution. The Veeco white light profilometer utilize a Mirau type interferometer [75] to measure the distance difference between the
reference mirror and the sample surface (Figure 3.4) and utilize a piezo drive system to vertically scan the sample surface. The measurement area of the NT3300 is 240µm by 183µm when using a 50x objective lens and a 0.5x field-of-view lens. The discrete points number in X and Y direction is 736 and 480.

![Schematic diagram of the white light interferometer microscope](image)

Figure 3.4 Schematic diagram of the white light interferometer microscope [75].

The optical scattering was measured by a home-built device shown in Figure 3.5 (a). The sample is shown at the right. It is irradiated with light from a 5 mw He-Ne laser shown at the left. The scattered light is sensed with the detector (Edmond 53-357, surface area 5.1mm²) shown at the upper center. The detector is mounted on a long arm which is attached to the Aerotech ADRT-200 rotary stage so that the detector can swing in an arc about sample. The direction of the laser can be adjusted to place the laser beam directly over the axis of the Aerotech rotary stage. The sample is mounted on an adjustable stage configured so that it can be translated to select the point where
the laser beam hits. It can then be rotated about vertical and horizontal axes so that the surface of the sample lies on the axis of the Aerotech rotary stage. The sample is oriented so that the normal to the sample surface is at an incident angle of 5 degrees to the laser beam. The detector rotates in an arc centered about the axis of the rotary stage and in a plane perpendicular to its axis. Its range is from 2 degrees from the sample surface normal to 90 degrees in 0.1 degree increments.

Figure 3.5 Optical scattering measurement device: (a) Setup of the scattering measurement device, (b) Scattering measurement device control system.
The measurement system was fully computerized as shown in Figure 3.5 (b). The computer is schematically shown at the bottom. It performs two functions. First it controls the angle of the rotary stage through the drive shown at the left. Second the computer records the detector current increased by the amplifier shown at the right.

Figure 3.6 shows both surface profile measurement results and the optical scattering measurement results from a typical diamond turned sample. Figure 3.6a shows a typical three-dimensional surface profile measured by the Veeco profilometer. In Figure 3.6a the X axis is along the tool feed direction, Y axis is along the cutting direction and Z axis is the height of the surface variation. From the measured 3D surface profile data, the surface profile spectrum can be calculated using the discrete Fourier transform. Figure 3.6 (b) shows the associated 1D surface profile spectrum obtained by first funding the 2D surface spectrum and then superimposing all the spectrum in the tool feed direction (X axis). In Figure 3.6b, the peaks 1 to 9 are the harmonics of the periodic tool marks. Figure 6 (c) shows the direct optical scattering measured by the home built device described early. Figure 3.6 (c) shows the optical scattering plotted as a function of spatial frequency (the spatial angle was changed to spatial frequency by \( \nu = \frac{\sin \theta - \sin \theta_i}{\lambda} \), where \( \theta \) is spatial scattering angle, and \( \theta_i = 5^\circ \) is the incident angle). In Figure 3.6 (c), neglecting the specular reflection (the 0 order) 13 diffraction peaks can be seen. It can be seen that the optical scattering is similar to the surface profile spectrum. Figure 3.6 (d) compares the signal-to-noise ratio of the harmonic peaks (Figure 3.6 (b)) obtained by Veeco measurement and the diffraction peaks (Figure 3.6 (c)) obtained by the optical scattering measurement. In each case the
signal-to-noise ratio was calculated as the ratio of the amplitude of peaks to the amplitude of the background noise (amplitude at the bottom of each peak). The high signal-to-noise ratio at peak 6 and peak 9 was caused by the shape of the tool marks of this sample and is not common for all samples. This will be studied in future works. Because the Veeco measurement cannot achieve high magnification and large view field at same time, and also because the Veeco measurement is discrete, the Veeco measurement has lower sensitivity and signal-to-noise ratio than the optical scattering measurement does.

Figure 3.6 Comparison of typical Veeco profilometer and optical scattering measurements. (a) 3D plot showing typical surface profile measured by profilometer; (b) Calculated surface profile spectrum in x direction based on Veeco measurement; (c) Directly measured optical scattering in x direction for the same sample; (d) Comparison of the signal-noise ratio of the Veeco profilometer and direct optical scattering measurements.
Figure 3.6 continued
3.4 Optical Effects of Surface Finish by Ultraprecision Single Point Diamond Machining

In this section, the results of all 5 sets of tests will be presented and the relationship with the machining process will be discussed. In Section 3.4.1 the diamond turning process with large radius tools is considered; the diamond turning process with small radius tools is discussed in Section 3.4.2; while in Section 3.4.3 and 3.4.4 we consider the Slow Tool Server process and Broaching process respectively; a model for the diamond turned surface is presented in Section 3.4.5.

For each test, four different sets of plots will be displayed. The first plot is the first-order diffraction peak intensity normalized to the incident light peak intensity as a function of machining parameters, specifically tool mark spacing, feedrate, and spindle speed. The second plot is the ratio of the specular (zero-order) reflection light peak intensity to the incident light peak intensity as a function of the same machining parameters. The third plot is the surface roughness \( (R_a) \) as a function of machining parameters. The forth plot is the periodic tool mark depth, which was calculated by first identifying the periodic harmonies from the spectrum and then plotting the associated surface profile. The tool mark depth is then the peak to peak value of the plot. This is also presented as a function of machining parameters. The data of the first and second plots were obtained by the direct optical scattering measurement and the data of the third and fourth plots were obtained by the surface profile measurement. The error bars in these plots were obtained by making a second measurement.
3.4.1 Diamond Turning Process with Large Radius Tools

The regular diamond turning process with large radius tools (3.048mm and 2.54mm) is first evaluated. There are two sets of data in this part. In the first set the relationship between the surface quality and the tool mark spacing is presented. The data used in this set comes from the samples of VST_1, VST_2, and the diamond turning samples of STSC and BC test. The second set of data concerns the relationship between the surface quality and feedrate/spindle speed. The samples used in this analysis were come from CST test.

3.4.1.1 Relationship between Surface Quality and Tool Mark Spacing

Figures 3.7 compare the four sets of diamond turning data that were obtained using large radius (3.048 mm and 2.54 mm) tools. These include all the samples of VST_1 and VST_2 tests and all the diamond turning samples of STSC and BC tests. VST_1 test was performed using a worn 3.048 mm radius tool; STSC and BC test were performed using a new 3.048 mm radius tool; VST_2 test was done using a new 2.54 mm radius tool.
Figure 3.7 Experimental results of diamond turning tests, including all the samples of VST_1, VST_2 and the turning samples of STSC and BC. (a) Normalized first order diffraction intensity; (b) Normalized specular reflectivity; (c) Surface roughness measured by Veeco profilometer; (d) Theoretical and measured tool mark depths all versus tool mark spacing.
Figure 3.7 (a) shows the first order diffraction intensity normalized to incident light intensity vs. tool mark spacing for several different tools. The data were acquired from the direct optical scattering measurements. In figure 3.7 (a), it can be seen that the first order diffraction intensity decreases as the tool mark spacing decreases. For different tools, the diffraction intensity is different. The diffraction of the samples machined by the worn tool is higher than that of the samples machined by the new
tool. The diffraction of the samples machined by new and different tool is at the same level. There is shown a critical level below which the diffraction caused by the tool marks can be neglected (for example, we choose when only 0.05% of the incident light was diffracted), and the position of this critical point, where the first order diffraction crosses the critical level, depends on the condition of the tool used. In this test, only some samples machined by the worn tool were above this level.

Figure 3.7 (b) shows the normalized specular reflectivity versus tool mark spacing. The specular reflectivity is affected by diffraction associated with the periodic tool marks and by random scattering. The specular reflectivity remains in the region 0.83-0.88 for tool mark spacing between 20 μm – 2 μm and decreases rapidly for tool mark spacing less than 2 μm. For samples of VST_1, the diffraction intensity associated with the tool marks is higher than that of samples of other tests; the specular reflectivity is lower than that of samples of other tests as well. The reason for specular reflectivity rapidly decreases demands further study. It can be seen that the samples machined by worn tool machined samples have smaller specular reflectivity than the samples machined by new tools. If the specular reflectivity were used as an indicator, a critical tool mark spacing could be identified in figure 7 (b) for diamond turning process (the straight dash light). Specular reflectivity above this line (we choose 85%) is acceptable for most of our applications. This includes all samples machined with new tool and tool mark spacing greater than three microns.

Figure 3.7 (c) shows plots of surface roughness $R_a$ versus tool mark spacing. The surface roughness comes from two contributions, the first is the periodic tool
marks, and second is the random roughness. For VST_1, at wide spacing where residual tool mark depth is large, the surface roughness increases with an increasing spacing. All but one of the values are below the critical level. That one sample is machined by worn tool. At very small spacing, because the machining time is long so that the external effects such as vibration and spray maybe significant, the random roughness also increases. Otherwise the surface roughness has no obvious relationship with the tool mark spacing.

Figure 3.7 (d) shows the residual tool mark depth versus tool mark spacing. As described earlier the data were obtained from the Veeco measurements. The residual tool mark depth has the same trend as the first order diffraction intensity (Figure 3.7 (a)) and decreases as the spacing decreases. For different tools, the residual tool mark depth is different and the new tools tend to form lower residual tool mark depth. Comparing the measured residual tool mark depth with the theoretical tool mark depth, the actual depth is much larger than the theoretical value at large spacing and is closer to the theoretical predicted depth at small spacing. A critical tool mark spacing exists below which the periodic tool mark depth can be neglected. For these samples, we choose 15 nm, which is the same level of the surface roughness of these samples as shown in Figure 3.7 (c). Because in that case the periodic tool marks cannot be easily separated from the random surface variation if only the surface roughness is considered [44].
3.4.1.2 Relationship between Surface Quality and Feed Rate and Spindle Rotation Speed

Figures 3.8 (a)-(d) show the comparison of the normalized first order diffraction, specular reflectivity, surface roughness, and residual tool mark depth of CST tests versus feed rate and spindle speed. In this test, 5 sample surfaces were diamond turned using a 3.048 mm radius tool at different feed rates and spindle speeds (Table 3.3) and the tool mark spacing was constant at 5μm. Figure 8a shows the first order diffraction ratio. It can be seen that higher spindle speeds and feed rates tend to generate higher diffraction. Figure 8 (b) shows the specular reflectivity which was not affected by the spindle speed and feed rate. Figure 8 (c) shows the surface roughness, which increased as the spindle speed and feed rate increase. In Figure 8 (d) we see the residual tool mark depth. It can be seen that the tool mark depth at higher spindle speed and feed rate is larger than that at lower spindle speed and feed rate. Comparing to the data in Figures 3.7, the diffraction and tool mark depth in Figures 3.8 is larger and this is because the tool used in this test is worn.
Figure 3.8 Experimental results of CST tests. (a) Normalized first order diffraction intensity; (b) Normalized specular reflectivity; (c) Surface roughness; (d) Measured and theoretical tool mark depths all versus feedrate and spindle speed.
3.4.2 Diamond Turning Process With Small Radius Tool

Figures 3.9 (a)-(d) shows the results of DTT test (Table 3.4). It can be seen that Figures 3.9 (a) and 3.9 (d) have trends similar to those Figures of the larger radius tools (Figures 3.7 (a) and 3.7 (d)). The differences are the amplitude and the decrease/increase rate. The comparison of Figures 3.9 (b) and 3.9 (c) to 3.7 (b) and 3.7 (c) is not very obvious. The small radius tool brings much stronger diffraction, much
higher residual tool mark depth, and much larger surface roughness at large tool mark spacing. When machining using the small radius tool (2.5 μm), the tool mark spacing needs to be less than the light wavelength otherwise the diffraction may not be ignored.

Figure 3.9 Experimental results of DTT tests. (a) Normalized first order diffraction intensity; (b) Normalized specular reflectivity; (c) Surface roughness; (d) Measured and theoretical tool mark depths all versus tool mark spacing.
3.4.3 Slow Tool Servo Process

The STSC tests (Table 3.5) give a comparison of the Slow Tool Servo (STS) process and regular diamond turning process. From the plots in Figures 3.10 (a)-(d), it is seen that the surfaces machined with the STS process have the same quality as diamond turned surfaces. The diffraction caused by the periodic tool marks of STS machined samples is in general slightly higher than that of diamond turned surfaces.
The specular reflectivity of slow tool servo process machined surfaces is about 2% less than that of diamond turned surfaces on average (Figure 3.10 (b)). At very small spacing, the surface specular reflectivity of the surfaces machined with the slow tool servo process become notably worse due to longer machining time. Figure 3.10 (c) shows the surface roughness of the STS machined surfaces and diamond turned surfaces. The STS machined surfaces have much larger surface roughness at very small spacing, while the surface roughness at larger spacing is at the same level of diamond turned surfaces. Figure 10 (d) shows the residual tool mark depth of both the STS machined surfaces and diamond turned surfaces. The STS machined surfaces in general have slightly larger tool mark depth than that of diamond turned surfaces.

Figure 3.10 Experimental results of STSC tests. (a) Normalized first order diffraction intensity; (b) Normalized specular reflectivity; (c) Surface roughness; (d) Measured and theoretical tool mark depths all versus tool mark spacing.
Figure 3.10 continued
3.4.4 Broaching Process

The BC test (Table 3.6) compares the slow tool servo broaching process and the regular diamond turning process. From the measured data, the broaching process machined surfaces have the same quality of diamond turned surfaces (Figure 3.11). The diffraction from the periodic tool marks off the surfaces machined by broaching process is slightly higher than that of diamond turned surfaces (Figure 3.11a). The specular reflectivity difference between surfaces machined by broaching and diamond turning is within 2% (Figure 3.11 (b)). Figure 3.11 (c) shows the surface roughness of the broaching machined surfaces and diamond turned surfaces. The surface roughness of the broaching machined surface is slightly higher than that of diamond turned surfaces. Figure 3.11 (d) shows the residual tool mark depth of both the broaching machined surfaces and diamond turned surfaces. The tool mark depth of these two type of surfaces are almost at the same level.
Figure 3.11 Experimental results of BC tests. (a) Normalized first order diffraction; (b) Normalized specular reflectivity; (c) Surface roughness. (d) Measured and theoretical tool mark depths all versus tool mark spacing.
3.4.5 Model for Diamond Machined Surface

In this section are presented two mathematical models for the relationship between first order diffraction and the machining parameters (tool mark spacing, diffraction angle, and tool condition) for large radius tools (3.048 mm and 2.54 mm). These two empirical models were based on all the related diamond machined samples (VST_1, VST_2, CST, STSC, and BC) demonstrated previously.
Figure 3.12 Models for the relationship between tool marks caused diffraction and tool mark spacing

Figure 3.12 (a) is a log-log plot showing the relationship between the normalized intensity of the first order diffracted beams $I_i/I_i$, tool mark depth $d_i$, and diffracted angle $\theta$, as Eq. 8:
\[ I_1/I_i = 6.64 \times 10^{-7} \cdot e^{2.3 \cdot \text{ctg} \theta \cdot d_i} \]  \hspace{1cm} (3.16)

where \( I_i \) is the first order diffraction intensity, \( I_1 \) is the incident light intensity, \( d_i \) is the magnitude of the first order harmonic coefficient of the periodic tool marks, and \( \theta \) is the diffraction angle (in our setup, the diffraction is along \( X \) axis). From Figure 3.12a, it can be seen that the normalized first order diffraction intensity has an exponential relationship with the term \( d_i \cdot \text{ctg} \theta \). The points with larger \( I_1/I_i \) come from both larger tool mark depth and smaller diffracted angles and also worn tools. For diffraction off the periodic tool marks, there is a critical value below which the diffraction level is acceptable (i.e. we choose \( I_1/I_i = 0.05\% \), the red dash line as shown in figure 3.12 (a)). From Figure 3.12 (a), the critical value of \( d_i \cdot \text{ctg} \theta \) can also be found once the critical diffraction level \( I_1/I_i \) is chosen. In our tests, the critical value of \( d_i \cdot \text{ctg} \theta \) is about 60.

Figure 3.12 (b) shows the relationship between \( d_i \cdot \text{ctg} \theta \) and the tool mark spacing for the same group of samples used in Figure 3.12 (a). Both tool mark depth and diffraction angle are affected by the tool mark spacing and the tool mark depth is also affected by tool condition and machining conditions (machining process, spindle speed and feedrate). In Figure 3.12 (b), there are seven different lines corresponding to different tools and different machining conditions. It can be seen that worn tools tend to generate higher tool mark depth. The worn tools has larger cutting edge radius than the newer tools. According to the review and discussion in Chapter 2, we can propose
a hypotheses that the tool cutting edge radius can affect the tool mark depth thus affect
the amount $d_1 \cdot \text{ctg} \theta$. For new tools, the tool mark depth is at the same level no matter
which process (turning, STS, or broaching) was used. From this model, we can find the
optimal tool mark spacing for each tool. For tool 1, to obtain critical value 60 for
$d_1 \cdot \text{ctg} \theta$, the tool mark spacing needs to be below 6 $\mu$m. For tool 3, 5 and 6 up to 20 $\mu$m
tool mark spacing is acceptable.

This model can be used to select optimal machining condition for diamond
machining process. Only the first order diffraction was considered in this model.
Several other criteria can also be considered, such as specular reflectivity, and surface
roughness.

3.5 Summary

In this chapter, the optical effects of diamond machined surfaces are studied.
We consider the influences from machining parameters, such as tool mark spacing,
feedrate, spindle speed, tool radius, tool condition and different diamond machining
process.

First, the analytical analysis for the calculation of the diffraction and scattering
from diamond machined surface was carried out. The diffraction is the combination of
three parts, the specular reflection, higher order diffraction and random scattering.
Both the diffraction field and diffraction light irradiation can be obtained after
knowing the surface characteristic parameters.
Then, the relationship between the machining conditions and the optical performance of the diamond machined surfaces was studied experimentally.

For the large radius tool single point diamond turning process (Section 3.4.1), it is shown that the normalized first order diffraction intensity caused by periodic tool marks decreases as the tool mark spacing decreases, and there exists a critical tool mark spacing value under which the diffraction can be neglected. This critical value is related to the tool condition, spindle speed. The worn tools and large spindle speeds tend to generate higher diffraction. For worn tools the critical tool mark spacing is about 5 μm while the critical tool mark spacing can be as large as 20 μm for the new tools.

The normalized specular reflectivity of a test sample also varies as the tool mark spacing changes (Section 3.4.1 to 3.4.4). To maintain high specular reflectivity, the tool mark spacing cannot be very small (feedrate cannot be very low). For our tests, the minimal acceptable tool mark spacing cannot be less than 2 μm and still have good specular reflectivity. The minimal value is also affected by the tool condition, tool size, spindle speed, and machining process used.

The diffractive diamond tools used for diffractive optics machining generate much more diffraction than large radii tools due to the small nose radii (Section 3.4.2). Therefore for machining of diffractive optical elements, the tool mark spacing need be less than the light wavelength.
The surfaces machined by slow tool servo and broaching processes have optical effects similar to those of the diamond turned surfaces, and their quality is at the same level (Section 3.4.3 and 3.4.4).

Finally, an empirical relationship between the machining conditions (feed rates and tool condition) and the first order diffraction of the diamond machined surface was setup. This model can be used to select optimal machining condition for diamond machining process, in particular for slow tool servo machining or broaching of freeform optical surfaces, including micro and diffractive optical elements.
CHAPTER 4: SPDM APPLICATION: MICROLENS ARRAY AND 3D
MICROLENS ARRAY PROJECTION

Micro-optical devices have been used broadly in recent 20 years. Microlens arrays are the most studied and best developed micro-optical device because microlens array has simple structure and extensive usage. Simply speaking, a microlens array is a combination of several of a number of lens the diameter of which is from several micrometers to several millimeters. In this range, the geometry optical theory can still apply and the diffraction is not dominant. The best noticeable advantage of the microlens array is the compact size and high efficiency. Microlens array has been used in numerous fields since its first appearance, for example in measurement, detecting, imaging, beam steering, machining, and communication [76; 77; 78; 79; 80; 81; 82; 83].

In general, there are two types of microlens arrays, one is using the geometry profile to form the lenslet and the other is using the material property to form the lenslet [84]. Numerous fabrication methods for microlens array were investigated. Among the fabrication methods for the geometry profile shaping, one is directly shaping and the other is duplicating. The directly shaping method use some 'tools' like laser beam, ion beam, thermal, UV light, and diamond cutters [85; 86; 87; 88; 89; 90] to make the profile of the microlens array directly. The duplicating method also uses
some ‘tools’ to fabricate a mold and then replicate the shape of the mold to substrates [91; 92; 93; 94; 95].

Among these fabrication methods, ultraprecision single point diamond machining process has some overwhelming advantages. For example, SPDM and micro machining process are capable of true 3D machining, have optical surface finish and dimension accuracy, have very large dimension span, can be used for both direct machining and mold machining, have lots of machinable material choice, and the process are very flexible and suit for many different design. Of course, SPDM and micro machining also have some disadvantages, like machinable structure limited by the tool, residual tool marks, and tool wear. Microlens array can also be considered as a special type of freeform surface. Thus the slow tool servo process may be used for machining microlens array structures and regular single point diamond turning will also be involved for substrate surface machining.

In this chapter, the procedure of design, fabrication, and test of microlens array by using SPDM will be discussed in Section 4.1. In section 4.2 gives an application example by using 3D microlens array machined by using SPDM.

4.1 Design and Fabrication of Microlens Array by Using SPDM

The design and fabrication of the microlens array by using SPDM mainly include four steps, optical design, tool trace design, machining process design and machining, and testing and measurement. In this section, these four steps will be discussed and several microlens array examples will be given.
4.1.1 Optical Design

For the microlens array machined by using SPDM, the design process includes the design of each micro lenslet and the design of the distribution and layout of the micro lenslets on a substrate surface. If the diameter of the lenslet is not too small (> several microns), geometry optical theory can still be approximately used for the optical design. The optical design is principally the same as regular lens design and is based on the application demanding. However there are some unique features to the microlens arrays machined by other methods:

1. Unlike the microlens arrays machined by other methods where the lenslet can only have spherical or parabolic like shape. The lenslets of the microlens arrays machined by SPDM can be aspherical or even freeform as long as the slop of the profile is less than the clearance angle of the diamond tool. Thus better optical design like aberration correction can be applied to the lenslet.

2. The shape of the lenslets in a microlens array doesn't need to be the same, which means these micro lenslets can have different profile according to the requirement of the application.

3. The distribution of the micro lenslets is optional and not restrict to matrix or circular as long as the lenslets do not interfere with the tool.
4. The layout of the micro lenslets is not restricted to flat surface, therefore the micro lenslets can be scattered on a curved surface like sphere, parabolic, or even freeform surface.

These properties will greatly enlarge the application range of the microlens array and also improve the quality of the microlens array.

Next, the design of two different microlens arrays will be given. The first one is a matrix arranged microlens array mold on a flat surface, thus the lenslets are concave. The second one is a circular arranged microlens array on a spherical surface, and the lenslet is also a plano-convex type.

For design one, the microlens array consists of 5x5 spherical concave micro lenses cavities as shown in Figure 4.1. Each micro lens is spherical in shape. The diameter of the lens cavity is 2 mm and the sag is 100 μm. The center to center distance is also 2 mm.
For design two, each micro lenslet has a plano-convex shape and the curvature radius of the convex sphere is 1.5 mm. The diameter of the aperture for each micro lenslet is 0.6 mm, and the distance between the neighboring micro lenslets is 0.9 mm. The micro lenslets are distributed on a spherical substrate surface and the axes of all the micro lenslets point to the center of the substrate sphere. The radius for the top surface of the substrate is 50.5 mm and the radius for the bottom surface of the substrate is 48.5 mm, thus the thickness of the substrate along the sphere radius direction is 2 mm, plus the height of the lenslet sphere above the substrate, the thickness of the micro lenslet is 2.030 mm and the design focal length was 3.677 mm from the front surface. In this design, the micro lenslets were circularly distributed on the substrate sphere surface. There were 11 circles of micro lenslets in the 10 mm radius, and the total number of the micro lenslets was 340. Figure 4.2 (a)-(d) show the
layout, ray fan, spot diagram, and MTF of the micro lenslet of design two by using optical design software ZEMAX. It can be seen from Figure 4.2 that due to the small size of the microlens, the optical aberration is quite small. Figure 4.3 (a) shows the designed micro lenslet array distributed on a spherical surface. Figure 4.3 (b) shows the cross section of the 3D micro lenslet array from $r=0$ to $r=10$ at the 0° position (corresponding to $X=0$ to $X=10$ at $Y=0$ plane).

Figure 4.2 Optical design of a Plano-convex micro lenslet. (a) Layout of the lens, (b) Ray fan plot, (c) Spot diagrams, (d) MTF.
Figure 4.2 continued

(b)

(c)
Figure 4.3 Design of the microlens array on a spherical surface (a) isometric-view of the microlens array (b) cross sectional view of top surface of the 3D microlens array along 0° (Y=0) direction.
4.1.2 Tool Trace Design

The next step for machining the microlens array, as well as other freeform surfaces, by slow tool servo process is to generate the tool path. There are two different types of slow tool servo cutting methods. One is the rotational slow tool servo process and the other is the slow tool servo broaching process [96]. For design one, both rotational slow tool servo process and slow tool servo broaching process can be used. For design two, since the curved surface is spherical and the micro lenslets are circularly distributed, the rotational slow tool servo process was considered to be more appropriate.

Take the rotational slow tool servo process as an example, the tool path was obtained by first setting up the rotational center and then calculating the normal vector.
of the surface curvature and the micro lenslet curvature plus compensation of the tool radius according to the rotational center. In the calculation of the tool path code, one would need to ensure that the cutting tool will not interfere with the features to be cut and the clearance angle of the tool is large enough so not to scratch the machined surface. However, it is almost impossible to entirely eliminate that interference between the diamond tool and the feature to be machined, for example, the disrupted conjunction between two lines or two surfaces. In this situation, the structure need be redesigned according to the machining process unless the points of conflicts are not important, in that case, the tool path can be modified to smoothly connect two neighboring points.

For example, to fully machine the sphere part in figure 4.4a, the tool will interfere with the straight line section. If this junction section is not important, the design can be modified to a smooth curve as shown in figure 4.4b. It will be much more complicated for the real machining for the design are always 3D structure rather than the 2D plot shown in figure 4.4.
Figure 4.4 Example for the interfere during STS machining freeform surface. (a) original design where interfere happens (b) modified design.

Figure 4.5 and 4.6 show the CNC tool trace of design one and two for the rotational STS process. The tool trace start from the outside and spirally reach the center. To clearly show the trace, the number of passes was reduced. The actual number of passes is decided by the requirement for the dimension accuracy and surface roughness.
4.1.3 Machining Process

The machining process is also different for different microlens array designs. Proper machining process needs to be identified based on specific optical design, material used, and dimensions of the part.
The 5x5 micro concave lens array is machined on brass and the substrate can be directly set on the main spindle of the machine tool by simple fixtures. The machining process is described as follows. First the substrate material was diamond turned on both top and bottom surfaces. If the position of the micro lenses on the surface is important, the outside diameter of the cylinder also needs to be diamond turned in order to indicate the part of proper centering. Then, the microlens cavities machining can be carried out by applying the tool pass code which was programmed in the previous step. Figure 4.7 shows the machined microlens array.

![Machined freeform microlens array.](image)

The machining process for the 3D microlens array is schematically illustrated in figure 4.8. A piece of round polymethylmethacrylate (PMMA) substrate was first machined to rough dimensions (figure 4.8 (a)). Both the top and bottom surfaces were diamond turned to establish the flatness and parallelism of these surfaces. The outside
diameter was also diamond turned and can be used as a reference to center the part. The part was then mounted on the vacuum chuck and the bottom concave sphere surface ($R \ 48.5 \text{ mm}$) was machined right of the middle of the part by diamond turning (figure 4.8 (b)). Since the designed part is hollow and the thickness of the part is small, it cannot be mounted on vacuum chuck due to deformation. To support the PMMA part, an aluminum mandrel (as shown in figure 4.8 (c)) was machined to match the bottom surface of the PMMA part machined in the last step. The PMMA part was bounded to the aluminum mandrel using optical wax (figure 4.8 (d)) and the mandrel was directly mounted on the vacuum chuck of the diamond machine. The center of the PMMA part was aligned with the machine spindle using the outside circular surface as reference with an ultraprecision dial indicator (federal gage, model EHE-2056, www.mahr.com). The topside sphere on the PMMA part was first machined by diamond turning. Then the 3D microlens array on the top surface was fabricated by slow tool servo process using the tool path described previously (figure 4.8 (e), the micro lenslets were not shown in the plot due to their small size). The diamond tool used for contouring the 3D microlens array has a 0.2438 mm tool nose radius and 8° clearance angle. Finally, the aluminum mandrel and wax were removed to complete the construction of the 3D microlens array on a sphere surface (figure 4.8f).
Because the gaps between the micro lenslets and the target will generate stray light, a 3D micro aperture array was fabricated. The machining process is similar to the process shown in Figure 4.8. The differences are: 1) the material used is black thermo plastic olefin (TPO) instead of PMMA; 2) in Figure 4.8(e), the final thickness of the aperture array is about 0.2 mm instead of 2 mm for the microlens array; 3) in Figure 4.8(e), micromilling was used to drill the through holes on the thin sphere TPO aperture. Figure 4.9 (a) and 4.9 (b) show the fabricated 3D microlens array and the 3D micro aperture array respectively.
4.1.4 Measurement and Testing

There are two kinds of the measurements for the machined microlens array. The first kind is mechanical measurement including surface profile measurement and surface roughness measurement. The second kind is the optical testing.
4.1.4.1 Mechanical Measurement

For the first design, mechanical measurement was applied. The machined surfaces were measured using a contact type profilometer (surf 2000, Federal Gage Inc.). Figure 4.10 (a) demonstrates the measurement of three neighboring lenses. The measured curves were plotted against a best fit curve. This result has demonstrated that STS is capable of producing optical surfaces that meet or exceed precision optical application. The machined microlens array was measured on Wyko phase shift microscope for surface roughness. Figure 4.10 (b) shows the surface in a 3D format. For this surface, \( R_a = 34.5 \) nm, where \( R_a \) is evaluated over the 0.70 mm scan length. This value meets the requirements for optical applications. No post machining polishing is required. Such a result is critical because no process available today can be adapted to polishing a complicated optical surface without altering its shape.

The finished 3D microlens array was measured using a laser based noncontact profilometer. Figure 4.11 shows the measured surface profile using Fries Research & Technology-FRT GmbH’s Microglider [97]. Figure 4.11 (a) is the 3D surface profile of the fabricated microlens array. A 2D surface profile of the microlens array along the 0° direction (\( Y=10 \) in Figure 4.11a) and from the center to the edge was obtained and compared to the design micro lens profile described earlier in figure 4.3 (b). As shown in Figure 4.11 (b), the measured lens profile matches the design lens profile well. The maximum error of the micro lenslet profile in height was around 6 \( \mu m \) at \( X=9 \) mm (lenslet at the 11th circle).
Figure 4.10 (a) Profile of the micro lenses, (b) Surface finish of the slow tool servo diamond machined microlens array.
Figure 4.11 (a) Measured 3D surface profile of the microlens array (b) Measured 2D surface profile along the 0° ($Y=10$) from center to the edge

Notice that the large positive/negative error peaks mostly occurred at the junctions between the micro lenslets and the base spherical surface. This was largely
due to the shape and the size of the tool used in slow tool servo. However, since these errors appeared only at the edge of the micro lenslets, they will not affect the quality of the system performance. The error between the measured and design profile is a combination of the design error, machining error, measurement error, and data analysis error. The main source of errors includes: 1) the diamond tool’s radius error; 2) tool and part alignment error; 3) machine tool positioning error and movement error; 4) the spring back of the material; 5) measurement error; 6) design and measurement data fitting error. The affect of these errors to the final performance of the 3D microlens array and how to improve the machining and measurement accuracy will be discussed in future work.

4.1.4.2 Optical Testing

Optical testing has also been carried out for design two. First, the focal length of the micro lenslet was measured using a standard optical microscope (BH2, Olympus) with a 10x magnification objective lens. The schematic setup for the measurement of the micro lenslet’s focal length is shown in Figure 4.12. The 3D microlens array and the aperture array were placed on the microscope stage. To measure the focal length, first adjust the focus of the microscope to the surface of the micro lenslet. Second put a transparent object mask right on the field lens of the microscope and adjust the focus of the microscope until a clear image of the object mask was seen. The distance moved by the stage is $d_1$, and the distance from the object mask to the surface of the micro lenslet is $d_0$. The focal length of the micro lenslet can thus be obtained from lens equation:
\[ \frac{1}{f} = \frac{1}{d_0} + \frac{1}{d_1} \]  \hspace{2cm} (4.1)

The measured focal length for the micro lenslet at the center of the microlens array is 3.4730 mm from the front surface. Comparing to the design focal length 3.677 mm, the error was 5.5%.

![Schematic setup for measuring the focal length of the micro lenses.](image)

Figure 4.12 Schematic setup for measuring the focal length of the micro lenses.

The imaging quality of the micro lenslets was then evaluated by measuring the point spread function (PSF). Figure 4.13 shows the schematic setup for measuring the PSF. A He-Ne laser (\( \lambda = 0.6328 \ \mu m \)) was used as light source, and a microscope objective lens with a 50 \( \mu m \) precision pinhole was used to generate a point source. The 3D microlens array was placed behind the pinhole, and the distance between the 3D microlens array and the pinhole is 250 mm in this measurement. To evaluate the image of the point source, a zoom lenses imaging system (VZM\textsuperscript{TM} 450i, Edmund Optics, [www.edmundoptics.com](http://www.edmundoptics.com)) and a CCD camera (PL-B957F, pixeLINK, [http://www.aegis-elec.com/products/PL-B957F.html](http://www.aegis-elec.com/products/PL-B957F.html)) were used. The magnification of
the zoom lenses was set at 1.0x. The exposure time was set at 0.4 s, at this setting, the maximum incident intensity was just below the saturation level of the CCD camera.

Figure 4.13 Schematic setup for measuring the point spread function of the micro lenslet

The image of the point source formed by the micro lenses and the zoom lens is shown in figure 4.14 (a), indicating the uniform performance of the micro lenses. Due to the limited size of the sensor, not all the points imaged by the microlens array were shown in figure 4.14 (a). Figure 4.14 (b) shows the cross section light intensity distribution of the image of the point source by the micro lenslet at the center of the microlens array. From figure 4.14, it can be seen that the most of the energy was concentrated in the center and diffraction energy (loss) can hardly been seen. In figure 10 (b), a detailed plot of a single focal point, two diffraction rings can be seen and the diameter of the first dark ring is 39.7 μm.
Figure 4.14 (a) Image of a point source by the microlens array (b) cross section of the image of the point source by the lenslet at the center of the microlens array

4.2 Three Dimensional Micromachining by using Microlens Array Projection

Besides the prescribed applications, the microlens array can also be used for micro machining as the projection lithography optics. There already have some developed microlens projection system for micro machining [98; 99; 100], but they are
all used for micro machining on plane and therefore considered to be 2D micro machining.

In the past, numerous efforts have been tried to obtain microstructures on concave or convex surface using different techniques. These techniques belong to two different categories, the direct 3D micromachining method and photolithography/projection based method.

The well known direct 3D micromachining methods include laser micromachining, micro milling, and micro electrical discharge machining (EDM). These processes can be used to directly generate true 3D microstructures/patterns using physical tools on both planar and curved surfaces. These processes are however restricted by the design of the tools (the size and shape of the laser beam, the milling bit, or the electrode) and the resolution and the control of the machine.

Different to the direct 3D micromachining method, the photolithography or projection based method use modified lithography process like gray scale and multilayer exposure. However these processes have complicated operation and require precise alignment.

Although the prescribed photolithography or projection based methods are not true 3D micromachining like the direct micromachining methods, they have a major advantage, i.e., it is suitable for mass production. Compared to the direct machining process, such as laser micromachining and micro milling, the photolithography/projection based method can generated a large number of
microstructures in a single operation therefore has a higher efficiency for high volume production. Moreover, these methods have less restriction on the tool and the control of the machine.

A process realizing 3D microfabrication on curved surfaces can be developed based on the fabricated microlens array on curved surface. Obviously, this process will have the following characteristics:

1. True 3D process capability, in principle can be utilized to create complex microstructures on arbitrarily curved-substrates

2. A replication process partially based on lithography principle but without the use of cleanroom therefore allowing high volume and low cost manufacturing

3. Can be applied to wide selection of substrates including metals, polymers and other common engineering materials.

4.2.1 Three Dimensional Micromachining Process

The projection lithography is a high volume micro scale fabrication process. As illustrated in figure 4.15, the system used in this study consists of a precision stage that is computer controlled in real time down to submicron level, similar to the precision level on the 350 FG diamond machine. This system allows precise movement of the test sample in 3D space. One of the core components is this 3D micro projection optics, which can be a 3D microlens array, 3D diffractive optical elements, a 3D freeform micro optics or a combination of the aforementioned optics. Unlike the more
conventional optics, 3D micro projection optics will generally image on a non-flat surface.

In this study, the microlens array which was fabricated on a curved surface in the previous step was used as the 3D micro projection optics. The microlens array was placed above a substrate which also has a curved surface. The radius of the substrate sphere is 46.83 mm and the thickness of the shoulder is 1.67 mm. If the 3D microlens array and the substrate are very well aligned and the centers of these two sphere surfaces are coincident to each other, the 3D microlens will focus right on the top surface of the substrate for object at infinite distance.

In this experiment, the substrate is also made of PMMA and the curvature was machined by diamond turning. A shoulder was also machined on the PMMA substrate.
at the same time when the curved surface was created to ensure that the distance between the substrate and the 3D microlens array is 1.67 mm. This shoulder can also be fabricated separately as a spacer if the shoulder cannot be made directly on the substrate. To create the projected pattern, a thin layer of photoresist (SU8 2005, Micro Chem, [www.microchem.com](http://www.microchem.com)) was spin coated on the curved substrate. The spindle speed of the spin coater was 1,000 rpm (revolution per minute) and the thickness of the photoresist was estimated to be about 7 μm. After soft bake, the photoresist was exposed to UV light. A UV lamp (SUNRAY 400 SM, wavelength range 320nm – 390nm) was placed over a photomask of an Ohio State logo (Figure 4.16) made out of transparency using laser printer, the proper light distribution will be emitted on the photoresist surface. Afterward, the photoresist was baked and developed and 3D micro scale structures were created on the spherical surface of the substrate. Figure 4.17 shows the setup for the 3D microlens array projection system.

**Figure 4.16 Detailed mask with Ohio State logo pattern design.**
4.2.2 Results

Figure 4.18 illustrates one of the patterned OSU logo on a substrate surface. The exposure time for this sample was 60 seconds. From figure 4.18, this pattern was well developed. The dimension of the Ohio State logo is about 340 μm by 460 μm. Compare to the original mask size of 11.8 mm by 16.7 mm, giving an overall reduction of 34:1. The resolution of the 3D projection is high, i.e. the curvature of the edge of letter O was very smooth and the line width change of letter O is also very visible.
Figure 4.18 Patterned OSU logo on a substrate surface

Figure 4.19 (a) and (b) show the scanning electron microscope (SEM) pictures for 3D micro patterns generated on another substrate in this study. The exposure time for this sample was also 60 s. It can be seen that the micro patterns were well distributed on a curved surface. Because the microlens array was distributed on a curved surface, the viewing angles of these microlenses at different position to the same photomask were different. Thus the images of these microlenses were also different, similar to the case involved in the compound eyes of insects. In order to generate identical patterns at all places, the setup of the 3D micro projection system as shown in figure 4.15 need be modified. Figure 4.19 (b) shows the details of one of the logos.
Figure 4.19 (a) a group of the micro patterns by 3D micro projection (b) an individual pattern.

4.3 Summary

In this chapter, the design, machining and testing of microlens array by using SPDM process was introduced. Two microlens array examples were given. One is the matrix arranged concave micro lenses on flat brass substrate surface. The other one is
the circular arranged plano-convex micro lenses on a thin spherical substrate surface. From the measurement results, it can be seen that the machined micro lenses has very high dimension accuracy and optical surface finish. The optical testing shows that the focal length of the machined micro lenses agree with the design and has very little diffraction.

It shows that, compare to other methods, SPDM process is capable of true 3D machining, producing surfaces with optical surface finish and high dimension accuracy, has very large dimension span. SPDM can be used for both direct machining and mold machining, has lots of machinable material choice, and the process is very flexible and suit for many different design.

By using the fabricated 3D microlens array, a 3D micro projection machining system can be developed. The 3D micro projection required a substrate that was also machined to a spherical surface. The distance between the freeform microoptics and the substrate was 1.67 mm. This distance was precisely secured by the shoulders of the substrate. These features (shoulders) were machined on the 350 FG ultraprecision machine at the same time when the curved substrate surfaces were created to ensure their geometric tolerances. To complete the 3D microfabrication using projection, a PMMA spherical substrate was first spin coated a 7 μm thick SU8 photoresist layer. After soft bake, the substrate was placed under the 3D microlens array and aligned with the optics. The substrate was then developed in an SU8 developer after hard bake. The pattern on the photomask was projected on the substrate surface. The formed
micro pattern dimension was 340 μm by 460 μm, giving overall projection ratio of 34:1.

It has been demonstrated that a 3D projection system based on microoptics is capable of creating true 3D microstructures, resulting in a low cost and simple manufacturing process for true 3D micro scale structures on nonplanar substrates. The results can also be readily converted to producing micro size optoelectronic components for telecommunication, components with micro size channels for biomedical, medical applications as well as consumer products. It has the potential to replace cleanroom photolithography in some areas. It is also a high volume operation where multiple workpieces can be fabricated from the same projection system. Furthermore, the fabricated microstructures on proper materials such as steels or ceramics can be utilized as mold inserts to be used in other high volume production processes such as hot embossing, injection molding or glass molding.
CHAPTER 5: ULTRAPRECISION MICRO MACHINING APPLICATION:
DESIGN, FABRICATION, AND TESTING OF AN AFFORDABLE STATIC
MICRO MIXER

The demanding for functional microfluidic devices like micropumps, micromixers have been rapidly increased in the past decades. Many new fields, such as so-called Micro Total Analysis Systems (µTAS) or Lab-on-Chip (LOC) [101], are also based on these devices. The development of micro fluidic devices is benefited from the progress of the Micro-Electro-Mechanical System (MEMS) technology. The MEMS technology makes it possible to fabricate low cost and complicated silicon based micro devices. However the traditional MEMS technology has some disadvantages for micro devices used in biomedical and life sciences application. For examples, the silicon based devices are not biocompatible, and MEMS technology is expensive and inflexible for small volume fabrication. Thus the development of micro devices for biomedical application by alternate materials and methods is becoming an interesting field recently.

Micromixer is an important microfluidic device because the mixing of fluids in micro scale is a crucial and challenging work. Generally, there are two kinds of micromixers [102; 103]: passive micromixer and active micromixer. For each kind there are also many different types. The Split-and-Recombination (SAR) micromixer
is a passive micromixer and has become an attractive design for its high mixing efficiency and compact structure. More important, the theoretical minimum striation size obtained in a SAR micromixer can be controlled by the design.

Munson and Yager [105] utilized laminated multiple polymer layers to form their SAR micromixer. Before lamination, the polymer layers were cut to designed shape by a CO₂ laser. Schönfeld and coworkers [106] developed a five layers structure for their SAR micromixer. In their work, the five layers were made of PMMA (polymethylmethacrylate) and stainless steel. The machining methods they used include mechanical micromilling and laser cutting. The machining processes for the above two SAR micromixers are considered prototype device fabrication and are not suitable for mass production. Lee’s group [107] developed a cleanroom based process for fabrication of PDMS (Polydimethylsiloxane) SAR micromixer. This process can be used as mass production. Since it is cleanroom based and it includes a series of process steps such as coating, lithography, peeling, and bounding, the cost for this process is high and machining cycle is long. Later, Kim et al. [109] developed a mass production process by using injection molding. In their research, the two molds were machined by electroplating a layer of nickel on nickel disks and the structures were patterned in cleanroom before electroplating. Since they had two molds and both are made in cleanroom, the fabrication process is costly and inflexible.

For the SAR micromixer used in the lab-on-chip system, the requirements include compact size, biology compatible, affordable, and disposable. These
requirements have limited the choice of materials, manufacturing methods, and structures for the micromixer. In general, polymers are usually the choice of materials for micromixer because their biology compatibility, transparency, and low cost if manufactured by using injection molding.

The main motivation of this work is to develop an affordable polymer SAR micromixer using a low cost, high productivity, stable, and flexible process. Microinjection molding is selected as the mass production method and ultraprecision micromachining is selected as the mold fabrication method. In the following sections, the design, fabrication, and testing of an affordable polymer static micromixer will be discussed.

5.1 Design of the Micromixer

Unlike other SAR micromixer designs [104; 105; 106; 107; 108; 109], the ease with which the device can be fabricated especially the ease with which the device can be mass manufactured by available machining processes is a main consideration. The affordability of fabricated device need also be considered. For this reason, microinjection molding was selected as the mass production method and ultraprecision diamond turning and micromilling were selected as the mold fabrication method. According to the nature of microinjection molding and micromilling, a new SRA type micromixer was designed. This design was a compromise of the mixing performance and machining ability. The design is shown in Figure 5.1 (a). The splitting was realized
by dividing the channel to two sub channels, one leads to upper left and the other one leads to lower right direction.

Figure 5.1 (a) Schematic view of SAR micromixer design, (b) the cross section view of the flows in the micromixer at different stages.

As shown in Figure 5.1 (a), an inlet flow consists of two parallel running microfluidic components (shown as solid green and dashed red arrows respectively) enter the entrance to the first mixerlet. After entering the first mixerlet, the inlet flow is divided into two sub flows: one moves to the upper right direction and the other one moves to the lower left direction. Ideally, each of the sub flows contains same amounts of the green and red fluidic components. Then the two divided flows are horizontally rearranged by the shape changing of the sub channels. As a consequence, the upper right and lower left sub layers are now become right and left sub layers. Finally the two horizontally arranged sub layers recombined to one flow containing four layers. As a result, the number of the components included in the flow is increased 2 times.
Theoretically, after repeating this process for \( m \) times, the obtained number of striations \( N_s = 2^m \) and the minimum striation size is \( w_m = w_0 / 2^m \) where \( w_0 \) is the inlet component width and \( w_m \) is the outlet sub layer width. The cross section view of the theoretical distribution of the microfluidic components at four different locations in a mixerlet can be seen in Figure 5.1 (b). The numbers in Figure 5.1 (b) correspond to the locations denoted in Figure 5.1 (a).

For the purpose of fabricating micromixers by injection molding process, the design of the micromixer structure is shown in figure 5.2 and all the features in the micromixer are vertically arranged (normal to the mixer plate), i.e., the entire micromixer mold insert was machined straight down. In this design, the micromixer consists of two identical molded halves, therefore only one mold was needed.

Figure 5.2 Structure and dimensions of the micro mixer part (units: mm). ISO view of the molded mixer halve (right) and zoom view of several mixerlets (left).
The designed micromixer was composed of two identical molded parts as shown in figure 5.2. After assembly, an entirely sealed channel with mixing features was formed. The two splitting channels, the upper left channel and lower right channel, were in the upper and lower part respectively, and the cavities (i.e., the recombine section) were formed by combining the two halves. The features on two opposite parts needed to be precisely aligned so that no gap exist between the two halves to present leakage. For this purpose, two pairs of alignment pins and associated holes were machined on the part in a single operation. The dimensions of the micro mixer are shown in figure 5.2. The channel width is 1 mm and depth is 0.4 mm for each part. The splitting channels are 0.3 mm width and 0.4 mm depth. Each mixing unit is 1 mm in length. The designed micromixer includes 16 mixing units.

5.2 Fabrication of the Micromixer

The fabrication process for static micromixers includes three steps. (a) Fabrication of the micromixer mold by ultraprecision diamond machining and micromilling; (b) Fabrication of polymer micromixer parts by microinjection molding; (c) Assembly of the micromixers by hot compression or adhesion of two molded polymer halves.

5.2.1 Micromachining of the Static Micromixer Mold

As described in the previous chapters, the ultraprecision SPDM and micro machining have many advantages for the fabrication of meso/micro features and devices. Moreover, by combing with microinjection molding process, high quality and
affordable 3D polymer micro devices can be fabricated. Because the molded parts need to be precisely aligned and assembled to prevent fluidic leakage, the mold of the micromixer part needs to have very high tolerances (around microns). To ensure the dimensional accuracy, the molds were machined on an ultraprecision diamond machining and micromilling machine (ISO 6000, Professional Instrument, [www.airbearings.com](http://www.airbearings.com)). To ensure the mold assembly precision and high surface quality, diamond turning process was used first to create the outside diameter and top surface of the mold.

The features on the micromixer mold were machined by high speed micromilling. A 200 μm diameter flat end carbide milling bit was used and the spindle speed was 20,000 rpm (revolution per minute). To minimize the machining error, all the features, including the cavities for polymer pins and columns for the matching holes on molded parts, were machined in a single installation without re-chucking. Figure 5.3 shows one side of the machined mold (only the mold with mixer features). Figure 5.4 (a) and 5.4 (b) show both of the fabricated molds (including the flat mold) installed on the Sodick microinjection molding machine.
Figure 5.3 Fabricated micromixer mold

Figure 5.4 (a) Fabricated micro mixer mold installed in the microinjection molding machine, (b) The flat end mold installed at the other side of the molding machine.
5.2.2 Microinjection Molding of the Static Micromixer

The micromixer components were manufactured on the Sodick microinjection molding machine (TR30EH2, Plustech) as shown in figure 5.5. The machining condition is shown in Table 5.1. The molding material is polymethylmethacrylate (PMMA).
We measured the dimensions of the self-assembly pins and holes in the molded parts as indicators for machining accuracy. The opening of the self-assembly holes is 1.007 mm, which had a 0.7% error compared to the design. For the self-assembly pins, due to the filling and shrinkage of the PMMA during molding, the actual side walls of the pins were not straight up but tilted at a small angle. The measured dimensions of the pins at the top was 0.9316 mm, which had a 3.9% error, and at the bottom was 1.037, which had a 6.9% error. The relationship of the microinjection molding process and accuracy of the part dimensions will be discussed in another paper.

Table 5.1 Microinjection molding parameters

<table>
<thead>
<tr>
<th>Melt Temperature.</th>
<th>Injection Speed (mm/s)</th>
<th>Packing Press (MPa)</th>
<th>Packing Time (s)</th>
<th>Cooling Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(°C)</td>
<td>100</td>
<td>60</td>
<td>2</td>
<td>10</td>
</tr>
</tbody>
</table>

200
5.2.3 Assembly of the Static Micromixer

The static micromixer was assembled by bounding two identical molded polymer pieces. The bounding methods can be UV curable adhesive or hot compression. Before the bounding process, two holes at the inlets and one at outlet were drilled on one of the pieces. Figure 5.6 is a picture showing an assembled static micromixer bounded by hot compression in a laminator. The bounding temperature was 150°C.

![Assembled static micromixer](image)

Figure 5.6 Assembled static micromixer

5.3 Microfluidic Testing

Figure 5.7 illustrates mixing experiment setup. The setup includes a dual syringe pump (PUMP33, HARVARD), a fluorescent microscope (Nikon), and a micromixer. The solutions used in this experiment are colored water solutions, which
will be seen as green and red under fluorescent light respectively. In addition, sugar was dissolved in the solutions to increase viscosity ($0.03 \text{ Kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$) and reduce diffusion. The flow rate was 100 $\mu\text{l/min}$ during the mixing test.

![Micromixer](image)

**Figure 5.7 Setup for the mixing experiment**

Figure 5.8 shows the mixing experiment results. Figure 5.8 (a) shows two fluidic flows (green and red) at the inlet of the first mixerlet prior to being mixed. Figure 5.8 (b) to figure 5.8 (e) show mixing results throughout the micromixer. It can be seen that the two flows were divided into several sub layers after passing through a series of mixerlets. Figure 5.8 (f) is the flow at the micromixer’s outlet. Compared to the flows at the inlet, the flows at the outlet were mixed into multiple layers. It can be seen that the number of layers was less than that of the design. The main reason is the splitting structure. In order to simplify the manufacturing process, this splitting structure cannot evenly divide each fluid into two sub stream. Therefore one of the sub
stream is smaller than the other one. This problem can be improved by optimizing the structure.

Figure 5.8 Mixing experiment results, (a) inlet (b) mixerlet 1 and 2 (c) mixerlet 3 and 4 (d) mixerlet 7 and 8 (e) mixerlet 11 and 12 (f) mixerlet 16 and outlet
Figure 5.9 shows distribution of the two colors along the micro mixer channel cross section at different locations. These data are obtained by reading the RGB value of the pictures taken by the fluorescent microscope. These color data reflect the distribution of these two fluids. Due to the brightness difference, the maximal amplitudes of these two colors are different but the locations of the colors illustrate the mixing effects. At the inlet (figure 5.9 (a)), the red and green color can only be found at one side of the channel. At the exit of the 2nd mixing unit (figure 5.9 (b)), these two fluids had begun mixing. With the number of mixing units increasing, the two fluids gradually get mixed (figure 5.9 (c)-5.9 (e)). At the outlet of the channel (figure 5.9 (f)), the two color evenly distributed in the single outlet channel indicating that the two fluids have been mixed.

Figure 5.9 Fluid distribution at different locations. (a) Inlet; (b) exit of the 2nd mixerlet; (c) exit of the 6th mixerlet; (d) exit at the 10th mixerlet; (e) exit at the 14th mixerlet; (f) outlet.
The mixing efficiency of the micromixer can be calculated from the color distribution. We calculated the standard deviation of the normalized intensity of the green light and red light respectively as the mixing efficiency for the green fluid and red fluid [107]. Before flow into the mixing units, the two fluids are filled in only one half of the channel. If the width of the two fluids are the same, the mixing efficiency for both fluids is 0.5. If the two fluids are fully mixed and evenly fill the channel, the mixing efficiency is 0. Figure 5.10 shows the obtained mixing efficiency for each
mixing unit. The mixing efficiency at the outlet of the channel is 0.11 for the green fluid and 0.12 for the red fluid.

Figure 5.10 Mixing efficiency for the two fluids at different mixing units

5.4 Analysis and Improving of the Original Design

5.4.1 Improved Design

However, there are some problems in this original design. It is well known that fluids will run along a path that has the minimal resistance. For micro fluids, the Reynolds number \( \text{Re} = \frac{UD_h}{V} \) is small due to the small dimensions and the micro fluids are usually laminar flow. Therefore, in the original design (Figure 5.1) the inlet microfluidic component at the right side will most likely go to the upper right direction and likewise the inlet microfluidic component at the left side will most likely go to the
lower left direction. The split sub flows will not contain same amounts of the two inlet components and this is the main reason that the original design did not have very high mixing efficiency (Figure 5.10).

To solve this problem and at the same time not to increase the complexity of machining too much, a split improvement structure was designed (the manufacturing process will be covered later). This splitting improvement structure will force the inlet flow divides into two layers before entering the narrow sub channels (Figure 5.11). The resistance at where the splitting happens is less and evener and the two inlet components will be more equally divided.

![Splitting Improvement Structure](image)

Figure 5.11 Improved design of the static micromixer
5.4.2 Numerical Simulation

The mixing process of the designed micromixer was numerical simulated using a commercial computational fluid dynamics (CFD) program ANSYS CFX (release 11.0, ANSYS). Both inlet components to the micromixer were water (dynamic viscosity 0.0008899 Kg·m$^{-1}·$s$^{-1}$). The normal speed for both inlet flows was set to 0.00211 ms$^{-1}$ which correspond to a flow rate of 100 μl min$^{-1}$ according to the dimensions of the channel. Temperature was used as an indicator for mixing performance. The temperature of one inlet component was set to 500 K and the temperature of the other one was set to 0 K. The thermal conductivity of water was set to 0 to avoid temperature change caused by heat conduction. Laminar flow was chosen for simulation. In the simulations, tetrahedral mesh was used. The maximum size of elements was 0.1 mm and the total numbers of the volume elements was about 224,000.

A straight micro channel which did not has any mixing structures was used as a comparison for the mixing performance. The outside dimensions of this micro channel were the same as the designed micromixer. Figure 5.12 shows the resultant temperature distribution at the end of that straight channel. It can be seen that the temperature range at the observation plane were from 467.7 K to 32.2 K. The two inlet components still ran and kept remain one half of the channel and were not mixed at all.
Figure 5.12 Temperature distribution at the end of a straight channel without any mixing structure (two inlet components temperatures were 500 K and 0 K respectively).

The temperature distribution of the original design micromixer was shown in Figure 5.13. The observation plane was at the end of the last mixerlet and was also at the same location as that in Figure 5.12. The temperature range of the water at this plan was from 270.8 K to 228.6 K, which is much smaller than that in Figure 5.12. From Figure 5.13, it can be seen than the temperature distribution trend is analogous to that of Figure 5.12. The warm inlet flow still kept at right side while the cold inlet flow kept at left side. This means the two inlet flows was mixed but not completely.
Figure 5.13 Temperature distribution at the end of a static mixer of the original design.

Figure 5.14 shows the temperature at the same observation plane for the new design. The temperature range was now from 251.1 K to 249.0 K. The temperature distribution was much more uniform except at the far left and right edges. These results indicate that the two inlet flows were very well mixed.
Figure 5.14 Temperature distribution at the end of a static mixer of the optimized design.

If the standard deviation of the normalized temperature distribution at the observation plane as the mixing efficiency was used, the mixing efficiency of the three cases was 0.3487, 0.0506, and 0.0022 respectively. The new design has much higher mixing efficiency than that of the original design.

Stream line plots can also reflect the difference of these two designs. Figure 5.15 and Figure 5.16 show the stream lines at four stages, entrance, splitting, rearrange, and recombination, of these two designs. For the original design at the splitting stage (Figure 5.15(b)), most left side inlet component flowed to the upper left sub channel and most right side inlet component flowed to the lower right sub channel. At the exit of the mixerlet (Figure 5.15 (d)), the ideal four sub layers stream was not formed.
because the middle two sub layers were too small. Thus the mixing performance was not as good as design. As a comparison, the new design has better mixing. At the splitting stage (Figure 5.16 (b)), more component from right side flowed into the upper left sub channel than that in Figure 6.16 (b). At the recombination stage (Figure 5.16 (d)), the four sub layers stream was clearly formed though not very uniform. This problem can be solved by further optimizing the dimensions of the splitting improvement structure and the micromixer structures as well.

Figure 5.15 Cross section views of the steam lines in the mixing process of one static mixing cell of the original design.
Figure 5.16 Cross section views of the stream lines in the mixing process of one static mixing cell of the new design.
Besides simulate the mixing of two inlet flow at different temperatures, the particle tracking can be used to observe the flow of the micro fluids [110]. In the simulation, two same particles were added to both the inlet flows and one-way coupling was used for the liquid-solid couple so that the added particles will not affect the flow [111]. Figure 5.17 shows the flow condition of the original design. Figure 5.17 (a) shows the first 6 mixerlets and Figure 5.17b shows the last 5 mixerlets. Figure 5.18 (a) and b show the flow condition of the new design at the same locations corresponding to Figure 5.17. It can be seen that the splitting and mixing of the new design is much better than that of the original design. The simulation results by using particles (Figure 5.17) are very similar to the micro fluidic experiment results (Figure 5.8).
Figure 5.17 Simulation of the micro mixing of the original design by using particle tracking

Figure 5.18 Simulation of the micro mixing of the new design by using particle tracking
5.4.3 Machining Process

For the new design, a splitting improvement structure was needed. This structure was not straight down and cannot be molded together with the main mixer features. To keep the new design and to keep the machinability of the device, the splitting improvement structure was thus formed by using a standalone film (Figure 5.19). This standalone film should have structures that exactly match the major mixer feature and thus seal the channel very well. After assembling these three parts together, a formed device has the same structure as shown in Figure 5.11. By using this standalone thin film divider, the original design machining process and even the already fabricated molds do not need modification.
Compare to the original design, the fabrication process for new static micromixers includes four steps. (a) Fabrication of the micromixer mold by ultraprecision diamond machining and micromilling; (b) Fabrication of polymer micromixer parts by microinjection molding; (c) Machining of the splitting improvement film by micromilling for the new design; (d) Assembly of the micromixers of two molded polymer halves for the original design or of two molded polymer halves with one micromilled film for the new design. Except step (c), all the other steps are the same as the original design.

For the modified design, the standalone thin film divider need be machined. Due to the small thickness, it is not easy to be molded. Thus the divider was machined on a thin film by using an ultraprecision high speed air bearing spindle designed and built by Professional Instrument (ISO 6000, [www.airbearings.com](http://www.airbearings.com)). A 200 μm diameter flat end carbide milling bit was used and the spindle speed was 20,000 rpm.
The material for the film was a PMMA film of 100µm thickness (shinkolite®, Mitsubishi Rayon, www.mrc.co.jp).

In the assembly step, for the new design the thin film divider was sandwiched between the two molded halves and then the three parts were bounded by a laminator. The bounding temperature was 150°C. Figure 10 shows an assembled static micromixer of the improved design.

5.4.4. Microfluidic Testing

The microfluidic testing setup for the improved design is the same as previous design (Figure 5.7). Figure 5.20 shows the mixing experiment results of the new design. Figure 5.20 (a) shows the two fluidic flows (green and red) at the inlet. Figure 5.20(b) to figure 5.20 (e) show mixing results throughout the micromixer. In Figure 5.20 (b), it is very clear that the sub layer number in each sub channels changed from 2 to 4 when the fluids flowed from mixerlet 1 to mixerlet 2 and this indicates the number of sub layers doubled after passing every mixerlet. In Figure 5.20 (c) and (d), the number of the sub layers greatly increased and the thickness of each sub layer also graduate decreased. Compare to the same positions in Figure 5.8, the sub layers were more uniform in Figure 5.20. Figure 5.20 (e) and (f) are the flow at the last several mixerlets and outlet. The sub layers were too small to be seen, and the whole channel was filled with homogenous color. The mixing color of Figure 5.20 (e) and (f) does not look like yellow is because the intensity of the green fluoresce was much stronger.
than that of the red fluoresce. However both color were evenly appeared in the channel (as can be seen from Figure 5.21).

Figure 5.20 Mixing experiment results, (a) inlet (b) mixerlet 1 and 2 (c) mixerlet 3 to 5 (d) mixerlet 6 to 8 (e) mixerlet 11 and 12 (f) mixerlet 16 and outlet
Figure 5.20 continued

Figure 5.21 (a)-(d) show the distribution of the normalized intensity of the two colors in the micromixer cross section at inlets and outlets of the two designs. These data are obtained by reading the RGB (red, green and blue) value from the pictures taken by the fluorescent microscope. These color data reflect the distribution of these two fluids. At the inlet (Figure 5.21 (a) and (c)), the red and green color can only be found at one side of the channel. At the outlet of the channel (Figure 5.21 (b) and (d)), the two colors distributed in the single outlet channel indicating that the two fluids have been mixed. Compare Figure 5.21 (d) with (b), it can be seen that the mixing performance of the new design has been greatly enhanced.

Similarly the mixing efficiency at the end of the new designed micromixer was 0.065 for both flows. Compare to the mixing efficiency at the outlet of the original designed micromixer was 0.11 for the green fluid and 0.12 for the red fluid, the mixing efficiency of the new design has been improved two times. The measured mixing efficiency is lower than the CFD simulation results is mainly because the edge of the
channel is not clear and the surface of the device has brought noise to the light intensity. Moreover, the CFD simulation used temperature as indicator and the experiments used color as indicator, these two conditions are not fully comparable but can be used as reference to each other.

Figure 5.21 Mixing efficiency for the green and red fluids at different mixing units
5.5 Summary

In this chapter, a new affordable polymer SAR micromixer was developed. Specifically both the mixing performance and the fabrication process were carefully studied. An improved design of the SAR micromixer was also given. The results of this part of research are summarized as follow:

1. The original design has simple structure and machining process, the mixing experiment results indicate that this design can mix the inlet micro flows and the mixing efficiency can reach 0.11.

2. The developed machining process for the designed micromixer is very accurate, low cost, efficient, and flexible. This process is suitable for low cost high precision micro devices for biomedical and other applications.

3. For the original design, the major problem for the low mixing efficiency is due to the unevenly splitting of the inlet flows. The resistance at the entrance of the sub channel is higher for one side than for the other side.

4. A new design was given to solve the uneven splitting problem of the original design. By using an improvement structure of a split design, the splitting will happen prior to the entrance of the sub channel therefore reduce the uneven resistance.

5. The CFD simulation results show that both the micromixer designs can realize the mixing function and the new design has better mixing performance. The mixing efficiency for the original design and the new design were 0.0506 and 0.0022 when using temperature distribution as an indicator.

6. In order to not change the original machining process much, a standalone thin film divider was micromilled to form the new design. The basic machining steps are the
same as the previous design with a major change to the new design being that a step was added.

7. The micro fluidic experiments show that both of the micromixer design has good mixing performance. The mixing efficiency of the improved design is 0.065 which is much higher than the original design. Both designs can be used for micro mixing and the final selection of the product will depend on the balance between the mixing performance and the cost.

For biomedical applications, one of the most important requirements for the devices is their affordability and disposability. Therefore the cost of the machining process for the devices is very important. In this work, the developed machining process for the device is capable of achieving high productivity while it is still very flexible. Therefore the structure of the designed micromixer can be modified easily. Furthermore this process can be easily adapted for many other similar applications.
CHAPTER 6: CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

In this research, optical effects of the ultraprecision single point diamond machined surface and the applications of the SPDM and micro machining were studied. The ultraprecision single point diamond turning technology has been developed for over 40 years and has been applied to numerous fields. Though this technology has been very well developed, many problems still remain unresolved. One of the objectives of this research is to study one of the unsolved problems, i.e., the effects of the ultraprecision single point diamond machined surface finish to the optical performance of the device. Another objective is to extend the application of the SPDM by focus on developing new processes like slow tool servo and broaching for freeform micro devices fabrication. The last objective is to develop a high accuracy, low cost, and flexible machining process for affordable micro devices specifically for biomedical devices.

In chapter two, the basic mechanism and model of the ultraprecision single point diamond turning and micro cutting were reviewed and discussed. The related subjects to the SPDT and micro cutting were also involved. The SPDT and micro cutting have enormous different characteristics as compared to the conventional macro
scale cutting. Due to the small cutting depth, numerous factors that can be ignored in macro scale become ineligible or even significant. Due to the lacking of proper testing and analysis methods, many aspects of the SPDT and micro cutting are still unknown or uncertain.

In conventional macro scale cutting, the main cutting mechanism is shear deformation while in SPDT and micro cutting the material plastic deformation, extrusion, and ploughing become important or even dominant. There is common observed size effect in SPDT and micro cutting. Many amount including cutting force, specific energy, material property, abnormally increase at small cutting depth. The cutting forces is much smaller than that of macro scale cutting and several other forces such as thrust force, friction force become important in SPDT and micro cutting. The tool cutting edge radius becomes one of the important factors that affect the cutting mechanism and surface quality. The material properties such as crystallographic orientation, grain size, micro particles, micro hardness are critical to the cutting process. The material swelling and recovery are important to the surface roughness. Besides these, the chips movement, temperature variation, and cutting fluids are all very important to the SPDT and micro cutting process.

In chapter three, the optical effects of diamond machined surfaces are studied. The influences from machining parameters, such as tool mark spacing, feedrate, spindle speed, tool radius, tool condition and different diamond machining process were considered.
First, the analytical analysis for calculation the diffraction and scattering from diamond machined surface was carried out. The diffraction is the combination of three parts, the specular reflection, higher order diffraction and random scattering. Both the diffraction field and diffraction light irradiation can be obtained after knowing the surface characteristic parameters. Then, the relationship between the machining conditions and the optical performance of the diamond machined surfaces was studied experimentally. At last, an empirical relationship between the machining conditions (feed rates and tool condition) and the first order diffraction of the diamond machined surface was setup. This model can be used to select optimal machining condition for diamond machining process.

In chapter four, the design, machining and testing of microlens array by using SPDM process was introduced. Two microlens array examples were given. One is the matrix arranged concave micro lenses on flat brass substrate surface. The other one is the circular arranged plano-convex micro lenses on a thin spherical substrate surface. From the measurement results, it can be seen that the machined micro lenses has very high dimension accuracy and optical surface finish. The optical testing shows that the focal length of the machined micro lenses agree with the design and has very little diffraction.

By using the fabricated 3D microlens array, a 3D micro projection machining system can be developed. The pattern on the photomask was projected on a thin layer of photoresist on the spherical substrate surface. The formed micro pattern dimension was 340 μm by 460 μm, giving overall projection ratio of 34:1. It has been
demonstrated that a 3D projection system based on microoptics is capable of creating true 3D microstructures, resulting in a low cost and simple manufacturing process for true 3D micro scale structures on nonplanar substrates.

In chapter five, a new affordable polymer SAR micromixer was developed based on a high accuracy, low cost, and flexible micro machining process. Specifically both the mixing performance and the fabrication process were carefully studied. A improved design of the SAR micromixer was also given.

The original design has a simple structure and machining process, the mixing experiment results indicate that this design can mix the inlet micro flows and the mixing efficiency can reach 0.11. An improved design was given to solve the uneven splitting problem of the original design. By using a splitting improvement structure, the splitting will happen prior to the entrance of the sub channel and reduce the uneven resistance. The CFD simulation results show that both micromixer designs can carry out the mixing function but the new design has better mixing performance. The mixing efficiency for the original design and the new design were 0.0506 and 0.0022 when using temperature distribution as an indicator. The micro fluidic experiments show that both of the micromixer design has good mixing performance. The mixing efficiency of the improved design is 0.065 which is much higher than the original design. Both designs can be used for micro mixing and the final selection of the product will depend on the balance between the mixing performance and the cost.
For biomedical applications, one of the most important requirements for the devices is the affordability and disposability. Therefore the cost of the machining process for the devices is very important. In this work, the developed machining process for the device is capable of achieving high productivity and while it is also very flexible. Therefore the structure of the designed micromixer can be modified easily. Furthermore this process can be easily adapted for many other similar applications.

6.2 Future Work

The future works of the related research may include two fields, the fundamental research on the surface quality of the SPDM and the application of SPDM and micro machining.

For the fundamental research on surface quality, the main aspects are:

1. The material swelling and recovery mechanism and their relationship to the SPDM machining parameters and material property. The research can be carried out by both FEM analysis and experiment study.

2. Quantitatively connect the theoretical diffraction analysis and the experimentally measured SPDM surface diffraction and modify the theoretical analysis methods.

3. Explanation of the abnormity in the surface diffraction experiment results, such as the quick decrease of the specular reflection at very low feedrate.
4. Optical design method research for the microlens array and other microoptics.

5. Machining of aspherical microlens for correcting optical aberration.

6. Analysis and optimization of the 3D microlens array projection system.

7. Optimization of the micromixer dimension for higher mixing efficiency.

8. Modification the micromixer structure to further improve its machinability.

9. Integration of the micromixer with other functional microfluidic devices.
Appendix A: Surface Diffraction Calculation for Uniform Field and Flat Sample

Surface Using Scalar Method

A1. Diffraction at the Observation Surface

Now consider the light field $E_0(x_0, y_0, z_0)$ in Eq. 3.6. $E_0(x_0, y_0, z_0)$ is the light reflected off the sample surface. The diamond machined surface has a surface profile height variation $d(x_0, y_0)$. Assume the incident field is a uniform plane wave $E_i = E_0 e^{-j(k_0 x + y + z_k)}$, where $\vec{\kappa} = (\kappa_x, \kappa_y, \kappa_z)$ is the wavefront normal vector. If the surface roughness height $d(x_0, y_0)$ is much less than wavelength $\lambda$, sample surface can be viewed as mirror surface so the reflection is nearly specular. Fig. A1.1 shows the relation of the reflection light and the incident light in X direction. The tangential components of $\vec{E}$ are continuous at the interface, then $\kappa_x = \kappa_x'$. For the same reason, $\kappa_y = \kappa_y'$. Because $|\kappa_z'| = \sqrt{k_x^2 - \kappa_x'^2 - \kappa_y'^2} = |\kappa_z|$ and $\kappa_z'$ is in different direction with $\kappa_z$, $\kappa_z' = -\kappa_z$. 
The specular reflect wave is: \( E_r = E_0 e^{-j(x_0 \kappa_x + y_0 \kappa_y - z_0 \kappa_z)} \).

Due to the surface roughness, the output wave has a phase delay \( \phi(x_0, y_0) \) in \( z \) direction given by

\[
\phi = j \kappa_z 2d(x_0, y_0) \quad (A.1)
\]

The output wave is

\[
E_o = E_0 e^{-j(x_0 \kappa_x + y_0 \kappa_y - z_0 \kappa_z) + j \kappa_z 2d(x_0, y_0)}
\]

On plane \( z_0 = 0 \), the reflected electric field is

\[
E_o = E_0 e^{-j[x_0 \kappa_x + y_0 \kappa_y - \kappa_z 2d(x_0, y_0)]} \quad (A.2)
\]

Substitute into Eq.3.6:
\[ E_1(x_1, y_1, z_1) = \frac{jk}{2\pi r_i} \cos \theta_i e^{-jk} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E_{00} e^{-j(x_0 \kappa_x + y_0 \kappa_y - \kappa_z 2d(x_0, y_0))} e^{j\left(\frac{\kappa_z}{\kappa_x} \kappa_x \kappa_y + \frac{\kappa_y}{\kappa_z} \kappa_z \kappa_x\right)} \, dx_0 \, dy_0 \]

Rearrange:

\[ E_1(x_1, y_1, z_1) = \frac{jk}{2\pi r_i} \cos \theta_i e^{-jk} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E_{00} e^{jk \kappa_z 2d(x_0, y_0)} e^{\left[\frac{\kappa_z}{\kappa_x} \kappa_x \kappa_y + \frac{\kappa_y}{\kappa_z} \kappa_z \kappa_x\right]} \, dx_0 \, dy_0 \]

(A.3)

Define normalized variables \( u_0, v_0 \) and \( u_1, v_1 \) given by

\[ u_0 = \frac{x_0}{a}, v_0 = \frac{y_0}{b} \]

\[ u_1 = \frac{x_1}{r_i} - a \frac{\kappa_x}{2\pi} = \frac{x_1}{2\pi \sqrt{x_1^2 + y_1^2 + z_1^2}} - a \frac{\kappa_x}{2\pi} \]

\[ v_1 = \frac{y_1}{r_i} - b \frac{\kappa_y}{2\pi} = \frac{y_1}{2\pi \sqrt{x_1^2 + y_1^2 + z_1^2}} - b \frac{\kappa_y}{2\pi} \]

\[ \frac{du_0}{a} = \frac{1}{a} \, dx_0, \frac{dv_0}{b} = \frac{1}{b} \, dy_0 \]

giving

\[ E_1(u_1, v_1, z_1) = \frac{jk}{2\pi r_i^2} e^{-jk} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E_{00} e^{jk \kappa_z 2d(u_0, v_0)} e^{j2\pi(u_0 u_1 + v_0 v_1)} \, du_0 \, dv_0 \]

(A.5)

The surface roughness related phase term can be written as:
\[ e^{i\kappa_2 d(u_0, v_0)} = \cos(\kappa_x 2d(u_0, v_0)) + j \cdot \sin(\kappa_x 2d(u_0, v_0)) \]

If \( d(u_0, v_0) \ll \lambda \), then \( \kappa_x 2d(u_0, v_0) \ll \pi \), then we have:

\[ e^{i\kappa_2 d(u_0, v_0)} \approx 1 - \frac{(\kappa_x 2d(u_0, v_0))^2}{2!} + j \cdot \kappa_x 2d(u_0, v_0) + O(d^3(u_0, v_0)) \]

Neglecting higher order items while \( d(u_0, v_0) \ll \lambda \)

\[ e^{i\kappa_2 d(u_0, v_0)} \approx 1 + j \cdot 2\kappa_x d(u_0, v_0) \]

Substitute into Eq. A.5

\[ E_1(u_1, v_1, z_1) \approx \frac{jk}{2\pi} \frac{z_{ab}}{r_1^2} e^{-jkr_1} E_{00} \int_0^1 \int_0^1 (1 + j \cdot 2\kappa_x d(u_0, v_0)) e^{i2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 \]

\[ = \frac{jk}{2\pi} \frac{z_{ab}}{r_1^2} e^{-jkr_1} E_{00} \left( \int_0^1 \int_0^1 e^{i2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 + \int_0^1 \int_0^1 2\kappa_x d(u_0, v_0) e^{i2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 \right) \]

\[ = A \left( \int_0^1 \int_0^1 e^{i2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 + \int_0^1 \int_0^1 2\kappa_x d(u_0, v_0) e^{i2\pi(u_0 u_1 + v_0 v_1)} du_0 dv_0 \right) \]

\[ (A.6) \]

Where \( A = \frac{jk}{2\pi} \frac{z_{ab}}{r_1^2} e^{-jkr_1} E_{00} \).

\( d(u_0, v_0) \) is the sample surface profile. It includes items, periodic one dimensional tool marks \( d_m(u_0) \) and two dimensional random surface roughness \( d_r(u_0, v_0) \). The coordinate orientation is taken such that the tool marks are periodic in
the \( u_0 \), i.e. \( x_0 \) direction. The one dimensional tool marks can thus be written in the form of Fourier series:

\[
d(u_0, v_0) = d_m(u_0) + d_r(u_0, v_0) = \sum_{n=-L}^{L} d_n e^{j2\pi u_0 v_0} + d_r(u_0, v_0) \quad n = -L, \ldots, -1, 1, \ldots, L \quad (A.7)
\]

\( d_n \) are the Fourier series coefficients for the tool marks, the constant term is zero.

Substitute Eq. A.7 into the second item of Eq. A.6:

\[
E_1(u_1, v_1, z_1)
\]

\[
= A \left( \int_{0}^{1} \int_{0}^{1} e^{j2\pi (u_0 u_1 + v_0 v_1)} du_0 dv_0 + \int_{0}^{1} \int_{0}^{1} j2\kappa_z \left( \sum_{n=-L}^{L} d_n e^{j2\pi u_0 v_0} e^{j2\pi (u_0 u_1 + v_0 v_1)} \right) du_0 dv_0 \right)
\]

\[
+ \int_{0}^{1} \int_{0}^{1} j2\kappa_z d_r(u_0, v_0) e^{j2\pi (u_0 u_1 + v_0 v_1)} du_0 dv_0 \right)
\]

\[
= E_{ih}(u_1, v_1, z_1) + E_{lm}(u_1, v_1, z_1) + E_{ir}(u_1, v_1, z_1) \quad (A.8)
\]

**A2. Specular Diffraction Beam Irritation at \( \theta_{id} \)**

Let \( \delta \theta_1 = \theta_1 - \theta_{i0} \) and \( \delta \phi_1 = \phi_1 - 0 = \phi_1 \quad (A.9) \)

Since the detector is at constant distance \( r_1 \), we transform to spherical polar coordinate.

According to figure 3.2:
\( \kappa_x = -k \cos \theta, \kappa_y = -k \sin \theta, \kappa_y = k \sin \theta \sin \phi, \) \hfill (A.10)

According to figure 3.1:

\[
\frac{x_i}{r_i} = \sin \theta_i \cos \phi_i, \quad \frac{y_i}{r_i} = \sin \theta_i \sin \phi_i
\]  
(A.11)

We choose the direction of the incident light to be in the x-z plane so \( \phi_i = 0 \). Later we will choose \( \theta_i = -5^\circ \).

From Eq. A.4, A.10, and A.11

\[
u_i = \frac{x_i}{r_i} a - a \frac{\kappa_x}{2\pi} \frac{a}{2\pi} (\sin \theta_i \cos \phi_i + \sin \theta_i), \quad \nu_i = \frac{y_i}{r_i} b - b \frac{\kappa_y}{2\pi} \frac{b}{2\pi} = \frac{b}{2\pi} \sin \theta_i \sin \phi_i \]  
(A.12)

Substitute into Eq. 3.8:

\[
E_{in}(\theta_i, \phi_i, z_i) = A. \frac{\sin \left( \frac{\pi}{\lambda} (\sin \theta_i \cos \phi_i + \sin \theta_i) \right)}{\frac{\pi}{\lambda} (\sin \theta_i \cos \phi_i + \sin \theta_i)} e^{i \frac{2\pi}{\lambda} (\cos \theta_i \sin \phi_i)} \frac{\sin \left( \frac{b}{\lambda} \sin \theta_i \sin \phi_i \right)}{\frac{b}{\lambda} \sin \theta_i \sin \phi_i} e^{i \frac{2\pi}{\lambda} (\cos \theta_i \sin \phi_i)} \frac{k}{\lambda} \sin \phi_i \sin \phi_i \]  
(A.13)

This expression has a maximum at \( \theta_i = -\theta_i \) and \( \phi_i = 0 \). For simplicity we expand the expression in Eq. A.13 about the maximum. \( \delta \theta_i = \theta_i - \theta_i, \) and \( \delta \phi_i = \phi_i \), where \( \delta \theta_i, \delta \phi_i << \pi \).
(\sin \theta_1 \cos \varphi_1 + \sin \theta_i) \\
= \sin(\delta \theta_1 + \theta_{10}) \cos \delta \varphi_1 + \sin \theta_i \\
= \sin \theta_{10} \cos \delta \theta_1 \cos \delta \varphi_1 + \cos \theta_{10} \sin \delta \theta_1 \cos \delta \varphi_1 + \sin \theta_i \\
\approx \sin \theta_{10} + \cos \theta_{10} \delta \theta_1 + \sin \theta_i

Because \sin \theta_1 + \sin \theta_i = 0

\sin \theta_1 \cos \varphi_1 + \sin \theta_i = \cos \theta_{10} \delta \theta_1 \hspace{1cm} (A.14a)

And

\sin \theta_1 \sin \varphi_1 \\
= \sin(\theta_{10} + \delta \theta_1) \sin \delta \varphi_1 \\
= (\sin \theta_{10} \cos \delta \theta_1 + \cos \theta_{10} \sin \delta \theta_1) \sin \delta \varphi_1 \\
\approx (\sin \theta_{10} + \cos \theta_{10} \delta \theta_1) \delta \varphi_1 \\
\approx \sin \theta_{10} \delta \varphi_1

Substitute Eq. A.14a and A.14b into Eq. 1.13:

\[ E_{11}(\theta_{10}, \delta \theta_1, \delta \varphi_1) = A \cdot \frac{\sin \left( \frac{a}{\lambda} \cos \theta_{10} \delta \theta_1 \right)}{\pi \frac{a}{\lambda} \cos \theta_{10} \delta \theta_1} \cdot \frac{\sin \left( \frac{b}{\lambda} \sin \theta_{10} \delta \varphi_1 \right)}{\pi \frac{b}{\lambda} \sin \theta_{10} \delta \varphi_1} e^{i \frac{b}{\lambda} \sin \theta_{10} \delta \varphi_1} \]

(A.15)

During the measurement, the readout of the detector is related to the total light irradiance entering the detector. For the detector at any position \theta_{1d} around the specular reflection beam, the total light intensity entering the detector is the integration of Eq. A.15 at the detector’s surface, assume the detector’s width is \(D_x\) in x direction and angular width is \(D_y\) in y direction:
We define the angular width of the detector:

$$\alpha = \frac{D_x}{r_1}, \quad \beta = \frac{D_y}{r_1}$$

Then, the total irradiance measured by detector at position $\theta_{id}$ is:

$$I_{1e}(\theta_id, \theta_{10}, \alpha, \beta, r_1) = \frac{\beta}{\sin^2 \theta_{10}} \frac{d\theta}{d\theta_1}$$

$$\int_{\beta}^{\alpha} \int_{\theta_0}^{\theta_{10}} \left[ E_i(\theta_{10}, \delta \theta, \delta \phi) \right]^2 \frac{2 \sin \frac{\theta_0}{2}}{2 Z_0} \frac{d\theta}{d\theta_1} \frac{d\phi}{d\phi_1}$$

$$\approx \frac{1}{2Z_0} r_1^2 \sin^2 \theta_{10} \int_{-\beta/2}^{\alpha/2} \int_{-\alpha/2}^{\alpha/2} \left[ E_i(\theta_{10}, \delta \theta, \delta \phi) \right]^2 d\theta d\phi$$

Substitute Eq. A.15 into Eq. A.16, giving:

$$I_{1e}(\theta_id, \theta_{10}, \alpha, \beta, r_1)$$

$$= \frac{1}{2Z_0} r_1^2 \sin^2 \theta_{10} \int_{-\beta/2}^{\alpha/2} \int_{-\alpha/2}^{\alpha/2} \left[ A e^{i \frac{\pi a}{\lambda} \cos \theta_{10} \delta \theta} \sin \left( \frac{\pi b}{\lambda} \sin \theta_{10} \delta \phi \right) e^{i \frac{\pi b}{\lambda} \sin \theta_{10} \delta \phi} \right] d\theta d\phi$$

$$= \frac{|A|^2}{2Z_0} r_1^2 \sin^2 \theta_{10} \int_{-\beta/2}^{\alpha/2} \left[ \frac{\sin \left( \frac{\pi b}{\lambda} \sin \theta_{10} \delta \phi \right)}{\left( \frac{\pi b}{\lambda} \sin \theta_{10} \delta \phi \right)^2} \right] d\phi \int_{-\alpha/2}^{\alpha/2} \left[ \frac{\sin \left( \frac{\pi a}{\lambda} \cos \theta_{10} \delta \theta \right)}{\left( \frac{\pi a}{\lambda} \cos \theta_{10} \delta \theta \right)^2} \right] d\theta$$

(A.17)

A3. The $n^{th}$ Order Diffraction Light Irritation at $\theta_{id}$

Substitute Eq. A.12 into Eq. 3.10, The light field around the $n^{th}$ order diffraction is:
\[ E_{lm}(\theta_1, \varphi_1, z_i, n) \]

\[ = j2\kappa,A \left( \frac{b}{\lambda} \sin \left( \frac{b}{\lambda} \sin \theta_1 \sin \varphi_1 \right) e^{i\frac{b}{\lambda} \sin \theta_1 \sin \varphi_1} \right) \left[ \frac{\sin \left( \frac{a}{\lambda} \left( \sin \theta_1 \cos \varphi_1 + \sin \theta_1 \right) + f_n \right)}{\pi} \right] \]

(A.18)

Eq. A.18 has a maximum when \( \varphi_1 = 0 \) and \( \frac{a}{\lambda} \left( \sin \theta_1 \cos \varphi_1 + \sin \theta_1 \right) + f_n = 0 \), expand Eq. A.18 about the maximum:

\[ \delta \theta_1 = \theta_1 - \theta_{in} \] and \( \delta \varphi_1 = \varphi_1 \)

where \( \delta \theta_1, \delta \varphi_1 << \pi \)

Let \( \theta_{in} \) be the position of the \( n^{th} \) order diffraction.

According to figure 3.2, similar approximation relation can be obtain as Eq. A.15:

\[ \frac{a}{\lambda} \left( \sin \theta_1 \cos \varphi_1 + \sin \theta_1 \right) + f_n \approx \frac{a}{\lambda} \cos \theta_{in} \delta \theta_1 \] (A.19a)

\[ \sin \theta_1 \sin \varphi_1 \approx \sin \theta_{in} \delta \varphi_1 \] (A.19b)

Substitute Eq. A.19a and Eq. A.19b into Eq. A.18:

\[ E_{lm}(\theta_{in}, \delta \theta_1, \delta \varphi_1, r_i) \]
\[
I_{im}(\theta_{id}, \theta_{in}, r_1, \alpha, \beta) = j2\kappa, A \left| \sin \left( \frac{b}{\lambda} \sin \theta_{in} \delta \phi_1 \right) e^{j\pi \frac{b}{\lambda} \sin \theta_{in} \delta \phi_0} \sin \left( \frac{a}{\lambda} \cos \theta_{in} \delta \phi_1 \right) e^{j\pi \frac{a}{\lambda} \cos \theta_{in} \delta \phi_0} \right| \]

\[
= \frac{2\kappa, d_n, A^2}{2Z_0} r_1^2 \sin \theta_{in} \left( \int_{-\beta/2}^{\beta/2} \sin^2 \left( \frac{b}{\lambda} \sin \theta_{in} \delta \phi_1 \right) \left( \frac{a}{\lambda} \cos \theta_{in} \delta \phi_1 \right)^2 \right) d\delta \phi_1 \]

(A.21)

**A4. Random Scattering Light Irradiation at \(\theta_{id}\)**

We define \(\Phi_{est}(u_t, v_1) = \int_0^1 \int_0^1 \left| \int_0^1 \int_0^1 d_r(u_0, v_0) e^{j2\pi(n_0+\nu_0 z_0)} du_0 dv_0 \right|^2 du_1 dv_1 \) as the estimated power spectrum density of the random surface roughness [72].

Then the scattering light irradiance at point \((u_1, v_1, z_1)\) is:
\[ \langle I_{tr}(u_1, v_1, z_i) \rangle \]
\[ = \left\langle \frac{1}{2Z_0} |E_{tr}(u_1, v_1, z_i)|^2 \right\rangle \]
\[ = \left\langle \frac{1}{2Z_0} A^2 \kappa_z | \int \int d_r(u_0, v_0)e^{i2\pi \eta_{u_0}+\eta_{v_0}} du_0dv_0 \right\rangle^{2} \]
\[ = \frac{1}{2Z_0} A^2 \kappa_z | \langle \Phi_{ex}(u_1, v_1) \rangle \]  \hspace{1cm} (A.22)

We next change the variable from \( u_1, v_1 \) to \( \theta_1, \varphi_1 \), according to Eq. A.12,

\[ u_1 = \frac{a}{\lambda} (\sin \theta_1 \cos \varphi_1 + \sin \theta_1) \]

\[ v_1 = \frac{y_1}{r_i} \frac{b}{\lambda} - b \frac{\kappa_z}{2\pi} = \frac{b}{\lambda} \sin \theta_1 \sin \varphi_1 \]  \hspace{1cm} (A.23)

We can express the scattering light intensity density in terms of \( \theta_1, \varphi_1 \): \( \langle I_{tr}(\theta_1, \varphi_1, z_i) \rangle \)

Integral the scattering light intensity density over the whole detector surface is the measured intensity:

\[ I_r(\theta_{id}, \alpha, \beta, r_i) = \int_{-\beta/2}^{\beta/2} \int_{\alpha/2}^{-\alpha/2} \int_{1}^{1} |I_{tr}(\theta_1, \varphi_1, z_i)|^2 \sin \theta_1 d\theta_1 d\varphi_1 \]  \hspace{1cm} (A.24)
BIBLIOGRAPHY


24. *Nano-precision measurement of diamond tool edge radius for wafer fabrication.*


111. **ANSYS.** ANSYS CFX 11.0 Tutorial.