ABSTRACT

KONG, XIANGCHENG. Predictive Modeling and Optimization for Vibration-assisted AFM Tip-based Nanomachining. (Under the direction of Prof. Jingyan Dong and Prof. Paul H. Cohen)

The tip-based vibration-assisted nanomachining process offers a low-cost, low-effort technique in fabricating nanometer scale 2D/3D structures in sub-100 nm regime. To understand its mechanism, as well as provide the guidelines for process planning and optimization, we have systematically studied this nanomachining technique in this work. To understand the mechanism of this nanomachining technique, we firstly analyzed the interaction between the AFM tip and the workpiece surface during the machining process. A 3D voxel-based numerical algorithm has been developed to calculate the material removal rate as well as the contact area between the AFM tip and the workpiece surface. As a critical factor to understand the mechanism of this nanomachining process, the cutting force has been analyzed and modeled. A semi-empirical model has been proposed by correlating the cutting force with the material removal rate, which was validated using experimental data from different machining conditions. With the understanding of its mechanism, we have developed guidelines for process planning of this nanomachining technique. To provide the guideline for parameter selection, the effect of machining parameters on the feature dimensions (depth and width) has been analyzed. Based on ANOVA test results, the feature width is only controlled by the XY vibration amplitude, while the feature depth is affected by several machining parameters such as setpoint force and feed rate. A semi-empirical model was first proposed to predict the machined feature depth under given machining condition. Then, to reduce the computation intensity, linear and nonlinear regression models were also proposed and validated using experimental data. Given the desired feature dimensions, feasible
machining parameters could be provided using these predictive feature dimension models. As the tip wear is unavoidable during the machining process, the machining precision will gradually decrease. To maintain the machining quality, the guideline for when to change the tip should be provided. In this study, we have developed several metrics to detect tip wear, such as tip radius and the pull-off force. The effect of machining parameters on the tip wear rate has been studied using these metrics, and the machining distance before a tip must be changed has been modeled using these machining parameters. Finally, the optimization functions have been built for unit production time and unit production cost subject to realistic constraints, and the optimal machining parameters can be found by solving these functions.
Predictive Modeling and Optimization of Vibration-assisted AFM Tip-based Nanomachining

by
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To my parents, Fanxu Kong and Yan Wang, for their endless love and support.
BIOGRAPHY

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Figure A.17 Continued

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Figure A.19 Continued
CHAPTER 1 INTRODUCTION

1.1 Background

Nanotechnologies have been widely applied in many areas such as physics, chemistry, biological science, and engineering. To achieve these applications, nanofabrication techniques especially fabrication of master patterns and masks are critical. Many nanofabrication methods have been developed previously, such as X-ray lithography [1], e-beam lithography [2, 3], nanoimprint lithography [4], etc. Although these methods can achieve nanometer scale resolution, many of them still rely on e-beam lithography to fabricate the mold or mask, which is costly. Atomic Force Microscope (AFM) based nanomachining provides a low-cost, easy-to-setup alternative to the above-mentioned nanolithography methods.

The traditional tip-based nanomachining approach can directly modify the sample by plastic deformation with low-cost, while the major disadvantage of this method is its low efficiency. As the machined feature dimensions are mainly controlled by the AFM tip radius, multiple times of scratching are needed to make a relatively large feature. Moreover, poor controllability is another disadvantage of this method. Usually a large normal force is required to push the AFM tip into the workpiece surface and achieve desired feature depth [5]. Thus, the tip will wear out quickly. Previous researchers have demonstrated that by adding XY high frequency vibration, the feature width can be fully controlled. Also, the normal force and the tip wear can be greatly reduced [6].

For traditional machining process, such as turning and end milling, many studies have been conducted to understand the machining mechanism including: 1) modeling of the
cutting forces between the cutting tool and the workpiece surface, 2) providing a guideline for parameters selection, and 3) modeling of tool wear. [7-10] However, for machining in nanometer scale, the machining conditions are significantly different than those in conventional scale. For example, the dimensions of machined features in nanometer scale are close to the dimensions of the cutting tool. Moreover, for our vibration-assisted tip-based nanomachining process, the machining process involves many complex machining scenarios, such as rotary motion and partial engagement between the tip and the workpiece surface, so it is very difficult to understand the mechanism of material removal. There is little research on the understanding of nanomachining process, hence the importance of systematically analyzing and modeling the process.

1.2 Motivation

This vibration-assisted tip-based nanomachining process has been successfully applied to machine 2D or 3D patterns previously, and the machined patterns show good machining accuracy and surface finish [11]. However, the selection of machining parameters is usually based on operators’ experience, which may not be adequate for designed features and the role of machining forces is not well understood. Also, commercialization of this nanomachining technique will require potential users to effective apply the process through guidelines for process planning and answer the following questions:

1. As in conventional scale machining, it is critical to know what are the feasible machining parameters to achieve desired feature depth and width. In this vibration-assisted tip-based nanomachining process, three machining parameters may affect the machining process, including the setpoint force, the XY vibration
amplitude and the feed rate, so we need to understand the effects of these three 
machining parameters on the feature depth and width.

2. During this nanomachining process the AFM tip may become damaged (e.g. wear 
or fracture), which will greatly impact the machining accuracy and production 
efficiency. To avoid these issues and maintain the machining quality, we must 
monitor the machining process in real-time using the cutting forces, which could 
be obtained using the signal feedback system. However, to employ the cutting 
forces to monitor the machining process, we must understand the effects of 
machining conditions on the cutting forces, and can calculate the cutting forces 
under different machining conditions.

3. It is critical to provide the guideline for when to change the tip, because if we 
change the tip too frequently, the production cost will be high. However, if we fail 
to change the tip on time, the machining accuracy will be greatly affected and the 
surface finish will be bad.

4. For this tip-based nanomachining, based on our experience, the unit production 
cost is very high. Also, as the machining speed is μm/s scale, the total production 
time is long if we need to machine thousands of patterns. Thus, it is critical to 
optimize the machining process by minimize the production cost and maximize 
the production efficiency.

1.3 Research hypotheses

This novel research will explore the following hypotheses. First, the machined feature 
dimensions, such as depth and width, are significantly affected by machining parameters,
such as setpoint force, the XY vibration amplitude, and feed rate. Second, cutting forces during the machining process are proportional to the instantaneous material removal rate. Third, the tip wear is significantly affected by several factors, such as the machining distance, setpoint force, and feed rate. Finally, the production time and production cost are affected by machining parameters, such as setpoint force and feed rate, which can be optimized to achieve minimum production time or cost.

1.4 Outline

In Chapter 2, the current research advances in the tip-based nanomachining area is introduced, as well as modeling methods to predict interaction force and tip wear. In Chapter 3, the experimental platform used in this research is described. In Chapter 4, the interaction between the AFM tip and workpiece surface will be discussed; a numerical model will be proposed to estimate the contact area between these two. Then, a semi-empirical model will be proposed and validated to predict the feature dimensions under given machining parameters. Also, regression models are also developed as alternatives. The performance of these models will be discussed. In Chapter 5, to calculate the interaction forces between the tip and workpiece surface, a semi-empirical model is proposed by correlating the forces with material removal rate. Due to the difficulties of analytically calculating the material removal rate, the numerical model used in Chapter 4 is modified to calculate the volume of instantaneously removed material during machining cycle as well as material removal rate. To investigate different machining conditions, we conduct a factorial design experiment. The feature dimensions of machined patterns using each machining condition are predicted and validated using the predictive feature dimension model developed in Chapter 4. Then, the
proposed semi-empirical model is calibrated using the predicted feature dimensions and calculated material removal rate. Chapter 6 discusses tip wear during machining process. Several metrics are explored to detect tip wear including tip radius and pull-off force between the tip and workpiece surface. Then, to study the effects of machining conditions on tip wear, a factorial design experiment is conducted, and the tip wear is compared. In Chapter 7, process optimization models and their constraints are discussed. By solving these optimization models, optimal operation points are found to achieve minimum production time or production cost. Chapter 8 of this thesis briefly summarizes the results of this research and proposes extensions for future work.
CHAPTER 2 LITERATURE REVIEW

In this chapter, we will first introduce some of the commonly used AFM-based nanofabrication methods, such as dip-pen lithography, anodic oxidation lithography. Then, we will review some cutting force models for both conventional scale machining and nanoscale machining. Finally, we will introduce some tool wear models developed previously.

2.1 AFM-based nanofabrication methods

2.1.1 Dip-pen lithography

Dip-pen lithography nanolithography (DPN) is a nanofabrication technology that atomic force microscope (AFM) tip is used to create patterns on a substrate surface with a variety of inks [12]. This technology allows surface patterning with a resolution of 100 nm scale. DPN method has been applied to fabricate nanostructures with both organic and inorganic materials. One important application is to use an AFM tip to deliver molecules to a solid substrate via capillary transport. Hong et al. reported that DPN could be applied to pattern monolayers of different organic molecules, with nanometer scale separation [13]. Ki-Bum Lee et al. reported using DPN to construct protein arrays with feature dimensions between 100 to 350 nm [14]. For inorganic materials, such as metals, oxides, and magnetic compounds, the feasibility of DPN method has also been investigated. Carno et al. developed two methods to precisely position gold nanoparticles on SAM-covered Au substrate. And they found that the 3D positions of the nanoparticles could be precisely controlled by AFM, and particles within the nanopatterns can be characterized using the same AFM [15].
2.1.2 Anodic oxidation lithography

Anodic AFM-based nanolithography has been heavily studied previously. For this fabrication method, a bias voltage is applied between the AFM tip and the workpiece surface, which usually ranges from $10^8$ to $10^{10}$ V/m. With this bias voltage, the geometry, as well as the electro-physical properties of the workpiece surface, will be modified. The mechanism of this lithography method is that due to the humidity of the air, both the AFM tip and the workpiece surface are covered with a very thin water film. A water bridge will be formed if the distance between AFM tip and the workpiece surface is small enough, which is the result of the capillary effect. After applying a strong electronic field, the tip and the workpiece surface will behave like anode and cathode separately and the area right beneath AFM tip on the workpiece surface will be oxidized. AFM anodic oxidation method can be employed to fabricate oxide structures on semiconductors, metal etc. This method was first demonstrated by M. Yasutake et al. [16]. The AFM tip was applied with a negative voltage with respect to the silicon substrate. H. C. Day et al. applied AFM with a conductive tip to perform localized oxidation of silicon, the fabricated lines dimensions are within 100 nm [17]. P.M. Campbell et al. applied this oxidation method to fabricate nanometer scale side-gated silicon field effect transistors (FET) [18]. E. S. Snow et al. created a mask with linewidth around 10 nm by integrating anodic oxidation lithography with electron cyclotron resonance (ECR) source dry etching method [19]. H.T. Soh et al. used this method to fabricate a metal oxide semiconductor field effect transistor (MOSFET) on silicon with channel length in sub-100 nm scale [20]. Besides semiconductors, AFM anodic oxidation can also be applied to metals. E. S. Snow et al. fabricated metal wires and metal-oxide-metal junctions by anodic oxidation.
on Ti films [21]. The width of the wires and resistance of the junctions are controlled in real time. This method has also been applied to fabricate atomic point contacts on thin Al films.

2.1.3 Mechanical direct scratching

Due to its low cost and easy to setup properties, the AFM tip-based mechanical direct scratching method has been heavily studied in recent years. To modify the workpiece surface, a large normal force is applied to the AFM tip to push it into the workpiece surface. One advantage of this method is no subsequent transfer processes needed. Additionally, the final structure can be fabricated at one time; Usually, the workpiece surface is imaged before machining, and then after setup, the AFM tip is applied to scratch one line or multiple lines. After machining, the workpiece surface will be imaged again to obtain the patterns machined. As this tip-based direct scratching method only involves mechanical interaction between AFM tip and the workpiece surface, it can be applied to machine patterns on the surface of different substrate materials like polymer films, metals, etc. M. Malekian et al. applied retrofitted commercial AFM to study the cutting behavior on nanometer scale chromium workpiece [22]. T. Sumomogi et al. investigated the applications of direct mechanical scratching method by applying very sharp diamond AFM tips to scratch on pure metal surfaces including Ni, Cu, and Au [23]. X. Li et al. used this method to scratch the surface of the single gold nanowire to fabricate nano slot and nanopatterns [24]. Te-Hua Fang et al. simulated the nano scratching process on Au and Pt films with molecular dynamic (MD) simulation method. In the simulation, the effect of applied load, hold time, and machining temperature was analyzed, these results were also compared with experimental results [25].
AFM tip-based direct scratching method has also been reported to be applied to fabricate nanostructures on polymethylmethacrylate (PMMA) surface. S. Yamamoto et al. first fabricated the patterns on the ultra-thin PMMA film, then transferred the machined patterns to SiO\textsubscript{2} substrate by wet etching. The patterns fabricated on SiO\textsubscript{2} have a width less than 28 nm and depths of 10 nm [26]. This direct scratching nanolithography has been reported to be applied to fabricate patterns on polymers and monolayers.

Although this direct scratching approach has many advantages, such as easy to setup and low cost, a large normal force is usually needed to push the AFM tip into the workpiece surface, which results in a large friction, fast tip wear, and reduced tip life. Also, as the engagement between the tip and the workpiece surface is difficult to control, the interaction forces between these two can be very large, which will limit the machining speed. In recent years, many investigations have been conducted to overcome these disadvantages, improve the controllability and machining speed of this tip-based direct scratching process. Y. Yan et al. integrated a commercial AFM system with a precision stage, which is similar to conventional CNC machining system [5]. Diamond tips are employed as the cutting tool to scratch on the workpiece surface, and both 2D and 3D microscale and nanoscale structures were fabricated. Then, they further improved this fabrication method by applying close-loop control in this system for 3D machining, such as 3D portrait of human face, nanoline arrays of sine-wave and triangular nanostructures.

2.1.4 Dynamic plowing lithography

Dynamic plowing lithography (DPL) is another commonly used AFM tip-based nanolithography method. Unlike direct scratching approach, for this plowing lithography method, the workpiece surface is modified by the indentation of a vibrating tip under the
AFM tapping mode. With the assistance of the applied vibration, the controllability has been greatly improved.

AFM-based DPL method was first introduced by B. Klehn et al. They applied a vibrating AFM tip to indent on a photoresist layer [27], and transferred the machined patterns to SiO₂ layer by wet chemical etching. Then, they further transferred the patterns from SiO₂ layer to the Si substrate using KOH etching. With this method, 60 nm wide V-shape grooves were machined. M. Heyde et al. modified the PMMA surface using plastically indenting. They have verified that the workpiece surface can be either imaged or modified by changing the vibration amplitude of the cantilever or the indentation depth [28]. B. Cappella et al. studied the mechanism of DPL and polymeric debris formation process by analyzing the nanoindentation process with DPL method on PMMA and polystyrene (PS) films [29, 30]. They reported the stiffness and hardness of polymers can be modified by dynamic plowing method: Surrounding the fabricated patterns, the border walls or debris were created, whose dimensions were larger than the dimensions of the structures fabricated. The result indicated that the polymer entity was loosened after fast indentation of the AFM tip.

2.1.5 Ultrasonic force microscopy

In traditional machining, ultrasonic vibration has been widely used to reduce friction in many machining processes [31]. In nanoscale, the ultrasonic vibration has also been introduced to some AFM-based imaging method, such as ultrasonic force microscopy (UFM). The UFM is a microscope designed for nanoscale topographical and elasticity measurements for stiff materials which are difficult to analyze by traditional AFM. The combination of AFM and UFM generates a near field acoustic microscope image: the AFM tip is used to detect the ultrasonic waves and overcome the limitation of a wavelength that
occurs in the acoustic microscope. An image with much more details than the topography can be generated by analyzing the elastic changes. This ultrasonic force microscope was first proposed by O. Kolosov et al. to detect ultrasonic vibration of the workpiece surface in AFM using nonlinearity in the tip-workpiece interaction force curve $F(z)$ [32]. It was discovered that after the amplitude of AFM cantilever exceeded a threshold value, a strong repulsive force would be observed, which is caused by the nonlinearity in the tip-workpiece interaction. Also, an AFM cantilever could detect ultrasonic vibration with frequencies up to the MHz range. K. Yamanaka et al. successfully imaged subsurface with nanometer scale resolution using UFM and analyzed the subsurface images, as well as the effect of contact elasticity in UFM, were analyzed [33]. The mechanism of UFM can be explained as follows: when a sample is vibrated at a frequency which is much higher the resonant frequency of the AFM tip, the tip will be frozen and indent into the sample surface. By modulating the amplitude of ultrasonic vibration, the subsurface images have been acquired by the cantilever deflection. O. Kolosov et al. applied UFM to study the structure of strained Ge islands grown on a Si substrate [34]. By integrating the sensitivity of acoustic microscopy with a nanoscale resolution of atomic force microscopy. The local surface elasticity variations between Ge dots and the substrate were imaged with UFM, with a spatial resolution of around 5 nm. F. Dinelli et al. have demonstrated the capability of UFM to image surface elastic properties of stiff materials [35], the UFM was applied to image heterogeneous nanostructures with a lateral resolution of nanometers.

2.1.6 Rotating tip based nanomilling

When fabricating a pattern by scratching or plowing, the torsion of the cantilever will result in edge irregularities, which can be transferred onto the substrate. Many fabrication
parameters can potential affect the shape and regularity of fabricated patterns, such as material properties (hardness and stiffness), the AFM tip geometry, and some machining parameters (setpoint force, machining speed).

To overcome the drawbacks mentioned above, such as low material removal rate and low throughput, a rotating tip based nanomachining method has been developed by B. A. Gozen et al., which was named nanomilling [36, 37]. For this nanomachining method, the AFM tip is integrated with a three-axis piezoelectric actuator, which provides high-speed rotary movement. With this high precision nanopositioning stage, the machining depth and width become controllable, so the desired pattern can be machined in a single path, which means the production efficiency and product accuracy will be improved. The authors have demonstrated the nanomachining process has the capability of regulating feature dimensions on SU-8 polymeric film. They also studied in details about the design and evaluation of a mechanical system for the nanomilling process.

2.2 Cutting force modeling

For conventional scale machining, many investigations have been conducted to understand the machining mechanism and model the machining processes. The purpose of these investigations can be summarized into three categories: 1) optimizing machining conditions to achieve minimum production cost or production time, 2) selection of a feasible cutting tool and 3) selection of feasible coolant/lubricant. Different types of models have been proposed to model the machining processes, such as mechanical models, numerical models, empirical models, artificial intelligence (AI) based models.
Some models focus on the understanding of these mechanical variables, such as stresses, strains and machining temperature. Some are built to predict the process performance, such as tool wear and production time.

Mechanical models have been widely used to predict some machining parameters, such as the cutting forces, and temperature. Zhongtao Fu et al. proposed an analytical method to model the milling force in helical end milling process based on a predictive machining theory [38]. This model has many input variables such as material properties of the workpiece, the cutting tool geometry, the cutting conditions and the milling type. In their model, the cutting edges are discretized into infinitesimal elements along the cutter axis, and the cutting force applied to each element was predicted analytically. Then, the cutting forces were calculated by integrating all the forces along the cutter axis. The model was verified using data from previous publications. A. Moufki et al. applied predictive machining theory to study the peripheral milling process [39]. This predictive machining theory was proposed based on an analytical thermomechanical approach of oblique cutting. Some material characteristics, such as strain rate sensitivity, strain hardening and thermal softening, are considered. Umut Karagüzel et al. developed a process model for turn-milling operations [40]. In their research, the uncut chip geometry and tool-work engagement limits for orthogonal, tangential and co-axial turning-milling operations were defined. Then, a novel analytical turn-milling force model was developed, which was verified by experimental data.

For some machining processes, due to their complicated machining mechanism, it is very difficult to model using mechanical methods. So, numerical modeling methods like finite element method (FEM) have been employed to study these machining processes. S. Buchkremer et al. developed a 3D-FEM method to simulate the longitudinal turning process
based on the modified Bai-Wierzbicki material model [41]. The model was validated using data from longitudinal turning experiments conducted on AISI 1045 steel. They also investigated the longitudinal turning process using different cutting tools and process conditions. A high-speed camera was used to record the chip formation and chip flow process, which was compared with the simulation results. T. Özel et al. investigated the turning process of Ti-6Al-4V titanium alloy and IN100 nickel-based alloy with uncoated and TiAIN coated tools [42]. They built 3D finite element (FE) model to predict the turning forces as well as the induced stress fields. The predicted stress fields were compared with measured residual stresses. W.B. Lee et al. investigated the shear angle prediction and cutting force variation induced by crystallographic anisotropy [43]. To consider the effect of different crystallographic orientations on the cutting process, they implemented the constitutive equation of crystal plasticity by the finite element modeling of the chip formation at micro-scale. Two distinguished phases of pre-compression and steady-state cutting was revealed. The predicted patterns of cutting force variation agreed with published experimental results. Yao Xi et al. investigated the improvement in machinability during thermally assisted turning of the Ti-6Al-4V alloy with finite element modeling [44]. They developed a 2D thermally assisted model, and then validated this model by comparing the simulation data with experimental ones. The effect of workpiece temperature on the cutting force and chip formation process was analyzed. V. Vijayaraghavan et al. introduced a combined finite element based data analytics model. The finite element model was developed to predict the cutting forces while genetic programming method was used to obtain the mathematical relationship between the process variables and the cutting forces [45]. To predict process-induced residual stresses in high-speed dry cutting of Mg-Ca0.8 (wt%) alloy
using diamond tools, M. Salahshoor et al. developed a finite element simulation model of orthogonal cutting without explicit chip formation using the plowing depth approach [46].

In recent years, some fuzzy methods like artificial intelligence (AI) have been proposed to predict cutting forces during machining processes. Djordje Cica et al. investigated the prediction of parameters in turning using soft computing techniques [47]. The experimental research focused on the effect of different methods of cooling and lubricating of the cutting zone, such as the conventional method of cooling and lubricating with high-pressure jet-assisted machining, minimal quantity lubrication technique. To predict the cutting force, they created two different models, namely, artificial neural network and adaptive networks based fuzzy inference systems. Ali R. Yildiz developed an optimization approach based on artificial bee colony algorithm to search for the optimal cutting parameters in the turning operations [48]. Different evolutionary-based optimization techniques were also compared by the author to solve multi-pass turning optimization problems.

D. J. Waldrof et al. compared several models on the flow of workpiece material around the edge of an orthogonal cutting tool [49]. M. Fontaine et al. analyzed the effect of tool-surface inclination on cutting force for ball-end milling [50]. The study also studied the effect of different cutting conditions, such as plowing and inclination angle, on the cutting forces by building a predictive milling force model.

Like traditional machining, it is critical to estimate the cutting forces for the micro/nanomachining process. K.S Woon et al. investigated the effect of tool edge radius on the contact force in tool-based micromachining process [51]. To accurately calculate the cutting force for the micro-end-milling process, W.Y. Bao et al. proposed an analytical force
model [52]. M. Malekian et al. built models to study the machining factors that may affect micro-milling forces, which including plowing, elastic recovery, run-out and dynamics [53]. M.P. Vogler et al. analyzed the surface generation process in the micro-end milling for both single phase and multiphase sample materials [54]. To predict the effects of the cutter edge radius on the cutting forces, they also proposed a model by correlating the cutting force with the minimum chip thickness concept.

As the AFM-based nanofabrication methods can easily achieve nanometer-scale resolution, they have been used widely in recent years. Like conventional scale machining, it is crucial to understand their machining mechanism and model the cutting forces during the machining process. However, due to the complexity of these AFM-based nanomachining processes, such as nanometer scale resolution as well as partial indentation of the AFM tip, the above-mentioned modeling methods for conventional machining are not feasible. To analyze and model the nanofabrication processes, some approaches have been proposed, such as molecular dynamics (MD) method. The MD method was developed to study nanomachining processes by simulating the interaction between AFM tip and the workpiece surface, which can be applied to study the cutting forces, stress state, and machining energy. The diamond tool wear was modeled by K. Cheng et al. using MD simulation method. Its basic mechanism was revealed as the thermos-chemical wear [55]. X.S. Han et al. applied MD method to study the effect of tool angles and tool edge radii for the nanometric cutting process on single crystal silicon [56]. M.B. Cai et al. used MD approach to simulate the nanoscale ductile mode cutting of monocrystalline silicon wafer [57].

Although the MD simulation could be applied to analyze and model the interaction between the AFM tip and the workpiece surface, this method is computationally intensive.
Besides the MD simulation method, the interaction forces between the AFM tip and the workpiece surface can also be obtained by analyzing the feedback signal collected by the photodetector. Many investigations have been conducted using this method; L. Li et al. quantitatively studied the frictional properties of self-assembled alkanethiol monolayers on Au by analyzing the friction forces recorded by the photodetector [58]. Y. Yan et al. measured 3D force components after applying B. Bhushan’s calibration method and verified the method by friction coefficient measurement between the diamond tip and sample (sapphire) surface [59]. They claimed that the proposed method can be applied in the measurement of cutting forces in AFM tip-based nanomachining.

As the machining parameters may greatly affect the AFM-based nanomachining processes, many papers can be found in this area. The effects of some machining parameters, such as normal force, scratch directions, are discussed. S. C. Minne et al. studied the effects of the AFM tip geometry and scratching direction on the scratched patterns [60]. A pyramidal diamond coated Silicon tip was selected to scratch on the Ni$_{80}$Fe$_{20}$ coated Silicon substrate in four different directions. The Ni$_{80}$Fe$_{20}$ thin film was deposited on the Si substrate by an e-beam deposition process, so the film is nearly isotropic. During the machining process, a constant normal force is applied to the AFM tip. The results indicated that the direction of scratching had a significant effect on the machined feature dimensions. Tseng et al. have studied the relationship between the scratch force and the grooves’ dimensions (depth and width) for different materials like Si, Ni, and Ni$_{80}$Fe$_{20}$ [61]. The scratch force applied varies from 1 to 9 µN, and a logarithmic relationship has been built to describe the relationship between the dimension of grooves (depth and width) and the scratch force $F_n$, which is listed as equation 2.1 and 2.2:
\[ d(F_n) = \alpha_1Ln\left(\frac{F_n}{F_{t1}}\right) \quad 2.1 \]
\[ w_f(F_n) = \alpha_2Ln\left(\frac{F_n}{F_{t2}}\right) \quad 2.2 \]

where \( \alpha_1 \) and \( \alpha_2 \) are the scratch parameters defined as the scratch penetration depth and penetration width; \( F_{t1} \) and \( F_{t2} \) are the threshold forces based on the feature dimensions. The parameter of \( \alpha \) is a measure of the machining efficiency of the tip to a specific material, the threshold force \( F_t \) can be considered as the minimum normal force to scratch a measurable groove. These two equations have been verified by experimental data from several types of metals. As mentioned above, the parameter \( \alpha \) is defined as \( d/Ln(F_n/F_t) \), which is the ratio of the depth of the groove to the logarithm of the normalized cutting force. Based on the definition, the ratio \( \alpha \) can be viewed as a measure of the scratch efficiency of the tip to a specific material, which means, with higher \( \alpha \) value, the machined groove depth can be larger on given material. The threshold force \( F_t \) can also be used to determine the machinability.

With larger threshold, it will be more difficult to machine on this material, and larger normal force is needed to scratch a measurable groove. Tseng et al. defined a ratio, \( \alpha/F_t \), called scratch ratio (SR), to represent the scratch behavior. Similar to conventional machining processes, the SR should be considered as a material property used to quantify the machinability.

As mentioned above, the threshold force reflects the difficulties of machining on the surface of a specific material. To provide guidelines for the selection of applied force during scratching process, it’s important to investigate the theoretical value of threshold force based on material properties. Per the definition of threshold force, no starch occurs if the substrate is scratched at the threshold force, which implies the force is too small to generate plastic deformation or indentation into the substrate. Tseng et al. proposed a model to estimate the
threshold force, the relationship between the contact area $A_c$ and the normal contact force $F_c$, can be expressed as Equation 2.3:

$$A_c = C_c \left( \frac{3F_c R}{4E_c} \right)^{2/3}$$

Where $R$ is the radius of the tip, and $E_c$ is the contact elastic modulus, which is defined as Equation 2.4:

$$\frac{1}{E_c} = \frac{1 - v_t^2}{E_i} + \frac{1 - v_s^2}{E_s}$$

Where $E$ is Young’s modulus; $v$ is Poisson’s ratio, $v_t$ and $v_s$ corresponding to the material property of the tip and substrate. $C_c$ is a contact constant and equal to $2\pi$ based on JKR theory [62].

Tseng et al. then correlated the contact force with $E_c$, the hardness of the substrate $H$, the tip radius $R$. Then they compared the results calculated based on this model with the results from previous experiments [63-65]. The accuracy of this model for predicting the threshold force has been validated with a wide range of materials.

2.3 Tool wear models

For conventional tool wear, many analysis and modeling methods have been developed including numerical simulation, finite element analysis, and empirical modeling techniques. These modeling methods have been applied to different machining processes like turning, milling and cutting processes. Analytical models have been developed to describe the tool wear evolution during different machining processes. H. Shao et al. presented a
cutting power model in face milling operation [66]. The cutting conditions and average tool flank wear during milling process were considered in this model. This cutting power model was employed to calculate the normal cutting power for tool wear monitoring. M.S. Kasim et al. investigated the tool wear for a ball-type end mill [67]. The tool life and wear mechanism for machining Inconel 718 were examined using a physical vapor deposition (PVD) coated carbide tool under different cutting conditions. As the pitting was responsible for notching and flaking, they developed a mathematical model to predict the location of these pitting. Then the location calculated could be employed to estimate the location associated with the maximum load occurred during the cutting process. The results from the predictive model were very close to actual notching/flaking locations. K.D. Bouzakis et al. created a predictive model for the wear of the milling parts with complicated geometry [68]. The model correlated the tool wear evolution in milling process with other factors on the cutting edge entry impact duration, and the parameters of this model were determined based on experimental results. With this model, the expected tool wear evolution can be estimated during the numerically controlled milling process. F. Köppl et al. developed an empirical tool wear prognosis model to improve the predictability of the maintenance stops [69]. Based on the new Soil Abrasivity Index (SAI), this model could estimate the distance between maintenance stops and the required amount of cutting tools to be changed. The prognosis model was validated based on the original reference projects.

Due to the difficulties to build analytical models, numerical methods have also been adapted to predict the tool wear during machining processes. Jerzy Rojek et al. presented a thermomechanical discrete element model of rock cutting process [70], which considered both mechanical and thermal phenomena and their reciprocal influence. Then the
thermomechanical algorithm was implemented in a discrete element program and used to simulate the rock cutting with a single pick of a dredge cutter head. B. Haddag et al. used a multi-steps modeling strategy based on several numerical calculations [71]. The first step was using 3D thermomechanical analysis for the chip formation process. Some machining outputs like cutting forces, chip morphology chip flows direction and tool-chip interface parameters were obtained. The second step was to predict the tool wear using tool-chip interface parameters. Finally, a 3D thermal analysis of the heat diffusion was conducted by adequate thermal loading. The data obtained at each step were compared with experimental results. M. Kolahdoozan et al. investigated and optimized the tool wear in drilling process of difficult-to-cut nickel-based superalloy [72]. Mathematical models were deduced by Minitab software to display the effect of the main cutting variables including cutting speed, feed rate and tool diameter on tool wear. Based on finite element method (FEM), a wear process model of twist drill was built, which provided a novel approach to study the mechanism of drill wear. It was demonstrated that the simulated data matched with experimental data. To study the effect of microstructural changes and the cooling/lubrication effects during the cutting process, Giovanna Rotella et al. developed an FE model for describing the microstructural changes during dry and cryogenic cutting of Ti6Al4V [73]. The model was validated with experimental data. Yung-chang Yen et al. applied finite element method (FEM) to predict the tool wear evolution and tool life in the orthogonal cutting process [74]. In their model, they proposed three different parts. Firstly, they developed a tool wear model for the specified tool. Then, they modified the commercial FEM code to allow tool wear calculation and tool geometry updating. Finally, they validated this methodology with experimental results. A. Attanasio et al. developed a 3D numerical model to predict tool wear
in metal cutting operations [75]. They adopted simulation strategy to evaluate the tool wear, and the results were compared with some experimental data obtained from turning AISI 1045 steel using uncoated WC tool. Thanongsak Thepsonthi et al. used both experimental and finite element method (FEM) to study the effect of cBN coated tool in micro-machining of Ti-6Al-4V titanium alloy [76]. They conducted experiments to compare the performance of cBN coated and uncoated micro end mills regarding surface roughness, burr information and tool wear. Finite element method (FEM) were employed to study chip formation process in micro-milling to investigate the effects of cBN coated micro end mills with increased edge radius considering cutting force generation, tool temperature, and contact pressure, sliding velocity and tool wear rate. Then they utilized the simulation results to estimate the tool life based on a sliding wear rate model and the results were compared with experiments. The results showed the cBN coated carbide tool had better performance compared with the uncoated carbide tool in the generation of tool wear and cutting temperature. Durul Ulutan et al. studied the stress distribution on the rake and flank surface of the tool, and also the friction coefficients between the tool and the chip, tool and the workpiece [77]. They applied a determination methodology, which was applied to various tool edge radii. The stagnation point location on the tool edge was also solved by this method.

Due to the differences between the conventional scale machining and mic/nanometer scale machining, such as the dimensions of the cutting tools, many of these tool wear models in the conventional machining cannot be directly applied for micro/nanometer scale machining processes. In the following paragraphs, I will review the modeling methods used for micro/nanometers scale machining, e.g. finite elements method, molecular dynamics method (MD), Monte Carlo (MC) simulation method etc. In all AFM tip-based imaging or
fabrication processes, the tip radius is the most important factor that determines the image quality or feature accuracy. However, the tip wear is an inevitable byproduct of both tip-based imaging and machining processes. In practical applications, the consequences of tip wear can be severe, including image resolution degrades, false data, fabrication resolution degrades and reduced fabrication output. Although tip wear is inevitable, the tip wear processes can be analyzed and imaging or fabrication parameters can be optimized to minimize the tip wear.

Basically, there are two processes causing tip wear: engaging process and scanning process. Skarman et al. applied a high-resolution scanning electron microscope (SEM) to study the geometry of tips used in tapping mode [78]. The image deterioration was correlated with factors like tip cracking, tip contamination and tip supply vendors. Ho et al. reported that if an AFM probe contacts the surface by oscillation in each cycle, severe probe “wear” or damage is observed. If the probes oscillate in a “near-contact” tapping mode, image quality can be well preserved for longer scanning distance [79]. Bernd et al. applied a method to continuously monitor the tip radius during machining process [80]. They measured the tip radius based on the pull-off force between the AFM tip and sample surface, which is a 100-nm film of cross-linked polyaryletherketone spun cast on silicon. They observed several features: 1) the wear rate is generally low, 2) wear proceeds as a smooth process if no fracture occurs, and 3) the wear rate increases with increasing applied load and decreases at large sliding distance. The first two imply that the wear occurred during an atom-by-atom loss process, which was bond breaking process. To explain the third one, they argued that the activation barrier is reduced through bond stretching by shear stress.
2.4 Chapter Summary

In this chapter, some popular AFM tip-based nanofabrication methods were first introduced, such as Dip-pen lithography and Anodic oxidation lithography. For each of these nanofabrication methods, its mechanism and applications are described, followed by the discussion of their advantages and disadvantages. Then, some process modeling techniques for both conventional and micro/nanometer scale machining processes are introduced, such as Finite element (FE) analysis and Molecular Dynamic (MD) simulation. The advantages and limitations of these modeling techniques are discussed in detail. Some recent publications in modeling methods are also briefly introduced. Finally, some studies are discussed on tool wear for different machining processes, such as turning and cutting. The causes of tool wear are discussed in details, and some tool wear modeling methods, such as the cutting power model, are introduced. To better understand the tool wear for the AFM-based nanomachining processes, some recent advances on tip wear during direct scratching process were introduced.
CHAPTER 3 VIBRATION-ASSISTED TIP-BASED PLATFORM

In this research, a vibration-assisted AFM tip-based nanomachining process, which is developed before by Li Zhang [6], has been analyzed and modeled. The experimental platform is consisted of a commercial AFM, Park-70 (Park Systems Inc.), and a customized nano-vibration system. In this chapter, this experimental platform as well as the operations will be introduced.

3.1 Experimental platform

AFM is a powerful tool for nanometer scale imaging, measuring, and machining. To obtain the surface information, the sample will be scanned with sharp AFM probe. The precise imaging in XY direction and z direction is enabled by piezoelectric positioning elements with nanometer scale accuracy. Silicon and silicon nitride is usually used as AFM tip material. During the imaging process, the AFM tip contacts the workpiece surface, and the deflection of cantilever varies as the height of the workpiece surface varies, which is measured by an optical system. To improve the reflection of laser beam, the AFM cantilever has been coated with a reflective layer, which will reflect the laser beam onto the photodetector. The topographical and frictional information of sample surface is measured by the displacement of the laser beam on photodetector. In this study, this topographical and frictional information is collected for cutting force analysis. Park XE-70 is an AFM product from Park Systems, which consists of two independent close-loop XY and Z scanners for the sample and cantilever, a manual coarse stage, and vibration isolation stage. In the AFM system, the X-Y scanner has a scanning range of 50 µm by 50 µm. The Z-scanner maintains
feedback force or distance setting in the XEP software when it moves towards a sample surface. The maximum measurement range of Z stage is 12 µm. Park XE-70 has two imaging modes, contact mode, and tapping mode. In the following experiments, contact mode is used for nanomachining, while tapping mode is used for imaging before and after machining. The stage on XY scanner is detachable, so we can put customized nano-vibrator stage onto the XY scanner to provide the XY in-plane vibration.

3.2 Vibration-assisted nanomachining process

For this nanomachining process, the high-frequency XY vibration is introduced to increase the machining controllability as well as improving machining productivity; The schematic is shown in Figure 3.1. As shown in Figure 3.4, the high-frequency XY in-plane vibration is generated by a nano-vibrator system consisting of two piezoelectric actuators, which vibrates in two perpendicular directions. The outer edge of the trajectory of the tip circular motion, which is shown in Figure 3.2, can be viewed as a virtual cutting tool with a single tooth whose radius is controlled by the XY vibration amplitude. The schematic is like single tool fly-cutting in conventional scale. With the assistance of this XY vibration, the width of the machined features can be fully controlled, so unlike the directly scratching process, there is no need to scratch multiple times, which significantly reduced the production time. Also, as the XY vibration amplitude can reduce the interaction forces between the AFM tip and the workpiece surface, so the tip wear is also reduced.
Unlike direct scratching process, with the assistance of XY in-plane vibration, the cutting load is evenly distributed to each rotation cycle. And during each machining cycle, only a very thin slice of material (defined as feed per rotation) is removed, which is shown in Figure 3.3. In this way, the interaction force is greatly reduced.
3.3 Analysis of the experimental platform

The schematic of the experimental setup is shown in Figure 3.4. The platform is consisted of a commercial AFM, Park XE-70 (Park Systems Inc) and a lab-designed nano-vibrator system which includes two stack piezo actuators. With the XY nano-vibrator actuators, high-frequency XY vibration can be provided. Another nano-vibrator actuator, which is attached to the sample, can produce ultrasonic Z vibration. The cutting force signal is acquired by AFM through signal acquisition devices. In this dissertation, only the XY vibration is applied, and the driving signal is generated from signal generation device. The vibration-assisted nanomachining is performed on PMMA film, which is spin-coated on a silicon substrate and baked on a hotplate. PMMA is thermoplastic synthesis polymer, and Young’s modulus and shear modulus is 1800-3100 Mpa and 1700 Mpa respectively. The AFM cantilever used is DLC 190 with tip radius around 30 nm. The A-B, C-D data are acquired during this machining process.
As mentioned above, the driving signal for XY vibration is generated from signal generation device, the National Instrument USB-6259, which is a multifunction data acquisition module. This module could provide 4 analog output and 16 analog input channels with 1.25 MS/s sampling rates. The signal processing software, Signal Express, is applied for the output signal control, feedback signal acquisition, and basic signal processing during the machining process. In our system, NI USB-6259 is used for both signal generation and cutting force data acquisition. Analog output AO 0 generates 2 kHz command signal force y-axis while AO 3 generates 2 kHz command signal with 90° degree phase difference for X-axis vibration. Combining the vibration from both x-axis and y-axis, a rotational vibration in XY-plane will be provided. To study the interaction force during machining, we use Signal Access Module (SAM) from Park Systems to acquire the cantilever deflection signals for both vertical and lateral directions. When an AFM cantilever bends in the vertical direction, the topographic of the workpiece surface is measured by the photodetector as A-B signal.
The torsional motions of AFM cantilever, which can reflect the friction between AFM tip and the workpiece surface, is measured as C-D signal. For our vibration-assisted tip-based nanomachining process, both vertical and lateral motion of AFM cantilever is involved, A-B and C-D data are acquired simultaneously. The raw A-B and C-D voltage signals from photodetector are collected from SAM.

The surface topography of the workpiece can be imaged by AFM using the tapping mode, and analyzed using XEI, which is an image process software from Park Systems. Comparing the images of the workpiece surface before and after machining, the feature dimensions, such as depth and width of machined trenches, can be measured. The nanomachining control is realized in XEL, which is designed for nanolithography applications. A variety of different lithography modes can be achieved using XEL, such as Z scanner movement mode, Setpoint mode, and Bias mode. During this study, the Setpoint mode is applied to perform nanomachining, and machining parameters, such as setpoint force and feed rate are controlled.

To study the effect of machining parameters, straight trenches are machined. After imaging the workpiece surface before machining, the AFM cantilever is brought to contact with the workpiece surface under contact mode. To avoid affecting the sample surface as well as the AFM tip, a relatively small setpoint force (e.g. 5 nN) is applied. After approaching, the XEL is set to remote mode, and the AFM is taken over by the XEL software. Using the XEL interface, the desired patterns can be designed on the loaded pre-scanned image of the workpiece surface, and the cutting force and scan rate can also be set. Then, after clicking the “Start” button, the AFM cantilever will be moved to machine the designed pattern on the workpiece surface with the configured cutting force and feed rate.
Also, using the Signal Express interface, the XY-vibration is applied simultaneously. During this nanomachining process, the feedback signals are recorded through the signal feedback system.
CHAPTER 4 PREDICTIVE MODELING FOR FEATURE DIMENSIONS

In Chapter 3, we have introduced the experimental platform for this vibration-assisted tip-based nanomachining process. To better understand the mechanism of this nanomachining process, we need to analyze the relationship between machined feature dimensions and machining parameters including setpoint force, XY vibration amplitude and feed rate. In this chapter, we conducted a full factorial design experiment of these three machining parameters to analyze the relationship between feature dimensions and machining parameters. Based on the results of Analysis Of Variance (ANOVA), we determined the significant factors in determining the feature dimensions. The XY amplitude significantly affects the width, while the depth was significantly controlled by setpoint force, XY vibration amplitude, and feed rate. This analysis is valuable, but it is also critical to predict feature dimensions and provide the guideline for machining parameter selection. In this chapter, several models developed will be introduced to predict feature dimensions for this nanomachining process and their advantages and disadvantages will also be discussed.

4.1 Experimental design

In the vibration-assisted tip-based nanomachining process, the machining input parameters include setpoint force, XY vibration amplitude and feed rate. To fully understand the relationship between machined feature dimensions (depth and width) and these machining input parameters, a full factorial experiment was conducted. From our preliminary experiments, we determined a reasonable range of these parameters to machine observable features. For each input parameter, we set three different values corresponding to low,
medium and high levels of the parameter, yielding a three by three full factorial design experiment, which is shown in Table 4.1 below.

<table>
<thead>
<tr>
<th>Factor</th>
<th>Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setpoint force (nN)</td>
<td>120, 140, 160</td>
</tr>
<tr>
<td>XY vibration amplitude (mV)</td>
<td>35, 50, 65</td>
</tr>
<tr>
<td>Feed rate (μm/s)</td>
<td>0.6, 1, 1.4</td>
</tr>
</tbody>
</table>

4.2 Analysis of feature width

Based on the kinematics of the process, we anticipate that XY vibration will affect feature width. Also, based on our calculation, the distribution of residual is normal. So, ANOVA was used to determine if other machining parameters would also affect feature width. The results of ANOVA test (Table 4.2) showed that, among all these machining parameters, only the effect of XY vibration amplitude was statistically significantly in determining feature width (p-value < 0.0001), the effects of all other factors were not significant. To visualize the effect of XY vibration amplitude on the feature width, the feature width is plotted against XY vibration amplitude in Figure 4.1 with error bars, showing a strong linear correlation between feature width and XY vibration amplitude. A simple linear regression model has been built to predict the feature width, with Mean Square Error (MSE) of 0.83 nm, indicating that feature width can be accurately predicted.
Table 4.2 Significance test for feature width (x1: setpoint force, x2: XY vibration amplitude, x3: Feed rate)

<table>
<thead>
<tr>
<th></th>
<th>Setpoint force</th>
<th>XY vibration amplitude</th>
<th>Feed rate</th>
<th>Prob&gt;f</th>
<th>Setpoint force* XY vibration amplitude</th>
<th>Setpoint force* Feed rate</th>
<th>XY vibration amplitude * Feed rate</th>
<th>x1<em>x2</em>x3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prob&gt;f</td>
<td>0.99</td>
<td>&lt;0.0001</td>
<td>0.4436</td>
<td>&lt;0.0001</td>
<td>0.8075</td>
<td>0.2013</td>
<td>0.5638</td>
<td>0.3214</td>
</tr>
</tbody>
</table>

Figure 4.1 The relationship between feature width and XY vibration amplitude (35, 50, 65 mV separately). We can observe a strong linear correlation between width and XY vibration amplitude.

4.3 Analysis of feature depth

As previously mentioned, the XY vibration amplitude is the only statistically significant factor in determining the feature width. However, from our observations, the feature depth is affected by several factors including setpoint force, XY vibration amplitude, and Feed rate. To study the effects of these three factors, we conducted a factorial design experiment ($3^3$) of these three factors, which are shown in Table 4.3. The effects of setpoint force and feed rate on machined feature depth were visualized in Figure 4.2 (b) (d) (f), and strong correlations are observed. Based on calculation, the residual of feature depth follows
normal distribution. To verify these observations, ANOVA significance test was applied to determine significant factors for feature depth.

Table 4.3 Measured feature depth for all machining conditions

<table>
<thead>
<tr>
<th>N</th>
<th>Setpoint force/ nN</th>
<th>XY vibration amplitude/ mV</th>
<th>Feed rate/ µm/s</th>
<th>Depth/ nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>120</td>
<td>35</td>
<td>0.6</td>
<td>5.3</td>
</tr>
<tr>
<td>2</td>
<td>120</td>
<td>35</td>
<td>1</td>
<td>4.8</td>
</tr>
<tr>
<td>3</td>
<td>120</td>
<td>35</td>
<td>1.4</td>
<td>3.3</td>
</tr>
<tr>
<td>4</td>
<td>160</td>
<td>35</td>
<td>0.6</td>
<td>10.3</td>
</tr>
<tr>
<td>5</td>
<td>160</td>
<td>35</td>
<td>1</td>
<td>8.9</td>
</tr>
<tr>
<td>6</td>
<td>160</td>
<td>35</td>
<td>1.4</td>
<td>6.5</td>
</tr>
<tr>
<td>7</td>
<td>200</td>
<td>35</td>
<td>0.6</td>
<td>14.5</td>
</tr>
<tr>
<td>8</td>
<td>200</td>
<td>35</td>
<td>1</td>
<td>10.7</td>
</tr>
<tr>
<td>9</td>
<td>200</td>
<td>35</td>
<td>1.4</td>
<td>8.2</td>
</tr>
<tr>
<td>10</td>
<td>120</td>
<td>50</td>
<td>0.6</td>
<td>7.1</td>
</tr>
<tr>
<td>11</td>
<td>120</td>
<td>50</td>
<td>1</td>
<td>7.6</td>
</tr>
<tr>
<td>12</td>
<td>160</td>
<td>50</td>
<td>1.4</td>
<td>7.6</td>
</tr>
<tr>
<td>13</td>
<td>160</td>
<td>50</td>
<td>0.6</td>
<td>14.6</td>
</tr>
<tr>
<td>14</td>
<td>160</td>
<td>50</td>
<td>1</td>
<td>11.2</td>
</tr>
<tr>
<td>15</td>
<td>160</td>
<td>50</td>
<td>1.4</td>
<td>10.3</td>
</tr>
<tr>
<td>16</td>
<td>200</td>
<td>50</td>
<td>0.6</td>
<td>18.2</td>
</tr>
<tr>
<td>17</td>
<td>200</td>
<td>50</td>
<td>1</td>
<td>18.4</td>
</tr>
<tr>
<td>18</td>
<td>200</td>
<td>50</td>
<td>1.4</td>
<td>13.9</td>
</tr>
<tr>
<td>19</td>
<td>120</td>
<td>65</td>
<td>0.6</td>
<td>8.1</td>
</tr>
<tr>
<td>20</td>
<td>120</td>
<td>65</td>
<td>1</td>
<td>9.4</td>
</tr>
<tr>
<td>21</td>
<td>120</td>
<td>65</td>
<td>1.4</td>
<td>7.1</td>
</tr>
<tr>
<td>22</td>
<td>160</td>
<td>65</td>
<td>0.6</td>
<td>15.9</td>
</tr>
<tr>
<td>23</td>
<td>160</td>
<td>65</td>
<td>1</td>
<td>13.8</td>
</tr>
<tr>
<td>24</td>
<td>160</td>
<td>65</td>
<td>1.4</td>
<td>13.2</td>
</tr>
<tr>
<td>25</td>
<td>200</td>
<td>65</td>
<td>0.6</td>
<td>18.6</td>
</tr>
<tr>
<td>26</td>
<td>200</td>
<td>65</td>
<td>1</td>
<td>17.5</td>
</tr>
<tr>
<td>27</td>
<td>200</td>
<td>65</td>
<td>1.4</td>
<td>15.3</td>
</tr>
</tbody>
</table>

The AFM images of features after machining are shown in Figures 4.2 below. For each pattern, we show the AFM image, the measured depth and a plot of depth versus feed rate. Figure 4.2 (a) shows machined feature under different setpoint forces, feed rates with 35 mV XY vibration amplitude. Figure 4.2 (b) shows the corresponding depth. Figure 4.2 (c) shows the feature depth varies significantly under different machining conditions. Larger depths are achieved by increasing the setpoint force or decreasing the feed rate.
To find the significant factors in determining feature depth, we performed an ANOVA test. The test results are listed in Table 4.4, which indicates that the p values of all
main effects and the interaction between setpoint force and feed rate are smaller than 0.05, which means all these factors are statistically significant.

Table 4.4 Effect of significance test for feature depth

<table>
<thead>
<tr>
<th>Source</th>
<th>Prob &gt; f</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setpoint force</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>XY vibration amplitude</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>Feed rate</td>
<td>0.0001</td>
</tr>
<tr>
<td>Setpoint force * Feed rate</td>
<td>0.021</td>
</tr>
<tr>
<td>Setpoint force * XY vibration amplitude</td>
<td>0.1446</td>
</tr>
<tr>
<td>XY vibration amplitude * Feed rate</td>
<td>0.2879</td>
</tr>
<tr>
<td>Setpoint force * XY vibration amplitude * Feed rate</td>
<td>0.5799</td>
</tr>
</tbody>
</table>

4.4 Predictive models for feature dimensions

As discussed in Chapter 4.3, the results from ANOVA test indicated that XY vibration amplitude, setpoint force, feed rate and their interaction effect are all statistically significant in determining feature depth. To predict the feature depth after machining, we need a predictive model which includes the effects of all these factors. For the tip-based scratch process, the interaction force between tip and sample surface is usually correlated with the contact area between these two. For this vibration-assisted tip-based nanomachining process, we also try to correlate the contact force (setpoint force in our case) with the contact area. Due to the rotary movement between AFM tip and the workpiece surface, it is very difficult to calculate the contact area analytically. To solve this problem, we will first analyze
the geometry of the interaction area between AFM tip and the workpiece surface, and then we will develop a 3D voxel-based numerical model to calculate the contact area. With the calculated contact area and the setpoint force we set, the proposed semi-empirical model can be calibrated and verified with experimental data. The calibrated model has a high accuracy in predicting feature dimensions. Although this semi-empirical model has a very high accuracy, it is time-consuming to implement. To improve efficiency, we also try to develop regression models to correlate feature depth with machining parameters, which have also been proved to have good accuracy.

4.4.1 (a) Estimation of the contact area between the tip and sample surface

As mentioned above, it is critical to calculate the contact area between the AFM tip and the workpiece surface. However, the geometry of the interaction area is complicated. Unlike direct scratching process, for this vibration-assisted tip-based nanomachining process, the tip only removes a small slice of material during each machining cycle, which is shown in Figure 4.3 (a). As we can see, the tip-sample engagement keeps changing as the tip rotates. Intuitively, the contact area between the tip and the workpiece surface depends on the AFM tip location, which induces time-varying forces.
To calculate the contact area during the machining process, we first need to analyze the geometry of the engagement between the AFM tip and workpiece surface during each machining cycle. Based on the SEM images of AFM tips, the geometry of the tip is semi-sphere, and the manufacturer specified value of the tip radius is 30 nm. With the assistance of XY vibration, the relative movement between the AFM tip and workpiece surface is a combination of rotary movement and linear movement during the machining process.

When cutting a slot in the vertical direction, the top view of in-plane AFM tip movement during one machining cycle is shown in Figure 4.3 (a). In one rotation cycle, AFM tip starts machining from position “1”, and go through position “2”, and finish machining at position “3”. The current and previous machined edges are represented by the pink and red colored semi-circles separately. The path of the AFM tip center is represented by the sky-blue semicircle. For different cutting depth, the view of AFM tip movement in the XY plane is similar, but the parameters are different such as effective tip radius and virtual tool radius. Figure 4.3 (b) demonstrates the instantaneously removed material in the 3-D view.
In the tip-based nanomachining process, the AFM tip, as the cutting tool, is intrinsically blunt with negative rake angle, and the dimensions of the tool are comparable to the dimensions of the material removed, which is quite different with conventional scale machining process using tools with a sharp cutting edge.

Since the geometry of the interaction area between the AFM tip and surface is complicated, it is very difficult to calculate the corresponding contact area analytically. In this chapter, we developed a 3D voxel-based numerical method, which could effectively estimate the contact area at each tip location during the machining process. In this numerical method, the region under machining is discretized into 3D voxels (Figure 4.4 (a)). The initial value for each voxel is set as ‘0’. Then, if a voxel is machined by the AFM tip during a machining cycle, the value of this voxel is set to be ‘1’. Thus, if the feature dimensions (feature width and depth) are measured, at each tip location, by counting the number of voxels that are changed from ‘0’ to ‘1’, we can determine the instantaneously removed area and calculate the corresponding contact area.
Step 1: Discretize the machining region and construct the voxel matrix. Number all the voxels from 1 to n (For example, the whole region in Figure 4.4 is discretized in 150 * 150 * 150 voxels, then n=150 * 150 * 150), assign “0” to each voxel.

Step 2: For each voxel, evaluate if this voxel is within the region overlapped by the AFM tip at current tip position, which corresponds to the gray area in Figure 4.4 (c). If the answer is “Yes”, executes step 3; Otherwise, this voxel was not removed at this specific tip location and the value of the current voxel will be kept as zero. Then the next voxel will be inspected.

Step 3: Evaluate if the voxel is within the region of the AFM tip, and outside the previously machined region, which is illustrated in Figure 4.4 (d). If the answer is “Yes”, execute step 4; Otherwise, this voxel is not machined at this tip location, the value of the current voxel will be kept as zero. The algorithm will move forward to inspect the next voxel.
Step 4: Evaluate if the voxel is outside of the previous tip position. This region corresponds to the materials that are machined at the current tip location, as shown in Figure 4.4 (e). If the answer is “Yes”, execute step 5. Otherwise, this voxel is not within the contact area. Here we use the center of the voxel to evaluate which region it belongs to. For the partially overlapped voxel, if the center of the voxel is in a specific region, the value of the voxel is assigned accordingly. The volume of this voxel is added to the total volume of instant removed material; Otherwise, keep the value of the current voxel as zero, and move to the next voxel.

Step 5: After scanning through all the voxels, the instantaneously removed region can be determined. To obtain the geometry of the contact area, the voxels within the instantaneously removed region and directly contact with the AFM tip were selected, which is shown as Figure 4.5. As the dimensions of these voxels are extremely small (1 nm by 1 nm by 1 nm), the value of contact area can be estimated by adding the side area of all voxels within the area.

![Figure 4.5](image)

**Figure 4.5** The instantaneous contact area (The blue area corresponding to the contact area between AFM tip and sample surface). The blue area is discretized into voxels and its area can be calculated by counting the number of voxels.
In summary, in this adapted 3D discrete voxel method, we first discretize the working area into 3D cubic voxels (1 nm by 1 nm by 1 nm). To define the contact area, we first find the instant removed area, which is a slice of material removed in one machining cycle. Then the contact area is defined as the layer of voxels that directly interact with the AFM tip, which is shown as the blue zone in Figure 4.5. To estimate the area of this blue zone, we just count the total number of voxels occupied by this zone. As the dimension of the voxel is small enough, it is reasonable to estimate the contact area by adding all the side area of voxels in the area.

4.4.1 (b) Development of semi-empirical model for feature depth prediction

In this study, we tried to understand and model the effect of machining parameters on the feature dimensions. It is well known from the indentation process that applied force is related to the contact area between the workpiece surface and the indenter. If the geometry of the indenter is known, the depth of the indentation can be correlated to the applied force. A similar idea is applied for the modeling the nanomachining process to correlate the feature depth with the tip-sample interaction force (i.e. setpoint force). However, in the nanomachining process, the tip-sample interaction is much more complex than static contact in nano-indentation. The tip-sample contact is continuously changing during each machining cycle. Here a model structure considering the machining mechanism was proposed, and its coefficients were calibrated through experiments. Then, further experiments were performed to test the results from the semi-empirical model.

In nanoindentation and nano-scratching processes, the effect of scratch force on feature dimension is given as $F_c = kd + F_{tc}$, where $F_c$ is applied setpoint force, $F_{tc}$ is the threshold contact force based on the tip dimension and the material properties of the
substrate, and $k$ reflects the efficiency of the tip to machine a specific material[61]. The threshold contact force $F_{tc}$ can be considered as the minimum normal force needed to machine given material. The contact area between tip and substrate can be expressed as $A = C_c \left( \frac{3F_c R}{4E_c} \right)^{\frac{2}{3}}$, where $R$ is the tip radius, $C_c$ is a process related constant, $E_c$ is the contact elastic modulus defined as: 

$$E_c = \frac{1}{E_t} \left( \frac{1-v_t^2}{E_t} + \frac{1-v_s^2}{E_s} \right),$$

here $E_t$, $v_t$ and $E_s$, $v_s$ are Young’s modulus and Poisson’s ratio of the tip and sample, respectively. Based on Johnson-Kendall-Roberts (JKR) model of elastic contact [81], the relationship between contact area and applied force can be derived as:

$$\sigma_c = 1.5 \frac{F_c}{A_c},$$

$$F_c = \frac{2\sigma_c A_c}{3} = \frac{4\pi^3 R^2 \sigma_c^3}{3E_c^2}.$$  

$\sigma_c$ is the contact stress, the $A_c$ is the contact area. As observed from Equation 4.2, the contact force can be correlated with the contact area. Though this model has been mainly applied to elastic materials like metal, it has also been verified to successfully describe the direct scratching process for polymer films like PDMA [61]. As shown in Equation 4.2, for nanoindentation or tip-based direct scratching process, with larger contact force, the contact area will increase. However, for this vibration-assisted nanomachining process, besides the contact force, which is the setpoint force applied, the contact area may also be affected by several other machining parameters, such as XY vibration amplitude and feed rate. Based on the analysis in Chapter 4.3, with larger setpoint force and XY vibration amplitude or smaller
feed rate, the feature depth increases, which results in larger contact area. So, inspired by Equation 4.2, a model structure was proposed to describe the effects of these machining parameters on the contact area for this vibration-assisted tip-based nanomachining process, which is shown in Equation 4.3.

\[
F_{set} = k \frac{A_c^m \text{feed}^q}{V_{xy}} - b \quad 4.3
\]

\[
A_c = A(\text{Depth, width}) \quad 4.4
\]

\(F_{set}\) is the setpoint force applied (nN), \(V_{xy}\) is the XY vibration amplitude (mV), \(A_c\) is the contact area between the AFM tip and the workpiece surface (nm²). In this model, the tip-sample contact area is correlated with the applied force, XY vibration amplitude and feed rate on the tip with power terms \(m, n\) and \(q\), and coefficients \(k\) and \(b\). The tip-sample contact area is a nonlinear function of feature depth and width, as shown in Equation 4.4. If the coefficients can be identified properly, Equation 4.3 and 4.4 together describes the nonlinear relationship between the applied force and machined feature depth. It is difficult to explicitly express the feature depth at a given setpoint force. However, the feature depth can be solved by Newtonian Iteration Method from Equations 4.3 and 4.4. We can start with an initial value of feature depth, then the contact area can be calculated from Equation 4.4 and setpoint force can be derived from Equation 4.3. If the derived setpoint force differs from the given setpoint force, the feature depth can be improved by iteration until the resulting setpoint force is within a preselected tolerance band of the given setpoint force.

Using experimental data, the optimal parameters in the model, \(m, n, k,\) and \(b\) can be estimated by minimizing the mean square error between the experimental data and model prediction using Equation 4.3 and 4.4. The final model is given as Equation 4.5. As we can
see, the power of feed rate was determined as 0. However, the effect of the feed rate is still reflected in the calculation of contact area $A_c$. Based on the 3D voxel-based numerical model developed previously, the contact area increases with larger feed rate.

$$F_{set} = 58.86 \frac{A_{0.56}}{V_{xy^{0.51}}} + 47.7$$

With the fitted semi-empirical model, Equation 4.5, the feature depth can be calculated for a given setpoint force by Newtonian Iteration Method. Using this method, we plot the predicted and measured feature depth and the relative prediction error in Figure 4.6.

In general, good model prediction can be obtained and most of the relative prediction errors are within ±20%. Given the relatively large process variability at nanometer scale for nanomachining process, such relative error indicates we have a reasonable prediction of depth using the semi-empirical model.

Figure 4.6. (a) The measured depth (blue) and predicted depth (red) of the semi-empirical model for experiments from Table 4.3. (b) The relative error of the model prediction.
4.4.2 Regression models for feature depth prediction

Although the semi-empirical model can give a good prediction of the feature depth, it is computationally intensive and relatively complex to implement for process planning. Therefore, we have developed regression models for fast and efficient feature depth estimation. Both linear and non-linear regression models were built to reflect the impact of significant machining parameters on the feature depth.

From the analysis of Table 4.4, all the process parameters (i.e. setpoint force, XY vibration amplitude, and feed rate) and the interaction term between setpoint force and feed rate are significant (e.g. $p<0.05$) in the linear regression model. Using these four factors, a linear regression model was developed with both variables centered, as shown in Equation 4.6:

$$D_p = -9.49 + 0.101*F_{set} + 0.17*V_{xy} - 4.13*feed - 0.07*(F_{set} - 160)*(feed - 1)$$

where $D_p$ is the predicted feature depth (nm), $F_{set}$ is the setpoint force (nN), $V_{xy}$ is the XY vibration amplitude (mV), and, $feed$ represents the feed rate during machining process (µm/s). The $R^2$ for the above linear regression model is 0.9245. Both the model predicted results and the measured ones are shown in Figure 4.2 (a) (with the red dots are the predicted depth, the blue dots are measured ones, and the sequence number is the trench number corresponding to Table 4.3). The relative errors for each machined trench were plotted in Figure 4.2 (b). As we can see, for most machining conditions, the predicted depths fit very well with measured ones, and most of these relative prediction errors are within ±20%. Considering the large process variability and the measurement error in nanometer scale, the linear model provides a good prediction of feature dimensions.
However, the linear model was developed without considering much physical meaning of the process. From our understanding of the tip-based nanomachining process, the effect of different machining parameters may not be directly addable. Thus, a nonlinear model may better describe the process than a linear model. For the nanomachining process, from our results in Table 4.3, the feature depth increases with larger setpoint force and XY vibration amplitude, while decreases with larger feed rate. To describe this relationship between the feature depth and these machining parameters, a nonlinear model was proposed to describe this relationship, which is shown in Equation 4.7:

\[ D_p = k_1 \frac{F_{set}^a V_{xy}^b}{feed^c} \]  

where \( D_p \) is the predicted feature depth (nm), \( F_{set} \) is the setpoint force (nN), \( V_{xy} \) is the XY vibration amplitude (mV), and, \( feed \) represents the feed rate during machining process (µm/s). \( k_1 \), a, b, and c are empirical coefficients. This model can provide better physical meaning than the linear model, and clearly reflects the facts that the feature depth increases with the increasing of setpoint force and XY vibration amplitude, and decreases with the increasing of feed rate.

![Figure 4.7](image)

Figure 4.7 (a) The measured depth (blue) and predicted depth (red) of the linear model for experiments from Table 3. (b) The relative error of the model prediction.
Using the least square method, we determine all the parameters $k_1$ and $a, b, c$ in the Equation 4.8:

$$D_p = 0.000126 F_{set}^{1.576} V_{xy}^{0.857} set \frac{xy}{Feed}^{0.348}$$

The results from nonlinear model prediction and the experimental results are shown in Figure 4.8 (with the red dots are the predicted depth, the blue dots are measured depth, and the sequence number is the number of trench corresponding to Table 4.3). For most machining conditions, the depths from the nonlinear model fit very well with the measured ones with relative error mostly below 20%.

4.5 Model validation and comparison

The previous results show good prediction capability of both the semi-empirical model and regression models. To further verify the accuracy of these models, we designed experiments with different machining conditions (setpoint force from 130 nN to 190 nN, XY vibration amplitude from 40 mV to 62.5 mV and feed rate from 0.7 µm/s to 1.3 µm/s) to

![Graphs](image)

Figure 4.8. (a) The measured depth (blue) and predicted depth (red) of the nonlinear model for experiments from Table 3. (b) The relative error of the model prediction.
cover different machining conditions. We plotted both the predicted depth and measured depth in Figure 4.9 (a), and also plotted the relative error between the calculated values and measured ones in Figure 4.9 (b).

![Figure 4.9](image)

Figure 4.9 (a) The measured depth (blue) and predicted depth (red) of the semi-empirical model for experiments from Table 3. (b) The relative error of the model prediction.

As we can see from Figure 4.9 (a) and Figure 4.9 (b), the values of predicted depth from the contact force model are very close the values of measured depth of verification group. All these three models were compared by calculating their corresponding root mean square of relative errors as shown in Table 4.5.

Table 4.5 The root mean square of relative errors for all of three predictive models

<table>
<thead>
<tr>
<th>Errors/ nm</th>
<th>Semi-empirical model</th>
<th>Linear model</th>
<th>Nonlinear model</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.1%</td>
<td>15.3%</td>
<td>15.9%</td>
<td></td>
</tr>
</tbody>
</table>

From Table 4.5, we can see all these three models have a relatively small root mean square of relative error, which indicates they have good prediction capability. Further refinement of the semi-empirical mechanical model and numerical methods should further improve the accuracy. For the linear model, we considered the interaction effect between setpoint force and feed rate, which is reasonable in our machining process, as feed rate can
affect the interaction force between AFM tip and the workpiece surface. For the nonlinear model, the format is easy to understand and, the relationships between machining parameters and feature depth are clearly shown.

4.6 Chapter summary

In this chapter, we have investigated the relationship between feature dimension (width and depth) with machining parameters (setpoint force, XY vibration amplitude and feed rate) for the vibration-assisted tip-based nanomachining. Experiments with different machining conditions were conducted, and the results were analyzed using statistical methods to determine the significant factors. Feature width was found to be affected by XY vibration amplitude while feature depth was found to be affected by several factors, such as setpoint force, XY vibration amplitude and feed rate. Then a semi-empirical model for the contact force was adapted to describe the relationship between feature depth and setpoint force as well as XY vibration amplitude. Then, both linear and nonlinear regression models were built to reflect the effect of feed rate. Based on the prediction results from the testing data, all models shown good prediction capability. In summary, predictive feature dimension models have been successfully developed, which provides us the guideline for process planning.
In Chapter 4, we discussed the effect of machining parameters on machined feature dimensions, and successfully developed the predictive feature dimension models by correlating the machined feature dimensions with the machining parameters, such as setpoint force, feed rate, and XY vibration amplitude. Besides predicting the feature dimensions, it is also critical to understand the cutting forces involved in the nanomachining process, which is important to plan the process properly. In conventional scale machining, many models have been developed to predict the cutting forces during the machining process. These models are usually developed using a mechanical modeling approach, which uses the chip load, cutter geometry, and other cutting conditions to predict the cutting forces. Similarly, many cutting force models have been developed for micromachining processes. These force models are used during process planning to increase the material removal rate, reduce the tool deflection and improve the machining quality.

Due to the complicated mechanics and physics involved, cutting force modeling for nanometer scale machining is very complex. Many methods have been proposed. Molecular dynamic simulation method was adopted by many researchers to study the scratching-based nanomachining processes, which investigated the molecular interaction during machining processes [56]. While this molecular dynamics (MD) method can predict the cutting force, it is computationally intensive and time-consuming, which greatly limits its applications to relatively simple machining processes.

To understand this nanomachining process, a cutting force model was developed and validated. The model correlated the cutting forces with the instantaneous material removal rate, which is determined by the specific machining conditions (i.e. setpoint force, XY
vibration amplitude and feed rate). In this chapter, we will first analyze the interaction between the cutting tool (AFM tip) and the workpiece surface. As mentioned previously, this nanomachining process is complicated, so it is difficult to model the cutting forces analytically. To solve this problem, a discrete voxel model was adopted to estimate the material removal rate during the machining process. Then the cutting force model was developed by correlating the cutting force with the material removal rate. A set of experiments was performed at different machining conditions to calibrate and evaluate the model.

5.1 Numerical model to calculate material removal rate

As mentioned in Chapter 4, we have developed a numerical algorithm to determine the instantaneously removed volume and calculate the contact area at different tip locations. Similarly, we can apply this numerical algorithm to calculate the volume of instantly removed area and material removal rate. The adapted algorithm is illustrated in Figure 5.1. In one tip rotation cycle or one machining cycle, the volume of removed material is significantly different at various tip locations, which is shown in Figure 5.2 (a). After we obtain the volume of instantaneous removed material, the material removal rate can be calculated as:

\[ R(\theta) = \frac{V(\theta)}{\Delta T} \]

Where \( R(\theta) \) is the material removal rate at the rotation angle of \( \theta \), \( V(\theta) \) is the volume of removed material from two positions with a time interval of \( \Delta T \), and \( \theta \) is the tip rotation angle in the machining cycle. The material removal rate for machining a slot at
different tip rotation in a machining cycle is plotted in Figure 5.2 (b). As the tip rotates from the 0°, where the tip begins to engage with the sample, to 180° degree, where the tip moves off from the sample, different material remove rate is obtained with the maximum material removal at around 90° degree. From 180° to 360°, the tip loses the contact with the material, thus theoretically have zero material removal
Figure 5.1 Numerical algorithm to estimate the volume of instantaneously removed material.
5.2 Predictive modeling for feature dimensions

The force model will rely on the voxel-based method to estimate the material removal rate, which assumes the feature dimensions (feature width and depth) are known. In our previous work, we measured the feature dimensions after machining for calculating the material removal rate and calibrating the force model. However, measurement after machining reduces the applicability of the machining force model in process planning and other applications. In this work, we aimed to develop the force model to correlate the input parameters of the machining process with the resulting dynamic machining force, to predict the machining force using the machining conditions without post-machining measurement.

Based on our previous research, the machined feature dimensions can be predicted by machining parameters including the setpoint force, XY vibration amplitude, and feed rate. The feature depth was found to be significantly affected by the setpoint force, XY vibration amplitude and feed rate, while the feature width is predominately determined by XY vibration amplitude. Using the similar approach, for the AFM tip employed in this study, we
applied the predictive feature dimension model to predict the feature depth and width with respect to different process conditions. For the nanomachining process, from our observation, the feature depth increases with setpoint force and XY vibration amplitude and decreases with larger feed rate. We selected a nonlinear expression to describe the relationship between the feature depth and width at different process conditions by:

\[
D_p = 0.0018 \frac{F_{set}^{1.01} V_{xy}^{0.85}}{feed^{0.28}}
\]

\[
W_p = 24.63 + 0.55 V_{xy}
\]

where \(D_p\) is the predicted feature depth (nm), \(F_{set}\) is the setpoint force for the machining process (nN), \(V_{xy}\) is the XY vibration amplitude (mV), \(feed\) represents the feed rate of nanomachining (µm/s), and \(W_p\) is the predicted feature width (nm). The coefficients of the feature depth and width model were identified experimentally using a set of tests with different machining conditions, which are shown in Table 5.1.

With the predictive feature dimension models, the feature depth and width under the given machining conditions can be estimated. Table 5.1 lists a set of machining conditions we used for the machining force modeling, covering a broad range of the machining conditions. From Table 5.1, for such a wide range of machining parameters, the predictive feature dimension model can accurately predict the feature dimensions with the Mean Square Error (MSE) of depth and width between predicted and measured about 1.3 and 2.1 nm separately. With the predicted feature dimensions, the material removal rate under different machining conditions can be calculated using the numerical voxel-based algorithm.
Table 5.1 Machining tests for force modeling with the predicted and measured feature depth and width by predictive feature dimension models

<table>
<thead>
<tr>
<th>No.</th>
<th>Force (nN)</th>
<th>V_XY (mV)</th>
<th>feed μm/s</th>
<th>Predicted depth (nm)</th>
<th>Predicted width (nm)</th>
<th>Measured depth (nm)</th>
<th>Measured width (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>150</td>
<td>30</td>
<td>1</td>
<td>5.3</td>
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<td>4.9</td>
<td>40.3</td>
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<td>2</td>
<td>150</td>
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<td>8.2</td>
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<td>49.7</td>
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<td>150</td>
<td>70</td>
<td>1</td>
<td>10.9</td>
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<td>10.7</td>
<td>41.1</td>
<td>10.8</td>
<td>42.6</td>
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<td>300</td>
<td>50</td>
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</tr>
<tr>
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<td>450</td>
<td>30</td>
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<td>49.4</td>
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<td>0.5</td>
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<td>54.9</td>
<td>12.7</td>
<td>56.8</td>
</tr>
</tbody>
</table>

5.3 Dynamic cutting force modeling in nanomachining process

In conventional scale machining, the cutting forces are usually correlated with the material removal rate. Intuitively if the material removal rate is larger, during unit time the area that the cutting tools must break bonds will also increase, which results in a larger cutting force. For this vibration-assisted tip-based nanomachining process, it is difficult to analytically calculate the cutting forces during machining process, so we have tried to correlate the cutting forces in both the normal and lateral direction with the instantaneous material removal rate. As mentioned above, the material removal rate can be calculated using
the feature depth and width by the 3D voxel-based numerical model developed in Chapter 5.1. Also, with Equations 5.2 and 5.3, the feature depth and width can be predicted using the machining parameters, such as setpoint force, feed rate and XY vibration amplitude.

To study the cutting forces during machining process, a Signal Access Module (SAM) from Park System is employed to access the deflection signals of cantilever in both vertical and lateral directions. When machining a trench, due to the interaction forces between the AFM tip and the workpiece surface, the AFM cantilever bends in the vertical direction, which can be measured by photo detector as A-B signal. Also, the torsional movement of the AFM cantilever is measured by the photo detector as C-D signal. The A-B data and C-D data are simultaneously acquired through National Instrument (NI) data acquisition module during machining process. In our cutting force model, the cutting force is extracted from A-B signal, and divided into lateral component \( F_L \) and normal component \( F_N \). When machining a trench, a lateral force component exists in the direction parallel to the cantilever axis, which induces a moment on the free end of the tip, and modifies the A-B signal. In this way, the A-B signal does not capture only the machining forces, so it is difficult to derive actual force values from this cutting force model.

The model for the normal and lateral component of the cutting force, expressed as normal force \( F_N \) and lateral force \( F_L \), are given as Equations 5.4 and 5.5:

\[
F_N = c_1 R^{k_1} = c_1 R^{k_1} \left( D_p, W_p \right) = c_1 R^{k_1} \left( F_{set}, V_{xy}, feed \right) \tag{5.4}
\]

\[
F_L = c_2 R^{k_2} = c_2 R^{k_2} \left( D_p, W_p \right) = c_2 R^{k_2} \left( F_{set}, V_{xy}, feed \right) \tag{5.5}
\]
where $F_N$ is the normal cutting force (V), $F_L$ is the lateral cutting force (V). $c_1$ and $c_2$ are normal and lateral force coefficients, $R$ is material remove rate ($nm^3/s$), and $k_1$, $k_2$ are exponent coefficients for the normal and lateral force. These parameters in the cutting force model will be identified experimentally.

To calibrate the cutting force model in Equations 5.4 – 5.5, a set of machining tests were performed using vibration-assisted nanomachining process with different cutting conditions. The machined results were imaged by AFM, and as mentioned above, the machining forces were recorded by measuring the raw cantilever normal deflection. Figure 5.3 shows the machining results from the first nine conditions in Table 5.1. The instant material removal rates at different conditions were calculated from the voxel-based method using the predicted feature depth and width. The machining force model was calibrated using the calculated material removal rate and the measured machining force in the normal and lateral directions.

![Figure 5.3 The machined slots for the machining conditions 1-9 in Table 1. From the cross-section profile, the feature width and depth can be measured.](image-url)
To model the dynamic cutting forces in the vibration-assisted nano-machining process and make data from different machining conditions comparable to each other, we normalize the measured data by subtracting the voltage before machining (corresponding to the setpoint force), to only study the dynamic force components for nanomachining at different experimental conditions. With the calculated material removal rates and acquired peak value of the cutting forces from conditions 1-9 (from Table 5.1), we can train the model and calibrate the unknown coefficients in the force model (Equation 5.4 and 5.5). The empirical coefficients in our force model \((c_1, c_2, k_1, \text{and } k_2)\) were obtained by minimizing the Mean square error (MSE) between the predicted cutting forces and measured ones, the calculated MSE for training data is \(2.3 \times 10^{-7} \text{V}^2\). The calibrated force model is as follows:

\[ F_L = 7.5 \times 10^{-5} \times R^{0.3093} \]
\[ F_N = 0.052 \times R^{0.0434} \]

Figure 5.4 (a) shows the typical material removal rate for six rotational cycles for the slots 6 in Figure 5.3. The corresponding lateral force and normal force were measured by the cantilever torsion and deflection, as shown in Figure 5.4 (b) and Figure 5.4 (c) as the solid curves. The results from model prediction were illustrated in Figure 5.4 (b) and Figure 5.4 (c) as the dashed curves. The force model fits well with the trends of the dynamic cutting forces and the peak value of the cutting force, which is most important. For the half rotational cycle, which ideally doesn’t have tip-sample interaction, we still observed a non-zero lateral force and normal force. The non-zero lateral force comes from the friction when the tip is sliding on the surface of the substrate, especially when the larger setpoint force is used. In our nanomachining process, we used the setpoint force to control the feature depth, and the
control system of the AFM always try to maintain the commanded setpoint force, even for the half cycle without machining. Thus, some friction force was produced, which generally has a smaller magnitude than the lateral force during machining. The force model can still predict the maximum force level or magnitude for tip-based nanomachining.

Figure 5.4 (a) calculated material removal rate during machining cycles. (b) Predicted and measured lateral force. (c) Predicted and measured normal force
The normal force in nanomachining is a little more complex to predict correctly as the cutting force is coupled with the setpoint force of the AFM system. For the normal force, the results from the force model and the experimentally measured force are compared in Figure 5.5 (c). Like the lateral force, even at the half rotational cycle without nanomachining, non-zero normal force is observed, which could come from some residual machining due to the setpoint force. But the model can still predict the peak value of the cutting force, which is one of the most important process variables that will affect tip wear and feature dimension. Since the lateral force is less affected by the setpoint force, we will focus on using lateral force to validate the developed force model. Figure 5.5 shows the predicted and measured cutting force for the first nine machining conditions in Table 5.1. For each process condition, we only compared the two forces in one machining cycle, as the cutting forces are periodic signals with fixed frequency. The cutting force model fits well with the trends of the dynamics cutting forces and the peak value of the cutting force. In machining conditions 1-9, we developed the cutting force model with different setpoint force and XY vibration amplitude. To further evaluate the effect of machining load (feed per rotation) to the cutting
force, a few more experiments were performed using different feed rates, which corresponded to the machining conditions 10-16 in Table 5.1. The feed rate was chosen to span a broad range from 0.25 µm/s to 5 µm/s. The machining results are displayed in Figure 5.6. As can be observed from the AFM image of the machined features using different feed rates in Figure 5.6, clearly with smaller feed rate or smaller feed per rotation, a small layer of material was removed in one tip rotation cycle, which results in relatively deeper features machined. With the cutting force model developed in Equation 5.6 and 5.7, both the lateral and normal cutting forces can be calculated at different feed rates. To validate the cutting force model, the cutting forces acquired from the AFM were compared with the calculated machining forces, both of which were plotted in Figure 5.7. As can be observed from Figure 5.7 (a), at different feedrates used in nanomachining, the cutting force model is very effective in predicting the lateral cutting forces for the given input process conditions, the MSE for this validation dataset is $4.9 \times 10^{-7}$. The force predicted from the model fits very well with the experimental results. For this set of experiments, even though the feed rates change significantly (by 20 times from 0.25 µm/s to 5 µm/s), the resulting cutting forces do not change as much. To better evaluate the force model, the machining power, defined as lateral force times feed rate $P = F_L \cdot f$, is introduced here, as the power will show more significant variances for different machining conditions.
Figure 5.7 (b) compares the machining power from the cutting force model and power calculated using experimentally measured force. With the developed cutting force model, the machining power can be successfully predicted with good accuracy across a large range of process conditions (different feed rates).

For all the experimental conditions given in Table 5.1, the cutting force model can successfully estimate the cutting forces from the input process parameters. Figure 5.8 compares the lateral force from the dynamic cutting force model with the experimentally measured lateral force for all sixteen conditions in Table 5.1. Over the wide range of the
cutting conditions, the force model can estimate the resulting cutting force very well. The maximum values of the cutting forces from the model prediction are very close to those measured from the experiments. The estimated lateral forces follow the trend of measured forces very well. The MSE of the model prediction here is $3.4 \times 10^{-7}$ V, which also indicates the high degree of correspondence between the predicted and actual cutting forces.

Figure 5.8 Lateral force from the machining force model and measured lateral force for all the conditions from table 5.1.

In this machining force model, we use feedback voltage from position-sensitive photodiode (PSPD) to represent the real machining force, so the unit of predicted machining force is V. When machining a trench, a lateral force component exists in the direction parallel to the cantilever, which induces a moment on the free end of the tip, and modifies the A-B signal. In this way, the A-B signal does not capture only the machining forces, so it is difficult to derive actual force values from this machining force model.

5.4 Chapter Summary

In this chapter, we successfully built and validated a dynamic cutting force model for the vibration-assisted nanomachining process. The interaction between the AFM tip and the workpiece surface during the vibration-assisted nanomachining process was studied numerically. A 3D discrete voxel method has been adopted to calculate the material removal rate (which is hard to calculate analytically). The voxel-based method can accurately
estimate the material removal rate given the width and depth of the machined features, which can be estimated by the machining parameters using a predictive model we developed before. Then a cutting force model was developed by correlating the cutting force with material removal rate and then the specific machining conditions. To calibrate the model, a set of nanomachining experiments was conducted using a broad range of machining conditions. The coefficients in the dynamic cutting force model were determined by comparing the predicted cutting force with the measured cutting force using mean square error (MSE) method. The model successfully predicted the cutting force in the vibration-assisted nanomachining process, which can provide potential guidelines to optimize the machining parameters to achieve higher productivity and reduce tip wear.
CHAPTER 6 MODELING OF TIP WEAR

Previously, we have developed models to predict the feature dimensions and dynamic cutting forces during this vibration-assisted tip-based nanomachining process. These models help us to understand the mechanism of this nanomachining process, and provide us the guidelines for process planning. When we developed these models, the tip radius was assumed constant during the machining process, which is reasonable for machining only a few patterns. However, if we apply this nanomachining process for high volume production, the tip could severely wear out, and its radius could become much larger than a new tip, which results in larger prediction error of these developed predictive models. Also, as we know, the tip wear could significantly impact machining accuracy and surface finish, so it is critical to understand the tip wear during this nanomachining process. In this chapter, we will first develop methods to detect tip wear, and then we will discuss factors that may affect tip wear and explain how we build the tip wear models.

6.1 Tool wear during machining process

During machining process, tool wear is generated by the direct contact and relative sliding between the cutting tool and the workpiece surface, or between cutting tool and the chip under the tool. When the tool wears, the cutting force, as well as the vibration and cutting temperature, will naturally increase, which will degrade the dimensional accuracy and surface quality of the features produced. Also, the tool must be replaced when its life comes to an end, which will increase the machining cost and decrease the productivity. In summary,
tool wear is a critical characteristic of the cutting process, which greatly affects quality and productivity.

For this vibration-assisted tip-based nanomachining, the effect of tool wear is even more significant as the dimensions of the machined patterns are close to the dimensions of the AFM tip. The radius of the AFM tip is only around 30 nm, while the depth of machined patterns is between 5 nm to 25 nm, so even if the radius of AFM tip increased by 5 nm, the dimensions of machined patterns would be greatly impacted.

For conventional scale, many models have been proposed to analyze the tool wear during the machining process. Some of them are based on one or more tip wear mechanisms while others are built by correlating tool wear with machining conditions. However, little research has been done in nanometer scale machining process. In this chapter, we will investigate the tip wear during the vibration-assisted tip-based nanomachining process.

6.2 Tip wear measurement through SEM images

To systematically study the tip wear during this nanomachining process, we have conducted a parallel study to study tip wear at different machining stages. Seven new tips were applied to machine different numbers of identical patterns. The number of machined patterns for each tip are shown in Table 6.1. Each designed pattern includes 32 identical trenches, and for each trench the setpoint force, feed rate, and XY vibration amplitude were applied as 1000 nN, 2 μm/s and 40 mV separately. All the machined patterns are shown in Appendix Figure A.1 to A.5. And a typically machined pattern by a new tip under the designed machining conditions is shown in Figure 6.1.
Table 6.1 Parallel study to analyze the tip wear during machining process

<table>
<thead>
<tr>
<th>Tip</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patterns machined</td>
<td>0</td>
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<td>2</td>
<td>4</td>
<td>8</td>
<td>12</td>
<td>20</td>
</tr>
</tbody>
</table>

With the ThreePointCircularROI, a plugin of Image J software, a circle was created based on three selected points on the tip cutting edge, whose radius equals the corresponding tip radius. With this method, the tip radius of all these seven tips were measured, which are shown in Appendix Figure A1 to Figure A5. The change in tip radius during machining process was observed and measured as shown in Figure 6.2.

Figure 6.1 (a) The pattern machined with a brand-new tip, (b) The pattern machined with a worn tip. As we can see, with a brand-new tip, the pattern quality is very high, and the machined feature depth is around 25 nm. However, using a worn tip, only some of the designed trenches was machined, and the machined feature depth is much smaller.
As shown in Figure 6.2, with more patterns machined (moving from Tip 1 to Tip 7), the tip became blunter. However, to study the tip wear at different stages, it is not enough to only qualitatively describe tip wear. So, we have tried to measure the tip radius to quantify the tip wear. For Tip 1 the radius was measured as 21 nm. In contrast, for Tip 7, which was applied to machine 20 patterns, the tip radius was measured at 208 nm. To better illustrate the wear of tip radius at different machining stages, we have plotted the value of tip radius in Figure 6.3. As we can see, with more patterns machined, the tip radius became larger.

Figure 6.2 SEM images for tip 1 to tip 7. As we can see, the tip is very sharp before machining, however, with more patterns machined, the tip became blunter, and the tip radius became larger.
6.3 Tip wear detection through pull-off force

Although the parallel study clearly shows us that the SEM can be used for tip wear detection, this process is time-consuming. To image the AFM tip, we need to uninstall the AFM tip, take the SEM images and reinstall the tip, which takes approximately one hour. Thus, the productivity will be greatly impacted. Also, as the hourly rate for SEM is very high ($30 to $50 USD/hour), this method will also increase the production cost. To solve this problem, we need to develop a low-cost, easy to implement method to detect the tip wear. Previous studies have correlated the pull-off forces with the AFM tip radius, which shows the
possibility of using pull-off forces to detect tip wear. In the following analysis, we will discuss the correlation between pull-off forces and tip radius during the machining process.

A typical force-distance curve obtained from AFM measurement is shown in Figure 6.4. The vertical axis represents the normal force applied on the cantilever due to the interaction between the tip and the workpiece surface, while the horizontal axis is the displacement of the cantilever. When the tip is far away from the workpiece surface, the cantilever will not deflect from the zero position. However, as the tip gradually approaches the workpiece surface, the tip snaps to the surface (“snap on peak”), and the cantilever is deflected toward the workpiece surface, which indicating there is an attractive force between these two. After the tip penetrates slightly into the sample, the cantilever is deflected away from the surface. Finally, when the cantilever is retracted from the surface, the tip-sample junction breaks at a value larger than the “snap-on peak”, which is called the the pull-off force. During the tip wear process, as the tip becomes blunter, there is a larger contact area between the tip and the workpiece surface, causing a larger force to be needed to retract the tip [82]. So, the pull-off force has been widely employed to study the tip geometry previously.

In this study, the force-distance curve can be easily measured right after machining. The workpiece used is silicon wafer with half of the surface covered by PMMA film. After machining on the PMMA film, the AFM tip was moved to the uncovered area, and the AFM was switched to the “Indenter mode”. As we know, humidity level will significantly affect the measured pull-off force [83], so all the measurements were conducted when the humidity in the room was between 16% and 21%. During the measurement, both the approach and retraction speed were set as 0.01 μm/s, and the applied normal force was set as 150 nN. After
the tip penetrates the surface, the cantilever is slowly retracted. The force-distance curves were plotted for both approach and retraction process, which can be employed to calculated the pull-off force.

![Force-distance curve obtained from AFM “Indentation mode”](image)

**Figure 6.4** Force-distance curve obtained from AFM “Indentation mode”. The X axis represents the displacement of the cantilever, and the Y axis represents the normal force applied on the cantilever. The red line represents the retraction curve, while the blue curve represents the approach curve. The force is measured by deflection of the AFM cantilever and the pull-off force is defined as the maximum attraction force during retraction of the tip for silicon surface.

When the setpoint force and feed rate were set as 1000 nN and 2 µm/s separately, the measured pull-off forces were plotted after machining process, which is shown in Figure 6.5. As the tip wears, the tip radius becomes larger, and a larger pull-off force is required to pull the tip away from the workpiece surface during the tip retraction process. In Figure 6.6, both the measured pull-off force and tip radius were plotted. As we can see, the variance of pull-off forces matches very well with the difference of tip radius, and the correlation coefficient between these two variables is calculated as 0.94. Therefore, the pull-off force is a reliable
alternative of measured tip radius by SEM images, which can be used to monitor the tip wear without removing it for SEM evaluation.

Figure 6.5 The measured pull-off forces during machining process under 1000 nN, 2 µm/s. As we can see, when the “Patterns machined” equals “0”, which corresponding to a new tip, the measured pull-off forces are around 20 nN. And with more patterns machined, the pull-off force gradually increased. After 15 patterns, no patterns could be machined with the tip and the measured pull-off force reached 170 nN. Then, with the machining parameters applied, even no patterns could be machined, the pull-off force continuously increased.

Figure 6.6 Both the measured tip radius and pull-off force are plotted. As shown in the figure, with more patterns machined, both the tip radius and pull-off force increased. Also, the pull-off force is strongly correlated with the tip radius, the rate of these two variables are close, which indicates the pull-off force could be employed to detect tip wear.
6.4 Tip wear under different machining conditions

Previously, we have shown that tip radius and pull-off forces could be used to detect tip wear during this vibration-assisted tip-based nanomachining process. However, it is not enough to only detect the tip wear, the tip change frequency must be investigated. If we change the tip too frequently, the machining cost will be greatly increased, and the productivity will be affected; However, if the tip is not changed in a timely manner, after the tip gets severely worn, the machining quality and accuracy will be impacted. Thus, it is critical to predict the tip wear and provide the guideline for the tip change frequency.

As we know, the rates of tip wear are different under different machining conditions, so it is essential to understand the effects of these machining parameters. Also, to provide the guideline for tip change frequency, it is critical to develop tip wear model to predict the machined distance before the tip must be changed. As discussed in Chapter 4, the feature width is only controlled by XY vibration amplitude. So, given the designed feature width, the XY vibration amplitude is determined. Then, to understand the impact of other machining parameters, such as setpoint force and feed rate, a full factorial design experiment ($2^3$) with these two factors was conducted. For each factor, three different values were assigned corresponding to the low, medium and high level of this factor, which is shown in Table 6.2.

To implement this factorial design experiment, nine new tips were applied to machine trenches with different machining parameters, which corresponding to Tip 7 to Tip 15 in Table 6.2. Under each machining condition, the tip was used to machine until several patterns after no trenches could be machined. Right after the machining process, the machined patterns were imaged with the same AFM using non-contact mode, and the pull-off forces were measured on clean silicon wafer surface using the “Indentation mode”.

76
Table 6.2 Factorial design experiments ($2^3$) for tip wear study.

<table>
<thead>
<tr>
<th>Tip number</th>
<th>Setpoint force /nN</th>
<th>Feed rate /μm/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tip 7</td>
<td>1000</td>
<td>2</td>
</tr>
<tr>
<td>Tip 8</td>
<td>500</td>
<td>1</td>
</tr>
<tr>
<td>Tip 9</td>
<td>500</td>
<td>2</td>
</tr>
<tr>
<td>Tip 10</td>
<td>500</td>
<td>3</td>
</tr>
<tr>
<td>Tip 11</td>
<td>1000</td>
<td>1</td>
</tr>
<tr>
<td>Tip 12</td>
<td>1000</td>
<td>3</td>
</tr>
<tr>
<td>Tip 13</td>
<td>1500</td>
<td>1</td>
</tr>
<tr>
<td>Tip 14</td>
<td>1500</td>
<td>2</td>
</tr>
<tr>
<td>Tip 15</td>
<td>1500</td>
<td>3</td>
</tr>
</tbody>
</table>

The machined patterns are shown from Appendix A.7 to A.14. As we can see, for the first few patterns, the machining quality is good. With more patterns machined, the quality rapidly degraded. Finally, no trenches could be machined. A typical example was shown in Figure 6.5. When the setpoint force and feed rate were set as 1000 nN and 2 μm/s separately, the quality of the first nine patterns are acceptable, while after the 10th pattern, the quality rapidly decreases, and only part of the designed pattern could be machined. Finally, after the 19th pattern, no trenches could be machined.
The values of measured pull-off force during machining process under all nine machining conditions were plotted in Appendix Figure A.15 (a) to (i). As we can see from these figure, under each machining condition, with more patterns machined, the pull-off forces increased. However, the rates of change of pull-off forces are different during the tip wear process. A typical example of the change of pull-off forces during the machining process is shown in Figure 6.8. As we can see, the pull-off force continuously increases during the machining process, however, the rate of change of pull-off force is during the
machining of the first nine patterns is significantly smaller than the one during the machining of the last eight patterns.

Also, to investigate the effect of different machining conditions, the rates of change of pull-off forces were calculated during the machining of the first 5 patterns for all these nine machining conditions, which were listed in Table 6.3 and visualized as the response surface in Figure 6.9. Obviously, the rates of change of pull-off forces increases with larger setpoint force or feed rate, which indicates faster tip wear.

Figure 6.8 The values of measured pull-off forces versus the number of patterns machined. As we can see, with more patterns machined, the pull-off force increases, but the rate of change of pull-off forces are different at different stages.
Table 6.3 The average rate of change of pull-off forces (nN/pattern) during the first five patterns under different machining conditions. After we can see, with larger setpoint force or feed rate, the average rate of change of pull-off forces are also larger.

<table>
<thead>
<tr>
<th>Tip number</th>
<th>Setpoint force /nN</th>
<th>Feed rate /μm/s</th>
<th>The average rate of change of pull-off forces/ nN/Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tip 8</td>
<td>500</td>
<td>1</td>
<td>1.4</td>
</tr>
<tr>
<td>Tip 9</td>
<td>500</td>
<td>2</td>
<td>3.2</td>
</tr>
<tr>
<td>Tip 10</td>
<td>500</td>
<td>3</td>
<td>4.8</td>
</tr>
<tr>
<td>Tip 11</td>
<td>1000</td>
<td>1</td>
<td>6.7</td>
</tr>
<tr>
<td>Tip 7</td>
<td>1000</td>
<td>2</td>
<td>6.7</td>
</tr>
<tr>
<td>Tip 12</td>
<td>1000</td>
<td>3</td>
<td>8.1</td>
</tr>
<tr>
<td>Tip 13</td>
<td>1500</td>
<td>1</td>
<td>11.8</td>
</tr>
<tr>
<td>Tip 14</td>
<td>1500</td>
<td>2</td>
<td>11.8</td>
</tr>
<tr>
<td>Tip 15</td>
<td>1500</td>
<td>3</td>
<td>13.3</td>
</tr>
</tbody>
</table>

Figure 6.9 Response surface of the average rate of change of pull-off forces during the first 5 patterns under different machining conditions. From this figure, we can clearly see that with larger setpoint force or feed rate, the average rate of change of pull-off forces is obviously larger.

As mentioned in Chapter 6.2, with more patterns machined, the tip becomes blunter and its radius gradually increases, which results in smaller machined feature depth. When the setpoint force and feed rate were set as 1000 nN and 2 μm/s separately, the values of...
machined feature depth were plotted in Figure 6.10 (The machined feature depth under all nine machining conditions were plotted in Appendix Figure A.16). As we can see, the measured feature depth decreases with more patterns machined, but the rates of change of pull-off forces are different at different stages.

![Graph](image)

Figure 6.10 The values of measured feature depth versus the number of patterns machined. As we can see, with more patterns machined, the feature depth decreases, and the rates of change of pull-off forces are different at different tip wear stages.

6.5 The effect of machining parameters on tip wear

In subchapter 6.4, we have discovered that the rate of change of pull-off force and machined feature depth are different under different machining conditions. To further analyze the effects of machining conditions, we need to quantify the rate of change of pull-off force and compare the results under different machining conditions. Both the pull-off forces and measured feature depth are plotted in Appendix Figure A.17 (a) to (i). Based on the rate of change of pull-off force and feature depth, we can divide this tip-based nanomachining process into three regions:
1. Initial tip wear region. The region usually occurs during the machining of the first few patterns, both the pull-off forces and the rates of change of pull-off forces are small. Also, the quality of machined patterns during this region are good.

2. Transition region. During this region, the pull-off force rapidly increases, while the depth of machined features rapidly decreases.

3. Tip failure region. During this region, no trenches could be machined on the workpiece surface. Both the pull-off forces and the rate of change of pull-off forces are relatively large.

A typical example of different tip wear regions during the machining process is shown as Figure 6.11. During the machining of the first nine patterns, the machined feature depth decreases slowly, and the pull-off force also increase gently. Between the machining of the 10th pattern and the 13th pattern, the depth of machined features rapidly decreases. Finally, after the 13th pattern, as shown in Figure 6.7, no trenches could be machined, the machined feature depth are zero while the pull-off force continuously increases.
During the machining process, the machined linear distance is defined as the distance that the AFM tip slide by, regardless of the machined trench is visible or not, which can be calculated by 160 times number of patterns machined. The pull-off forces during the initial tip wear region and tip failure region were plotted in Appendix Figure A.18 and A.19 separately. The X axis is the machined linear distance (μm), while the Y axis is the pull-off force (nN) measured after each machined pattern. For both the initial tip wear region and tip failure region, linear regression lines were fitted to correlate the pull-off forces with the machined linear distance under all machining conditions, which are defined as the local fitting lines. The equations of these local fitting lines are also shown in the figures. For the initial tip wear region, the slopes of these local fitting lines represent the rate of change of pull-off forces and the intercepts represent the pull-off force measured before machining for tip 7 to 15. As we can see, the slopes and intercepts of these local fitting lines are different under different machining conditions. The response surfaces of the slopes were plotted versus the corresponding setpoint force and feed rate in Figure 6.12 (a) (b).
To reflect the effect of machining conditions, a regression model was proposed to correlate the pull-off forces with the machined linear distance during the initial tip wear region, both the slope and intercept was correlated with machining parameters, which is shown as Equation

\[ F_{initial} = slope \times D_{linear} + \text{intercept} \]

\[ slope = k_1 \left( \frac{F_{set}}{1000} \right)^{k_2} \times \text{feed}^{k_4} + k_4 \]

\[ \text{intercept} = k_5 \left( \frac{F_{set}}{1000} \right)^{k_6} \times \text{feed}^{k_7} + k_8 \]

\[ F_{initial} \] is the pull-off forces measured during the initial tip wear region (nN), \( D_{linear} \) (µm) is the machined linear distance, \( \text{Feed} \) is the feed rate (µm/s), \( F_{set} \) is the setpoint force applied (nN). \( slope \) and intercept are the slope and intercept of the regression model, \( k_1, k_2, k_3, k_4 \) and \( k_5 \) are the coefficients. With the pull-off forces and corresponding machining parameters applied, this regression model was calibrated and all the coefficients were determined, which was shown as Equation 6.2.

---

Figure 6.12 The response surface of the slopes of the local fitting lines. As we can see, the slope increases with larger setpoint force or feed rate. Also, under the same machining condition, the slope during the tip failure region is obviously larger than the one during the initial tip wear region.
\[ F_{\text{initial}} = \text{slope} \ast D_{\text{linear}} + \text{intercept} \]
\[
\text{slope} = 0.019 \ast \left( \frac{F_{\text{set}}}{1000} \right)^{2.76} \ast \text{feed}^{0.23} + 0.0083 \quad 6.2
\]
\[
\text{intercept} = 26.56
\]

As we can see, the slope increases with larger setpoint force or feed rate, and the intercept is calculated as 26.56 nN, which is close to the average of measured pull-off forces for tip 7 to tip 5 before machining. Similarly, a regression model was proposed and calibrated for the tip failure region, which is shown as Equation 6.3.

\[ F_{\text{failure}} = \text{slope} \ast D_{\text{linear}} + \text{intercept} \]
\[
\text{slope} = 0.066 \ast \left( \frac{F_{\text{set}}}{1000} \right)^{1.78} \ast \text{feed}^{0.55} - 0.0089 \quad 6.3
\]
\[
\text{intercept} = -101.57 \ast \left( \frac{F_{\text{set}}}{1000} \right)^{1.72} \ast \text{feed}^{0.62} + 33.66
\]

where \( F_{\text{failure}} \) is the pull-off forces measured during the initial tip wear region (nN). Like the regression model for initial tip wear region, the slope increases with larger setpoint force or feed rate. However, the intercept is no longer a constant, it is also determined by the setpoint force and feed rate. In Figure 6.13 (a) (b), the pull-off forces were plotted versus the machined linear distance when the setpoint force and feed set as 1000 nN and 2 μm/s separately. The green lines are the global fitting lines corresponding to Equation 6.2 and 6.3, and the red lines are the local fitting lines. As we can see, for both the initial tip wear region and tip failure region, the global fitting lines are close to the local fitting lines, which indicates the calibrated regression models fit well for the pull-off forces.
In figure 6.14, the global fitting lines for both the initial tip wear region and tip failure region are plotted, and their cross point is represented by the yellow dot. As mentioned above, the slopes of the global fitting lines represent the rate of change of pull-off force, so their cross-point is the point that the rate of change of pull-off forces rapidly increases. The machined linear distance when the cross-point occurs is equal to the machining distance when the calculated $F_{\text{failure}}$ equal to $F_{\text{initial}}$ under each machining condition.
6.6 Modeling the tip change frequency

As we know, the patterns machined during the initial tip wear region are usually acceptable, while during the tip failure region, the tip rapidly wears out, and no trenches could be machined. To provide the guideline for the tip change frequency, we must identify the point where pattern quality rapidly decreases, which is termed as the “Transition point”. As mentioned above, the cross-point of the global fitting lines during initial tip wear region and tip failure region is the point that the rate of change of pull-off forces rapidly increases, which indicates the rate of tip wear rapidly increases at this point. So, the cross-point can be used as the “Transition point”. The calculated machined distance when cross-point occurred were listed in Table 6.4.

<table>
<thead>
<tr>
<th>Setpoint force/ nN</th>
<th>Feed rate/ µm/s</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td></td>
<td>1328</td>
<td>1456</td>
<td>1504</td>
</tr>
<tr>
<td>1000</td>
<td></td>
<td>2032</td>
<td>1952</td>
<td>1872</td>
</tr>
<tr>
<td>1500</td>
<td></td>
<td>2624</td>
<td>2320</td>
<td>2208</td>
</tr>
</tbody>
</table>

Besides the above-mentioned cross-point method, another method has been developed to estimate the transition point. For AFM tip-based direct scratching process, the machined feature depth and width is correlated with the force applied and the threshold force [61], which is shown as the Equation 6.4.

$$d(F_n) = \hat{d}_1 Ln(F_n/F_{\text{th}})$$
$$w_f(F_n) = \hat{d}_2 Ln(F_n/F_{\text{th}})$$

6.4
where $\partial_1$ and $\partial_2$ are the coefficients, $d$ and $w_j$ are the machined feature depth and width separately, $F_n$ is the force applied on the tip, and $F_{i1}, F_{i2}$ are the threshold forces. Per this equation, a trench can be machined only when the applied force is larger than the threshold force. Then, the threshold force was correlated with contact area $A_c$, and maximum contact stress $\sigma_c$, which is expressed as Equation 6.5.

$$F_{tc} = \frac{2\sigma_c A_c}{3}$$  \hspace{1cm} 6.5

Where $F_{tc}$ is the threshold force (nN), $\sigma_c$ is the maximum contact stress, $A_c$ is the contact area between the tip and sample surface ($nm^2$). If the force applied on the tip is larger than the threshold force $F_{tc}$, the tip could machine trenches. Otherwise, there will be no plastic deformation or indentation on the sample surface. During the machining process, with more patterns machined, the tip radius as well as the contact area between the tip and sample surface will be larger. So, the corresponding threshold force needed to make plastic deformation on the sample surface increases. As mentioned in chapter 6.2, the contact area $A_c$ between the tip and sample surface is correlated with the pull-off force $F_{\text{pull-off}}$ (nN), which indicates the measured pull-off force is positively proportional to the threshold force needed. Inspired by Equation 6.5, a threshold force model was proposed for this vibration-assisted tip-based nanomachining process, which is shown as Equation 6.6.

$$F_{tc} = b_1 * F_{\text{pull-off}} + b_2$$  \hspace{1cm} 6.6

With larger measured pull-off force, the contact area $A_c$ between the tip and sample surface is also larger, which results in larger threshold force. It is difficult to measure or calculate the threshold force during machining process, so the corresponding pull-off force
was applied to determine if the tip should be changed. As we know, when the threshold force reaches the force applied on the tip, no trenches could be machined and the pull-off force measured is termed as “Cut-off pull-off force”. With the quality of machined patters, we have identified the cut-off pull-off force using Appendix Figure A. 17, which is shown as Table 6.5. A regression model was proposed by correlating the cut-off pull-off force with the corresponding machining conditions, such as setpoint force and feed rate, which is shown as Equation 6.7. Then the model was calibrated using the first six data points, which is shown as Equation 6.8. Then, the model was tested using the last three data points, and the calculated Root Mean Square Error (RMSE) is only 6 nN, which indicates the cut-off pull-off force model has a high accuracy in predicting the cut-off pull-off forces.

\[ F_{\text{cut-off}} = c_1 \cdot F_{\text{set}}^{c_2} \cdot \text{feed}^{c_3} + c_4 \]

6.7

<table>
<thead>
<tr>
<th>Training Data</th>
<th>Setpoint force/ nN</th>
<th>Feed rate/ μm/s</th>
<th>Cut-off pull-off force/ nN</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>1</td>
<td>42</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>2</td>
<td>39</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>2</td>
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</tr>
<tr>
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<td>3</td>
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<td>Testing Data</td>
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<td>500</td>
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<td>1000</td>
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<td>81</td>
<td></td>
</tr>
<tr>
<td>1500</td>
<td>1</td>
<td>118</td>
<td></td>
</tr>
</tbody>
</table>

\[ F_{\text{cut-off}} = 2.7 \times 10^{-4} \cdot F_{\text{set}}^{1.74} \cdot \text{feed}^{0.46} + 31.4 \]

6.8

where \( F_{\text{cut-off}} \) is the cut-off pull-off force (nN), \( F_{\text{set}} \) is the setpoint force (nN) and \( \text{feed} \) is the feed rate (μm/s). As we can see, the cut-off pull-off force increases with larger setpoint force or feed rate. Using this model, the cut-off pull-off forces were calculated under different machining conditions. Then, with the measured pull-off forces, we estimated the “cut-off
point” of tip wear, which is the point when the measured pull-off force reaches the cut-off pull-off force under each machining condition. Also, the corresponding number of patterns machined before the measured pull-off force reached the calculated cut-off pull-off force. As shown in Table 6.6, the values of estimated number of machined patterns were compared with the number of machined patterns estimated using the cross-point method under different machining conditions.

Table 6.6 The number of machined patterns calculated using both cross-point method and cut-off pull-off force method.

<table>
<thead>
<tr>
<th>Setpoint force/ nN</th>
<th>Feed rate/ μm/s</th>
<th>Number of Machined patterns estimated by cross-point method</th>
<th>Number of Machined patterns estimated by cut-off pull-off force</th>
<th>Relative Error/°</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>1</td>
<td>8.2</td>
<td>11</td>
<td>34.15</td>
</tr>
<tr>
<td>500</td>
<td>2</td>
<td>9</td>
<td>8</td>
<td>-11.11</td>
</tr>
<tr>
<td>500</td>
<td>3</td>
<td>9.3</td>
<td>6</td>
<td>-35.48</td>
</tr>
<tr>
<td>1000</td>
<td>1</td>
<td>12.7</td>
<td>13</td>
<td>2.36</td>
</tr>
<tr>
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<td>2</td>
<td>12.1</td>
<td>12</td>
<td>-0.83</td>
</tr>
<tr>
<td>1000</td>
<td>3</td>
<td>11.8</td>
<td>11</td>
<td>-6.78</td>
</tr>
<tr>
<td>1500</td>
<td>1</td>
<td>16.3</td>
<td>12</td>
<td>-26.38</td>
</tr>
<tr>
<td>1500</td>
<td>2</td>
<td>14.6</td>
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<td>-10.96</td>
</tr>
<tr>
<td>1500</td>
<td>3</td>
<td>13.7</td>
<td>14</td>
<td>2.19</td>
</tr>
</tbody>
</table>

As shown in Figure Appendix A.20 (a) to (i), both the transition point and cut-off point were plotted under different machining conditions. As we can see, under most conditions, these two points are close. A typical example is shown as Figure 6.14 when the setpoint force and feed rate were set as 1000 nN and 2 μm/s separately.
In this chapter, we first developed methods to detect tip wear both qualitatively and quantitatively. The SEM images of the used AFM tip is a straightforward method to detect tip wear, and the tip radius could be measured to quantitatively study the tip wear. However, this method is costly and time-consuming. Based on the parallel study, we have proved that the pull-off force between the used tip and pure silicon surface was highly correlated with the tip radius, which indicates the pull-off force could be employed as a low-cost alternative to study the tip wear. To systematically study the tip wear during machining process, a full factorial design experiment of two factors including setpoint force and feed rate was conducted, and the pull-off forces as well as the machined feature depth were measured. Based on the rate of change of both the pull-off forces and measured feature depth, three tip wear regions were identified during the tip wear process including initial tip wear region, transition region and tip failure region. Then, a linear regression model, which was termed as
the global fitting line in Figure 6.13, was developed to correlate the pull-off force with the machined distance for the initial tip wear region, and both the slope and intercept of this regression model were correlated with setpoint force and feed rate. A similar linear regression model was also developed for the tip failure region. As the slope of these two global fitting lines represent the rate of change of pull-off forces during the machining process, their cross-point is the point that the rate of tip wear rapidly changed, which is termed as “Transition point” and corresponds to the point the tip becomes unusable. Besides this cross-point method, another model was developed to predict the threshold (maximum) pull-off force under each machining condition. With this model, the point, which is termed as the “Cut-off point”, that the measured pull-off force reaches the cut-off one was calculated under each machining condition. The predicted points to change the tip were very close for most machining conditions.
CHAPTER 7 OPTIMIZATION MODELS FOR UNIT PRODUCTION TIME AND COST

In previous chapters, we have developed models to predict the machined feature dimensions, the dynamic cutting forces during machining process and tip life. These models deepen our understanding of the mechanism of this complicated vibration-assisted tip-based nanomachining process, and provide us the guideline for parameter selection. Although we can produce the designed feature dimensions using these provided machining parameters, the production time or production cost may be unnecessarily high. To improve the productivity or reduce the machining cost, we will develop optimization models for unit production time or unit production cost in this chapter, and calculate the optimal machining parameters.

7.1 Process modeling in conventional scale

In workshop practice, the machining conditions is usually selected by the experience of the machine operator. However, even for a skilled operator, it is very difficult to choose the optimum values each time. Several parameters may determine the quality of product, such as cutting speed, feed rate and depth of cut. For conventional scale machining, such as turning and cutting, both analytical and experimental methods have been investigated to optimize the machining parameters.

Geometric programming was employed to determine the values of feed rate and cutting speed that minimize the total cost of machining SAE 1045 steel with cemented carbide tools, subjected to some realistic constraints like the surface finish and machine power [83]. Besides geometric programming method, an optimization module, named PC-based generative CAPP system, has also been developed to determine process parameters for
turning operations. The objective function is based on minimization of production time, with the constraints such as power, surface finish, tolerance, workpiece rigidity, etc. This developed optimization function was solved by the combination of geometric and linear programming techniques [84]. Response surface methodology was also used to investigate three independent machining variables simultaneously for turning operation [85].

7.2 Process planning for vibration-assisted tip-based nanomachining

Previously, we have investigated the effects of machining parameters on this vibration-assisted tip-based nanomachining process, and developed predictive models for feature dimensions (depth and width). Like conventional scale machining, if we are given the desired feature dimensions, such as feature width and depth, we could plan the machining process by selecting feasible machining parameters.

As discussed in Chapter 4, the feature width is proved to be only controlled by the XY vibration amplitude, and a linear regression model has been developed to describe the relationship between these two, which is shown as Equation 7.1

\[ W = k_i \times V_{xy} + b_i \]  

\( W \) is the predicted feature width, \( V_{xy} \) is the XY vibration amplitude, and \( k_i \), \( b_i \) are the coefficients, which can be determined using measured data from the experiment. With this equation, we can easily estimate the feature width given the machining conditions, or, we can calculate the feasible XY vibration amplitude to achieve desired feature width.

Similarly, in Chapter 4, we have also discussed the effects of machining parameters on the feature depth. Based on the ANOVA test results, several factors may have statistically
significant effect on feature depth, such as setpoint force, XY vibration amplitude, feed rate and the interaction term between the setpoint force and feed rate. Also, several models have been developed to predict the feature depth, which can be employed to provide the guidelines for the selection of feasible machining parameters to achieve desired feature depth. Among these models, the nonlinear regression model, shown as Equation 7.2, will be used in the following discussion due to its advantages, such as low computation cost, and clear physical meaning.

$$D = \frac{k_2 * F_{set}^{k_3} * V_{SY}^{k_4}}{feed^{k_5}}$$

Equation 7.2

\(D\) is the feature depth (nm), \(F_{set}\) is the setpoint force applied (nN), \(V_{SY}\) is the XY vibration amplitude (mV), \(feed\) is the feed rate (μm/s), \(k_2, k_3, k_4\) are the coefficients, which can be determined using data from experiments.

Besides the above-mentioned predictive models for feature dimensions (depth and width), in Chapter 6, we have also analyzed the effects of machining parameters on tip wear, identified tip wear regions, and provided the guideline for when to change the tip under different machining conditions. The machining process was also analyzed in detail as well as the interaction area between the AFM tip and the workpiece surface, and the dynamic cutting forces were modeled.

Based on these developments an algorithm for process planning of vibration-assisted tip-based nanomachining process is proposed and shown in Figure 7.1.
7.3 Stop criterion to change the tip

As mentioned in Chapter 6, the “Transition point” is defined as the point that the tip must be changed, and the tip life $S$ is the machined distance before this transition point. With the measured feature depth, the values of tip life $S$ calculated using the “Transition point” are shown in Table 7.1, $S_1$ is the tip life calculated using the cut-off pull-off force model (μm), $S_2$ is the tip life calculated using the cross point of two global fitting lines during the initial tip life region and the tip failure region (μm), and the $S_{average}$ is the mean value of $S_1$ and $S_2$ (μm).
Table 7.1 The tip life calculated using transition point

<table>
<thead>
<tr>
<th>Setpoint force/nN</th>
<th>500</th>
<th>1000</th>
<th>1500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed rate/μm/s</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>$S_1$/μm</td>
<td>1760</td>
<td>1280</td>
<td>960</td>
</tr>
<tr>
<td>$S_2$/μm</td>
<td>1328</td>
<td>1440</td>
<td>1488</td>
</tr>
<tr>
<td>$S_{average}$/μm</td>
<td>1544</td>
<td>1360</td>
<td>1224</td>
</tr>
</tbody>
</table>

As we can see, the values of $S_{average}$ are different under different machining conditions, so a tip life model is proposed by correlating the tip life with setpoint force and feed rate, which is shown as Equation 7.3.

$$S = b_2 \left( \frac{F_{set}}{1000} \right)^{b_1} \times \text{feed}^{b_2} + b_3$$  \hspace{1cm} 7.3

$F_{set}$ is the setpoint force applied (nN), $feed$ is the feed rate (μm/s). Using the values of $S_{average}$ shown in Table 7.1, the tip life model can be calibrated, which is shown as Equation 7.4. The relative root mean square error (RMSE) is 4.9%.

$$S = 2751.25 \times \left( \frac{F_{set}}{1000} \right)^{0.31} \times \text{feed}^{-0.078} - 728.11$$  \hspace{1cm} 7.4

As mentioned above, “Transition point” can be used to determine the tip life. However, in real machining process, the tip change frequency may vary based on requirements. The criterion used to determine the tip change frequency is named “Stop criterion”, which is defined as the maximum acceptable decrease of machined feature depth before the tip must be changed. For example, given the machined feature depth is 20 nm with a new tip, under 10% stop criterion, the tip must be changed when the machined feature depth drops below 18 nm. Difference stop criterions may be employed under different requirements. If the customer requires the machined feature depth to be highly consistency,
smaller stop criterions should be chosen, such as 10%. Otherwise, larger stop criterion may be used. With different stop criterions, the tip life $S$, which is defined as the distance machined before the tip must be changed, may be different.

To calibrate this tip life model (Equation 7.3) under different stop criterions, the tip life $S$, which is the machined distance before the stop criterion, must be measured. As we know, during the machining process, debris may fall into the machined trenches, which increases the measurement error of feature depth. As shown in Figure 7.2, to compensate for this measurement error, a linear regression line was fitted for the pull-off forces (blue dots) before the transition region, which is shown as the yellow line. Also, as an example, the 20% stop criterion is plotted as the green line. The cross point of these two lines represents the point that the tip must be changed under 20% stop criterion. Using this method, the values of tip life were estimated accurately under different stop criterions (from 5% to 30%) and machining conditions, which were applied to calibrate the proposed tip life model.
The determined coefficients are listed in Table 7.2. As we can see, the values of relative root mean square error (RMSE) are below 15% under all stop criterions, which indicates that the tip life model fits the data well.

Table 7.2 The calibrated coefficients for Equation 7.7

<table>
<thead>
<tr>
<th>Stop criterion</th>
<th>b0</th>
<th>b1</th>
<th>b2</th>
<th>b3</th>
<th>Relative RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>5%</td>
<td>210.38</td>
<td>0.36</td>
<td>-0.61</td>
<td>146.32</td>
<td>7.0%</td>
</tr>
<tr>
<td>10%</td>
<td>431.10</td>
<td>0.35</td>
<td>-0.59</td>
<td>122.33</td>
<td>9.5%</td>
</tr>
<tr>
<td>15%</td>
<td>681.18</td>
<td>0.32</td>
<td>-0.55</td>
<td>69.14</td>
<td>11.0%</td>
</tr>
<tr>
<td>20%</td>
<td>961.50</td>
<td>0.30</td>
<td>-0.51</td>
<td>-14.25</td>
<td>11.8%</td>
</tr>
<tr>
<td>25%</td>
<td>1259.10</td>
<td>0.28</td>
<td>-0.48</td>
<td>-114.94</td>
<td>12.4%</td>
</tr>
<tr>
<td>30%</td>
<td>1588.79</td>
<td>0.26</td>
<td>-0.45</td>
<td>-247.71</td>
<td>12.8%</td>
</tr>
</tbody>
</table>

As mentioned in Chapter 7.1, given the designed feature depth, such as 20 nm, using the predictive feature dimension model, the relationships between machining parameters are determined, which are shown in Equation 7.5 and 7.6:
\[ W = 0.3 * V_{xy} + 23.1 \]  

\[ D = \frac{21.76 * \left( \frac{F_{set}}{1000} \right)^{0.59}}{feed^{0.15}} = 20 \text{ nm} \]

So, the setpoint force can be expressed using feed rate, which is shown as Equation 7.7:

\[ F_{set} = 866 * feed^{0.25} \]

And the tip life can be expressed only using feed rate, which is shown as Equation 7.8:

\[ S = b_0 * 0.866^{b_1} * feed^{0.25b_2} + b_3 = k_1 * feed^{k_2} + k_3 \]

<table>
<thead>
<tr>
<th>Stop criterion</th>
<th>( k_1 )</th>
<th>( k_2 )</th>
<th>( k_3 )</th>
<th>Relative RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>5%</td>
<td>199.76</td>
<td>-0.52</td>
<td>146.32</td>
<td>7.0%</td>
</tr>
<tr>
<td>10%</td>
<td>409.93</td>
<td>-0.50</td>
<td>122.33</td>
<td>9.5%</td>
</tr>
<tr>
<td>15%</td>
<td>650.53</td>
<td>-0.47</td>
<td>69.14</td>
<td>11.0%</td>
</tr>
<tr>
<td>20%</td>
<td>920.88</td>
<td>-0.44</td>
<td>-14.25</td>
<td>11.8%</td>
</tr>
<tr>
<td>25%</td>
<td>1209.39</td>
<td>-0.41</td>
<td>-114.94</td>
<td>12.4%</td>
</tr>
<tr>
<td>30%</td>
<td>1530.46</td>
<td>-0.39</td>
<td>-247.71</td>
<td>12.8%</td>
</tr>
</tbody>
</table>

\( k_1, k_2 \) and \( k_3 \) are the coefficients. As shown in Table 7.3, with larger stop criterions, both \( k_1 \) and \( k_2 \) increase, while \( k_3 \) decreases.

As shown in Equation 7.8, when the stop criterion is set, the tip life decreases with larger feed rate \( feed \). To illustrate this effect, the values of tip life were plotted versus feed rate under different stop criterions, which is shown in Figure 7.3. As we can see, with larger feed rate, to achieve the same tip life, the corresponding stop criterion is also larger. For example, to achieve the tip life of 1000 \( \mu \text{m} \), when the feed rate is set as 0.3 \( \mu \text{m/s} \), the corresponding stop criterion is 10%; However, if the feed rate is increased to 1.7 \( \mu \text{m/s} \), the corresponding stop criterion is 30%.
7.4 Process optimization for minimum production time

For conventional scale machining, the unit production time, which is defined as the time consumed to finish machining one pattern, is a critical factor to determine the productivity. Many optimization models have been developed to optimize the machining parameters for minimum unit production time. Similarly, for this vibration-assisted tip-based nanomachining process, we also try to develop a mathematical model for unit production time, and provide the optimal machining parameters.

The unit production time $t$ (Hour) is consisted of two parts: 1) The unit machining time $t_m$ (Hour), which the time during machining process for one pattern. The unit machining time is determined by designed machining distance of one pattern $L_0$ (μm) and feed rate $feed$ (μm/s). 2) The unit tip changing time $t_{change}$ (Hour), which is the time consumed to change tips during the machining of one pattern. The tip changing time $t_{change}$ (Hour) is
determined by single tip changing time $t_c$ (Hour) and the number of tips needed for to finish machining one pattern $N_t$. For this nanomachining process, $N_t$ is correlated with the designed machining distance of one pattern $L_0$ ($\mu$m) and the tip life $S$. So, the unit production time can be express as Equation 7.9:

$$t = t_m + t_{change} = \frac{L_0}{3600 * \text{feed}} + \frac{L_0}{S} * t_c$$ 7.9

For this nanomachining process, we also have some realistic constraints for machining parameters. Based on large number of experiments, the nanomachining process could produce high quality patterns when the setpoint force is set between 500 nN and 1500 nN, and the feed rate is set between 1 $\mu$m/s to 3 $\mu$m/s. As discussed in Chapter 7.3, the tip life model is calibrated under different stop criterions. So, when the stop criterion is 10% and the single tip changing time equals 5 minutes, the optimization model for unit production time can be summarized as Equation 7.10.

Objective function:
Minimize $t = t_m + t_{change}$

$$t_m = \frac{L_0}{3600 * \text{feed}}$$

$$t_{change} = N_t * t_c = \frac{L_0}{S} * t_c$$

$$S = 431.1 * \left(\frac{F_{set}}{1000}\right)^{0.345} * \text{feed}^{-0.59} + 122.33$$ 7.10

Constraints:
$1 \mu$m/s $\leq$ feed $\leq$ 3 $\mu$m/s
500 nN $\leq$ $F_{set}$ $\leq$ 1500 nN

The unit production time can be expressed using machining parameters, such as setpoint force and feed rate, which is shown as Equation 7.11. To illustrate the effect of these
two factors, we have plotted the unit machining time, unit tip changing time and unit production time as the response surface versus feed rate and setpoint force, which is shown in Figure 7.4 (a) (b) (c) separately. As shown in these figures, the unit machining time increases with smaller feed rate, the unit tip changing time $t_c$ increases with larger setpoint force or smaller feed rate and the unit production time increases with larger feed rate or larger setpoint force.

\[
t = \frac{L_0}{S} * t_c + \frac{L_0}{3600 * \text{feed}} = \frac{L_0}{431.1 * \left( \frac{F_{set}}{1000} \right)^{0.345} * \text{feed}^{-0.59} + 122.33} * t_c + \frac{L_0}{3600 * \text{feed}}
\]

7.11
As in Chapter 7.3, if feed rate and stop criterion are increased simultaneously, the tip life may not change. So, with larger feed rate and larger stop criterion, the unit machining time could be reduced, while the unit tip changing time could be maintained, which results in smaller unit production time. Therefore, the optimal feed rate to achieve minimum unit production time increases with larger stop criterion.

If the designed feature depth is given as 20 nm, using the Equation 7.9, the relationship between the setpoint force and feed rate is determined, and the optimal feed rate and setpoint force to minimize the unit production time.

Figure 7.4 The response surface of (a) the unit machining time (b) unit tip changing time and (c) unit production time versus setpoint force and feed rate when stop criterion is 10% and single tip changing time is 5 minutes. As we can see, the unit machining time increases with smaller feed rate, the unit tip changing time increases with larger setpoint force or smaller feed rate and the unit production time increases with larger feed rate or larger setpoint force.

As in Chapter 7.3, if feed rate and stop criterion are increased simultaneously, the tip life may not change. So, with larger feed rate and larger stop criterion, the unit machining time could be reduced, while the unit tip changing time could be maintained, which results in smaller unit production time. Therefore, the optimal feed rate to achieve minimum unit production time increases with larger stop criterions. If the designed feature depth is given as 20 nm, using the Equation 7.9, the relationship between the setpoint force and feed rate is determined, and the optimal feed rate and setpoint force to minimize the unit production time.
can be calculated. To analyze the sensitivity of this optimization model, the values of optimal feed rate were calculated and plotted as a response surface under different stop criterions and single tip changing time $t_c$, which is shown as Figure 7.5. As we can see, the optimal feed rate increases with larger stop criterions or smaller single tip changing time.

![Figure 7.5 The response surface of optimal feed rate under different stop criterions and single tip changing time. As we can see, the optimal feed rate increases with smaller single tip changing time or larger stop criterions.](image)

7.5 Process optimization to minimize production cost

Besides unit production time, unit production cost is also a critical factor for machining process. The unit production cost is defined as the cost to produce one pattern. In this subchapter, we will try to develop a mathematical model for the unit production cost, and investigate the effects of machining parameters.

In this study, the unit production cost $u$ ($) is defined as the production cost per pattern, which is consisted of two parts: (1) The unit machining cost $u_E$ ($$), which is the cost of electricity and labor per pattern. This cost is charged hourly, based on our experience, the hourly rate is $80 USD per hour. (2) The unit tip changing cost $u_T$ ($$), which is defined as
the cost of the tips consumed for machining one pattern. So, the unit production cost can be expressed as Equation 7.12.

\[
u = u_E + u_T = u_e \cdot (t_m + N_t \cdot t_c) + u_e \cdot N_t = u_e \cdot (t_m + \frac{L_0}{S} \cdot t_c) + u_e \cdot \frac{L_0}{S}
\]  

7.12

\(L_0\) (\(\mu m\)) is the desired machining distance for one pattern, \(u_e\) ($/hour) is the hourly rate for the equipment and labor cost, \(t_m\) (hour) is the machining time. \(N_t\) is the number of tips consumed to machine one pattern, which is correlated with \(L_0\) and \(S\). \(t_c\) (hour) is the time used to change one tip.

As mentioned in Chapter 7.4, we also have some realistic constraints for machining parameters. Based on large number of experiments, the nanomachining process could produce high quality patterns when the setpoint force is set between 500 nN and 1500 nN, and the feed rate is set between 1 \(\mu m/s\) to 3 \(\mu m/s\). So, when the stop criterion is 10% and the tip price equals $ 15 USD, the optimization model for unit production cost can be summarized as Equation 7.13.

Minimize \(u = u_E + u_T\)

\(u_E = u_e \cdot (t_m + N_t \cdot t_c) = u_e \cdot (t_m + \frac{L_0}{S} \cdot t_c)\)

\(u_T = u_e \cdot N_t = u_e \cdot \frac{L_0}{S}\)

\[S = 431.1 \cdot \left(\frac{F_{set}}{1000}\right)^{0.345} \cdot \text{feed}^{-0.59} + 122.33\]  

7.13

Constraints:

\(1 \ \mu m/s \leq \text{feed} \leq 3 \ \mu m/s\)

\(500 \ \text{nN} \leq F_{set} \leq 1500 \ \text{nN}\)
To illustrate the effect of setpoint force and the feed rate on the unit machining cost, we have plotted its response surface of unit machining cost, unit tip changing cost and unit production cost, which is shown in Figure 7.6. As we can see, the unit machining cost, the unit tip changing cost and unit production cost increase with larger feed rate or smaller setpoint force.

![Figure 7.6](image)

Figure 7.6 The response surface of (a) unit machining cost (b) unit tip changing cost and (c) unit production cost versus feed rate and setpoint force. As we can see, all these three cost increases with larger feed rate or smaller setpoint force.

To test the sensitivity of this unit production cost model, the values of optimal feed rate are calculated and plotted as the response surface under different stop criterions and tip price, which is shown as Figure 7.7. As shown in the figure, the optimal feed rate increases with smaller tip price or larger stop criterions.
Previously, the optimization models for both the unit production time and the unit production cost have been developed. To better understand these optimization functions, in this chapter we will implement these models in a machining task. Assume we receive an order to produce large number of patterns using the 32-trench design as shown in Chapter 6, the designed feature dimensions, single tip changing time and tip price are shown in Table 7.3, how could we perform this machining task? As we discussed in Chapter 7.2, process planning must be performed first. Using the calibrated predictive feature dimension model, the feasible XY vibration amplitude is calculated as 45 mV using Equation 7.14, and the relationship between setpoint force and feed rate is also determined, which is shown as Equation 7.15. Then, to achieve minimum unit production time, the setpoint force and feed rate must be optimized.

Figure 7.7 The response surface of optimal feed rate under different stop criterions and tip price. As we can see, the optimal feed rate increases with smaller tip price or larger stop criterions.
Table 7.4 The designed feature dimensions and single tip changing time

<table>
<thead>
<tr>
<th>Length of trench/μm</th>
<th>Depth/nm</th>
<th>Width/nm</th>
<th>Single tip changing time/Hour</th>
<th>Tip price/USD</th>
<th>Hourly rate/USD</th>
<th>Stop criterion</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>15</td>
<td>60</td>
<td>1/6</td>
<td>15</td>
<td>80</td>
<td>10%</td>
</tr>
</tbody>
</table>

\[
W = 0.3 \times V_{XY} + 46.5 = 60 \text{ nm}
\]

\[
D = \frac{21.76 \times \left( \frac{F_{set}}{1000} \right)^{0.59}}{feed^{0.15}} = 15 \text{ nm}
\]

As discussed in Chapter 7.4, with 10% stop criterion, the optimization functions of unit production time and realistic constraints are shown as Equation 7.16.

Objective function:
Minimize \( t = t_m + t_{\text{change}} \)

\[
t_m = \frac{L_0}{3600 \times feed}
\]

\[
t_{\text{change}} = N_t \times t_c = \frac{L_0}{S} \times t_c
\]

\[
S = 431.1 \times \left( \frac{F_{set}}{1000} \right)^{0.345} \times feed^{-0.59} + 122.33
\]

Constraints:
1 \( \mu \text{m/s} \leq feed \leq 3 \mu \text{m/s} \)

500 nN \( \leq F_{set} \leq 1500 \text{ nN} \)

Using numerical search method, the optimal feed rate to achieve minimum unit production time is calculated as 1.7 \( \mu \text{m/s} \), and the optimal setpoint force is 609.2 nN. Similarly, we can optimize the feed rate and setpoint force to achieve minimum unit production cost. The optimization functions are shown as Equation 7.17.
Objective function:
Minimize $u = u_E + u_r$

$u_E = u_e \cdot (t_m + N_t \cdot t_c)$

$u_r = u_r \cdot N_t = u_r \cdot \frac{L_0}{S}$

\[
S = 431.1 \cdot \left( \frac{F_{set}}{1000} \right)^{0.345} \cdot \text{feed}^{-0.59} + 122.33
\]  

Constraints:
$1 \mu m/s \leq \text{feed} \leq 3 \mu m/s$

$500 \text{ nN} \leq F_{set} \leq 1500 \text{ nN}$

Using a numerical search algorithm, the optimal feed rate to minimize the unit production cost is $1.6 \mu m/s$, the optimal setpoint force is $599.9 \text{ nN}$, and the minimum production cost is $8.0 \text{ USD/pattern}$.

7.7 Chapter Summary

In this chapter, the process planning algorithm was firstly reviewed. Using this algorithm, given the designed feature dimensions, the feasible machining parameters, such as setpoint force, feed rate and XY vibration amplitude, can be provided. Secondly, different criterions to determine the tip changing frequency have been discussed, and the tip life model has been proposed and calibrated under different stop criterions. Then, the optimization model for unit production time have been developed, and the effects of machining parameters have been visualized. To test the sensitivity of the model, the values of optimal feed rate under different stop criterions and single tip changing time are calculated and visualized as a response surface. Similarly, the optimization model for unit production cost was developed, and the effects of machining parameters have been discussed. The sensitivity of this
optimization model for unit production cost was also studied under different stop criterions and tip price. Finally, a case study was presented, both process planning and optimization were performed under for designed feature dimensions and machining configurations.
CHAPTER 8 CONCLUSION

8.1 Summary

In this work, the vibration-assisted tip-based nanomachining process is systematically studied, predictive models have been developed to predictive the machined feature dimensions, dynamic cutting forces and tip wear. Process optimization is achieved based on these predictive models.

Vibration-assisted AFM tip-based nanomachining technique was developed for low-cost nanometer scale machining. To commercialize this machining process, it is essential to understand the relationship between the machined feature dimensions and the designed machining conditions. Also, from process design point of view, to achieve the desired feature dimensions, a guideline is needed to choose machining parameters. The feature width was found to be only significantly affected by the XY vibration amplitude, so we developed a simple linear regression model to predict it. For the machined feature depth, based on the ANOVA test results, several machining parameters were statistically significant in determining its value including setpoint force, XY vibration amplitude, feed rate and the interaction term between setpoint force and XY vibration amplitude. To predict the feature depth after machining, the interaction area between AFM tip and workpiece surface has been analyzed, and a numerical model was adapted to estimate the contact area between them. With this numerical model, the contact area could be calculated using machining parameters including setpoint force, XY vibration amplitude and feed rate. Then, a semi-empirical model was proposed to predict the machined feature depth using the calculated contact area and was calibrated using data collected from a factor design experiment of three machining
parameters. This semi-empirical model has been proved to be able to predict the machined feature depth with high accuracy, however, to reduce the computation time, we also build regression models as alternatives. Both the developed linear and nonlinear regression models show good accuracy for the test data. By now, we could successfully predict both feature depth and width after machining under different machining conditions. Also, if the feature dimensions are provided, we could also provide the guideline to choose the proper machining parameters.

Besides predicting the feature dimensions, during the machining process, it is also critical to estimate the cutting forces, as it will greatly impact the tool life, product accuracy, and surface finish. To study the cutting forces during machining cycles, we modified the previous numerical model to estimate the material removal rate using the feature dimensions (depth and width) predicted by the developed predictive feature dimension models. Then, a model was proposed by correlating the dynamic cutting forces with the calculated material removal rate. This model was calibrated and validated using data collected from a full factorial design experiment.

After we have built the predictive feature dimension models and dynamic cutting force model, we studied the tip wear during the machining process. To quantize the tip wear, the AFM tips were imaged using SEM at different machining stages. With more patterns machined, the tip radius became larger, and the tip became blunter. Although tip radius could be used to detect tip wear effectively, it is time-consuming and costly. To find an alternative, we investigated the correlation between tip radius and pull-off force between AFM tip and the workpiece surface. A strong correlation was found between the tip radius and pull-off forces, which indicates that the pull-off forces could be applied to detect tip wear. Using pull-
off forces as an effective, low-cost tip wear detection method, we have developed investigated tip wear regions during machining process: Three regions were identified including initial tip wear region, transition region, and tip failure region. Regression models were developed for initial tip wear region and tip failure region, then the theoretical transition point, which is defined as the point that tip starts to fail to machine clear patterns. This calculated transition point could provide us a guideline for when to change the tip.

With all these predictive models, we have a good understanding of this nanomachining process and could provide the guideline to choose machining parameters for desired feature dimensions as well as when to change the tip. However, if we implement this nanomachining process for mass production, we need to consider the overall production time and cost. To minimize the production time or cost, we have developed process optimization models, with the realistic constraints for this nanomachining process. Using the optimal operation point, we could significantly reduce the production cost or time.

8.2 Future work

This investigation presents the predictive modeling and process optimization of this vibration-assisted tip-based nanomachining process. It has been demonstrated that with these predictive models, we can successfully predict the feature dimensions, estimate the dynamic cutting forces during machining process and provide the guideline for optimal machining parameters to achieve minimum production time or cost. Further improvements in the modeling and process optimization are set forth in the following sections.
8.2.1 Real-time process monitoring

In our present machining model, we could estimate the dynamic cutting forces during the machining process, which could give me the guideline to avoid improper machining parameters. However, during the machining process, the cutting force could be extraordinarily large due to several reasons including inhomogeneity of workpiece, wrong parameter set, etc. It is critical to have a real-time process monitoring system, which could be implemented by obtaining real-time cutting forces and comparing with the calculated normal cutting forces with the set machining parameters. If the real-time cutting forces are significantly larger or smaller than the normal cutting forces, the machining process should be terminated.

8.2.2 Process simulation

In this preliminary work, we have applied semi-empirical or statistical methods to model this nanomachining process. Further work may consider using simulation methods to study the cutting forces between AFM tip and workpiece surface, predict the machined feature dimension as well as the tip wear. As both the tip and machined feature dimensions are in nanometer scale, some simulation techniques, such as Molecular Dynamic (MD) Simulation could be used. As introduced in Chapter 2, Molecular Dynamic (MD) simulation has been successfully applied to study the nanometric cutting process by simulate the interaction within the surface and subsurface layers, which could be applied to simulate our vibration-assisted tip-based nanomachining process. Using this MD simulation technique, we could accurately calculate the cutting forces during machining process, and compare with the results from our dynamic cutting force model. Also, we can investigate the machining heat using the MD simulation, which will be helpful to understand the tip wear and debris formation.
8.2.3 Process optimization for machining 3D patterns

For our process optimization model, we only considered machining simple 2D patterns. As 3D nanomachining is an important feature of this vibration-assisted tip-based nanomachining method. Future work may try to optimize the process for machining 3D patterns. Like what discussed in Chapter 7, we may consider to optimize the unit production time for 3D machining. Unlike the 2D machining, the 3D machining process has more controllable machining parameters, such as the number of machining layers and the machined depth of each layer, so the optimization function may be much more complicated. Also, the 3D machining process may have more realistic constraints due to the complex of designed 3D patterns. Similarly, the unit production cost should also be investigated, and the guidelines to select the optimal machining parameters should be provided.
REFERENCES


[78] B. Skärman, L. R. Wallenberg, S. N. Jacobsen, U. Helmersson, and C. Thelander, "Evaluation of intermittent contact mode AFM probes by HREM and using


APPENDIX
Appendix A

Figure A.1 Patterns machined by Tip 2. Tip 2 has been applied to machined 1 pattern, with 32 trenches.

Figure A.2 Patterns machined by Tip 3. Tip 3 has been applied to machined 2 patterns, and each pattern has 32 trenches.
Figure A.3 Patterns machined by Tip 4. Tip 4 has been applied to machined 4 patterns, and each pattern has 32 trenches.
Figure A.4 Patterns machined by Tip 5. Tip 5 has been applied to machined 8 patterns, and each pattern has 32 trenches.
Figure A.5 Patterns machined by Tip 6. Tip 6 has been applied to machined 12 patterns, and each pattern has 32 trenches.
Figure A.5 Continued
Figure A.6 Patterns machined by Tip 8 under 500 nN, 1 μm/s condition.

Figure A.7 Patterns machined by Tip 9 under 500 nN, 2 μm/s condition.
Figure A.8 Patterns machined by Tip 10 under 500 nN, 3 μm/s condition.
Figure A.9 Patterns machined by Tip 11 under 1000 nN, 1 μm/s condition.
Figure A.10 Patterns machined by Tip 12 under 1000 nN, 3 μm/s condition.
Figure A.11 Patterns machined by Tip 13 under 1500 nN, 1 μm/s condition.
Figure A.12 Patterns machined by Tip 14 under 1500 nN, 2 μm/s condition.
Figure A.13 Patterns machined by Tip 15 under 1500 nN, 3 μm/s condition.
Figure A.14 Measured pull-off forces during machining process under different machining conditions. The measured pull-off increases with more patterns machined. However, the rates of change of pull-off forces are larger with larger setpoint force or feed rate.
Figure A.14 Continued

1000 nN, 1 \( \mu \)m/s

1000 nN, 2 \( \mu \)m/s

1000 nN, 3 \( \mu \)m/s

Patterns machined

Pull-off force/ nN

Patterns machined

Figure A.14 Continued
Figure A.14 Continued

1500 nN, 1 \( \mu \text{m/s} \)

1500 nN, 2 \( \mu \text{m/s} \)

1500 nN, 3 \( \mu \text{m/s} \)
Figure A.15 Measured feature depth during machining process under different machining conditions. With more patterns machined, the measured depth decreased, which indicates the tip became blunter. However, the values of decrease rate are different machining conditions.
Figure A.15 Continued
Figure A.15 Continued

- (g) 1500 nN, 1 μm/s
- (h) 1500 nN, 2 μm/s
- (i) 1500 nN, 3 μm/s
Figure A.16 Different tip wear regions during machining process. The yellow lines divide the tip wear process into three different regions, including 1. The initial tip wear region, which occurs during the first few patterns. 2. The transition region, which is the region when the machined feature depth rapidly decreased, the pull-off force quickly increased. 3. Tip failure region, which is the region when the tip could not machine patterns under the given machining condition. As we can see, with larger setpoint force, more patterns were machined during the initial tip wear region, which indicates larger setpoint force could raise the limit of maximum patterns could be machined of the AFM tip.
Figure A.16 Continued
Figure A.17 The global fitting lines and local fitting lines for pull-off force during the initial tip wear region. The green lines represent the global fitting lines, and its function is shown as Equation 6.1, which was fitted using all the data during the initial tip wear region. The red lines are the local fitting lines, which are fitted using the data during the initial tip wear region for each machining condition. The functions of local fitted lines are listed in the figure, and their slopes represent the rate of change of pull-off force under each machining condition, which are plotted in Figure 6.13 as the response surface under different machining conditions. The intercepts of these functions represent the values of initial pull-off forces (before machining) for each tip.
Figure A.17 Continued

1000 nN, 1 μm/s

\[ A = 0.0209 \times \text{linear} + 34.1667 \]  

1000 nN, 2 μm/s

\[ A = 0.0289 \times \text{linear} + 33.6147 \]  

1000 nN, 3 μm/s

\[ A = 0.0382 \times \text{linear} + 33.3200 \]  

1500 nN, 1 μm/s

\[ A = 0.0691 \times \text{linear} + 18.8227 \]
Figure A.17 Continued

- **1500 nN, 2 μm/s**
  
  \[ A = 0.0755 \times \text{linear} + 21.9179 \]  
  
  - **1500 nN, 3 μm/s**
  
  \[ A = 0.0819 \times \text{linear} + 24.6855 \]
Figure A.18 Pull-off forces during the tip failure region. The red lines are local fitted lines, which are determined by the points under each machining condition. The green lines are global fitted lines, which are determined by the points under all machining conditions during the tip failure region.
Figure A.18 Continued

1000 nN, 1 μm/s

(d)

A = 0.0623*linear - 70.0190

Machined linear distance/ nm

1000 nN, 2 μm/s

(e)

A = 0.1123*linear - 110.7573

Machined linear distance/ nm

1000 nN, 3 μm/s

(f)

A = 0.1379*linear - 176.7200

Machined linear distance/ nm

1500 nN, 1 μm/s

(g)

A = 0.1528*linear - 170.9476

Machined linear distance/ nm

Figure A.18 Continued
Figure A.18 Continued

(h) 1500 nN, 2 μm/s

A = 0.1971 * linear - 266.2679

(i) 1500 nN, 3 μm/s

A = 0.2519 * linear - 377.6201
Figure A.19 The boxes represent the measured pull-off forces, the red solid lines represent the fitting lines for the initial tip wear region, the green lines represent the fitting lines for the tip failure region. Red dash lines are the extension of red solid lines, and green dash lines are the extension of green solid lines. The yellow dots represent the transition region estimated by the cross points of the red dash lines and green dash lines. The blue dots represent the estimated transition point by transition point model.
Figure A.19 Continued
Appendix B

To study the pull-off forces during tip wear process, the AFM tip was moved to clean silicon wafer surface right after machining each pattern, and the pull-off force was measured 5 times using the Indentation mode of AFM. The measured pull-off forces under 9 different machining conditions are plotted in Figure 6.8, and recorded in Table B.1 to Table B.9 separately. The first row of the table shows the number of patterns machined before measuring the corresponding pull-off forces. If the number of patterns machined is shown as “0”, it means the corresponding pull-off forces were measured for a new tip.

Table B.1 Measured Pull-off forces (nN) under 500 nN, 1 μm/s.

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Table B.2 Measured Pull-off forces (nN) under 500 nN, 2 μm/s.

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Table B.3 Measured Pull-off forces (nN) under 500 nN, 3 μm/s.

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### Table B.4 Measured Pull-off forces (nN) under 1000 nN, 1 μm/s

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|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| M1| 19 | 33 | 45 | 52 | 54 | 62 | 56 | 60 | 67 | 69 | 71 | 73 | 76 | 81 |
| M2| 21 | 27 | 38 | 46 | 53 | 56 | 55 | 62 | 62 | 68 | 70 | 74 | 74 | 80 |
| M3| 22 | 30 | 40 | 46 | 54 | 54 | 57 | 65 | 60 | 67 | 73 | 70 | 75 | 82 |
| M4| 18 | 33 | 44 | 51 | 57 | 60 | 52 | 67 | 62 | 66 | 67 | 72 | 74 | 81 |
| M5| 22 | 27 | 47 | 52 | 58 | 69 | 64 | 67 | 82 | 82 | 86 | 82 | 86 | 86 |

### Table B.5 Measured Pull-off forces (nN) under 1000 nN, 2 μm/s

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### Table B.6 Measured Pull-off forces (nN) under 1000 nN, 3 μm/s

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Table B.7 Measured Pull-off forces (nN) under 1500 nN, 1 μm/s

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Table B.8 Measured Pull-off forces (nN) under 1500 nN, 2 μm/s

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157
To measure the depth of machined patterns, we evenly selected 6 out of 32 trenches, and the depth was measured at 5 different locations for each trench. The value of average depth is calculated by averaging all the measured data for each pattern. The average depth under different machining conditions are plotted in Figure 6.10 and recorded in Table B.10 to Table B.18 separately.

Table B.9 Measured Pull-off forces (nN) under 1500 nN, 3 μm/s

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Table B.10 Measured average feature depth (nm) under 500 nN, 1 μm/s

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To measure the depth of machined patterns, we evenly selected 6 out of 32 trenches, and the depth was measured at 5 different locations for each trench. The value of average depth is calculated by averaging all the measured data for each pattern. The average depth under different machining conditions are plotted in Figure 6.10 and recorded in Table B.10 to Table B.18 separately.
Table B.11 Measured average feature depth (nm) under 500 nN, 2 μm/s

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Table B.12 Measured average feature depth (nm) under 500 nN, 3 μm/s

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Table B.13 Measured average feature depth (nm) under 1000 nN, 1 μm/s

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Table B.14 Measured average feature depth (nm) under 1000 nN, 2 μm/s

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Table B.15 Measured average feature depth (nm) under 1000 nN, 3 μm/s

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159
### Table B.16 Measured average feature depth (nm) under 1500 nN, 1 μm/s

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### Table B.17 Measured average feature depth (nm) under 1500 nN, 2 μm/s

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