Predictive Modeling of Feature Dimension for Tip-based Nano Machining Process

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Abstract

The tip-based vibration-assisted nanomachining process can fabricate three-dimensional (3D) features with nanometer scale resolution. To control the feature dimension accurately in process planning, we need to understand the relationship between feature dimension and machining parameters including setpoint force, XY vibration amplitude and feed rate. In this article, we conducted full factorial experiments to analyze the relationship between feature dimension and machining parameters. Based on Analysis Of Variance (ANOVA), we determined the significant factors in determining the feature dimension. The feature width is mainly controlled by XY vibration amplitude, and the feature depth is controlled by XY vibration, setpoint force and feed rate. In order to predict the feature dimension in nanomachining and provide instructions for machining parameter selection, a semi-empirical mechanical model was built first. Then simplified regression models were also investigated, with all models displaying good predictive capability. The results show good fit between predicted feature depth and measured feature depth, for most machining conditions. These models provide good capability in process planning for implementation of this process.

Keywords: Nanofabrication, Tip-based nano machining, modeling of feature dimension

1 Introduction

Machining process modeling have been heavily studied in conventional scale, with many of these studies examining the modeling of cutting force and the prediction of the feature dimension after machining. Researches on modeling of dynamic metal cutting process is summarized[1], mechanical modeling approach has been used to predict the cutting force for the ball end milling process[2]. Cutting force models have been used to increase the material removal rate[3], and mechanistic methods have been widely applied for the force predictions and prediction of the associated tool deflections[4] and surface geometrical errors[5].

Besides mechanical modeling, simulation methods have also been used in the study of machining process. A surface topography simulation was studied to simulate the finish profile generated after a turning operation [6]. Finite element (FE) simulations were applied to analyze the orthogonal cutting process [7]. Predictions of machining induced microhardness and grain size are performed by using 3D finite element (FE) simulations of machining and machine learning models, which have been adapted to predict machining induced microhardness and grain size [8]. Finite element simulation has been applied to predict cutting force, tool stress and temperature in high-speed flat end milling [9]. Cutting force and chip formation under different tool edge geometry in the orthogonal machining process was analyzed with finite element method [10].

Statistical modeling approach has also been widely used to study the machining processes. Statistical models and artificial neural networks have been compared for predicting tool wear in hard machining [11]. Optimal cutting conditions for surface roughness were investigated using response surface methodology [12]. Cutting conditions for the hard turning process was optimized using Analysis Of Variance (ANOVA) and experimental design methods [13].

Processing modeling at nanometer scale is very difficult, due to the complex physics involved in the process. Molecular dynamic simulation is a useful method to study the machining process from the perspective of molecular responses to the process input. At the nanometer scale, the nanomachining of copper was simulated with molecular dynamics method [14]. Molecular dynamics simulation was also used to study the chip formation process during nanomachining [15], while this method can give predictive results for feature dimension after machining, it is computationally intensive and time consuming, which limits its application to relatively simple process. Experimental modeling has also been applied for nanomachining process. The effect of major scratching parameters on the nano structure were studied to estimate the force needed to scratch features with desired dimensions [16].

In this research, feature dimension prediction models of tip-based nanomachining process are developed and validated. We first use Analysis of Variance (ANOVA) method to determine statistically significant factors that influence feature dimensions, and then built a semi-empirical model to describe the relationship between feature dimension and machining parameters. Then simpler linear and nonlinear regression models were built to be compared with semi-empirical model. The effectiveness of these models were verified using experimental data.

2 Machining Setup and Experimental Design

2.1 Machining Setup

Figure 1. Experimental setup. (a) The vibration assisted tip-based nano machining system. The AFM system was customized, and signal feedback system was added. (b) Schematic illustration of tip movement in the XY plane. (c) The top view of machining process.

The experimental setup includes a commercial AFM, Park XE-70(Park Systems Corp®), and a customized nano-vibration system, as shown in Figure 1(a). The detailed description of the nanovibrator has been previously reported [17]. The Signal Access Module from the Park Systems obtain the normal and lateral forces during nanomachining process, which are measured by cantilever deflection and torsion from the photo detector. The machining force measured from cantilever deflection and torsion are acquired by LabVIEW during machining through a data acquisition device (NI USB-6259), which is also used to generate a synchronized sinusoid signal with 90° phase difference to control the vibration of xy-piezoactuators as shown in Figure 1. A tapping mode cantilever with a nominal stiffness of 48 N/m and resonant frequency of 190 kHz is used in this study. The sample is mounted on the top of the nanovibrator, which is vibrated in the XY plane with the frequency of 2 KHz. In our experiment, vibration-assisted nano machining is applied to (PMMA) film. The PMMA film (950PMMA A4 as a 2% dilution in anisole) is spin-coated on a cleaned silicon substrate for 40s at 4000 RPM, and baked at 180°C for 90 s. The thickness of PMMA is 40nm and the machinable area is 2 μm × 2 μm .

During the machining process, the force applied by the tip to the sample is determined by setpoint force of the AFM, which corresponds to the deflection of cantilever. The larger setpoint force induces the larger interaction force between AFM tip and sample surface, which will produce the larger feature depth. As shown in Figure 1 (b), the sample was actuated by the nanovibrator to provide a XY in-plane vibration, thus the width of the feature is regulated by XY vibration amplitude. With high frequency circular xy-vibration, only a thin slice of material is removed in one machining cycle, which greatly enhances the machining speed and reduces tip-sample interaction force. Diameter of the virtual tool is controlled by the xy-vibration amplitude, which directly regulates the feature width that can be machined in one single machining path. Feed rate is the relative velocity of the AFM tip in the direction of machining. With larger feed rate, the AFM tip moves faster on the sample surface, and more material (feed per rotation) is removed in a revolution. The purpose of this study is to determine the relationship between feature size and machining inputs parameters.

2.2 Experimental Design

To fully understand the relationship between feature dimension and machining input parameters, a full factorial design was developed. The machining input parameters includes the setpoint force, the XY vibration amplitude and feed rate. From our preliminary experiments, we determined the feasible range of each parameter to machine an observable feature. For each input parameter, we set three different values corresponding to low, medium and high values of the parameter, yielding a 3^3 full factorial design. The full experimental design is given in Table 1 below. The machined features are scanned with the same AFM, and for each feature, we measure 10 times from randomly selected positions, with the mean values used for our analysis.

Table 1. Full factorial 3^3 experimental design

Factor	Levels
Setpoint force (nN)	120, 140, 160
XY vibration amplitude (mV)	35, 50, 65
Feed rate ($\mu\text{m/s}$)	0.6, 1.0, 1.4

3 Analysis of Feature Width

Based on the mechanism of the process, we anticipate that XY vibration will predominantly affect the feature width. In this study, ANOVA was used to determine if other process variables also affect the feature width. The analysis (Table 2) showed that XY vibration alone determines feature width with a level of significance that exceeds 0.0001. The feature width is plotted as a function of XY vibration amplitude in Figure 2 with error bars. The standard deviation is 0.83, indicating that the process width can be carefully controlled.

Table 2. Significance test for feature width

Sources	Setpoint force	XY vibration amplitude	Feed rate	Setpoint force*Feed rate	Setpoint force *XY vibration amplitude	XY vibration amplitude*Feed rate	Setpoint force*XY vibration amplitude*Feed rate
Prob>F	0.99	<0.0001	0.4436	0.8075	0.2013	0.5638	0.3214

Figure 2. The relationship between feature width and XY vibration amplitude (35 mV, 50 mV and 65 mV)

4 Analysis of Feature Depth

The control and prediction of feature depth is more complicated than feature width. Setpoint force will directly affect the machined feature depth, while the feedrate and xy-vibration amplitude will change the tip-sample interaction, thus also affect the resulting feature depth. We studied the effect of process parameters to feature depth experimentally. For all 27 experiments designed in Section 2.2, the trench features were machined and the feature depth was measured in 10 random locations. The mean of the depths measured is shown in Table 3.

Table 3. Measured feature depth for all machining conditions

Sequence number	Setpoint force/ nN	XY vibration amplitude/ mV	Feed rate/ $\mu\text{m/s}$	Depth/ nm
1	120	35	0.6	5.3
2	120	35	1	4.8
3	120	35	1.4	3.3
4	160	35	0.6	10.3
5	160	35	1	8.9
6	160	35	1.4	6.5
7	200	35	0.6	14.5
8	200	35	1	10.7
9	200	35	1.4	8.2
10	120	50	0.6	7.1
11	120	50	1	7.6
12	120	50	1.4	14.6
13	160	50	0.6	11.2
14	160	50	1	11.2

15	160	50	1.4	10.3
16	200	50	0.6	18.2
17	200	50	1	18.4
18	200	50	1.4	13.9
19	120	65	0.6	8
20	120	65	1	9.4
21	120	65	1.4	7
22	160	65	0.6	15.9
23	160	65	1	13.8
24	160	65	1.4	13.2
25	200	65	0.6	18.6
26	200	65	1	17.5
27	200	65	1.4	15.3

Figure 3. Feature machined under different setpoint force and feed rate with 35 mV XY vibration amplitude: (a) features for sequence numbers 1-9, (b) depth of each feature, and (c) relationship between setpoint force and depth at different feedrate.

The AFM images of features after machining are shown in Figures 3 to 5 below. For each feature, we show the AFM image as well as a sample scan of depth, and a plot of depth as a function of setpoint force and feed rate. Figure 3 (a) shows feature machined under different setpoint forces and feed rates with 35 mV XY vibrato in amplitude. Figure 3 (b) shows the corresponding depth at each condition. Figure 3 (c) shows the feature depth are significantly affected by machining conditions of setpoint forces and feed rates. Larger depths are achieved by increasing the setpoint force or decreasing

Figure 4. Feature machined under different setpoint force and feed rate with 50 mV (a-c) and 65 mV (d-f) XY vibration amplitude: (a, d) machined features for sequence numbers 10-27, (b, e) depth of each feature, and (c, f) relationship between setpoint force and depth.

the feed rate.

Figure 4 and Figure 5 demonstrate the machined feature at different setpoint force and feed rate with 50mV and 65mV XY vibration amplitude respectively. Similarly, the feature depth are controlled by machining parameters of setpoint forces and feed rates. Larger depths are achieved by increasing the setpoint force or decreasing the feed rate.

Figures 3 and 4 show the effect of setpoint force, feed rate and XY vibration amplitude on the machined feature depth. A statistical analysis was performed to evaluate the significance of these parameters in controlling feature depth. The p-value was calculated using JMP software. A linear model of the three factors and their cross terms yields an R^2 of 0.94, indicating a strong correlation between the depth and these three factors and their cross terms. Further analysis shows that all main effects and the interaction between setpoint force and feed rate are significant (e.g. $p < 0.05$) in the linear regression model. Table 4 shows the test of significance for each source of variability. The analysis of the effect of the process variables on feature width and depth now provides a framework for basic process understanding, process modeling, and future process planning.

Table 4. Effect of significance test for feature depth

Source	Prob>F
Setpoint force	<0.0001
XY Vibration	<0.0001
Feed rate	0.0001
Setpoint force*Feed rate	0.021
Setpoint force*XY Vibration	0.1446
XY Vibration*Feed rate	0.2879
Setpoint force*XY Vibration*Feed rate	0.5799

5 Prediction Models for Feature Dimension

Previous analysis finds the significant factors in determining the feature depth. In order to predict the feature depth accurately for nanomachining under given machining parameters or to provide guidelines for selecting machining parameters to achieve the desired feature depth, we need a quantitative model to describe the relationship between feature depth and significant machining parameters. Based on research on modeling of direct scratch process with AFM tip, the interaction force between AFM tip and sample is usually correlated with their contact area [16]. For our nanomachining process, we try to develop a semi-empirical model to correlate the feature depth with the tip-sample contact area and applied force, and then use experimental data to calibrate the model. This semi-empirical model takes the mechanism of tip-based nanomachining process in consideration, and shows good prediction capability of feature depth. As the semi-empirical model is relatively complex to implement and time-consuming, we developed regression models to correlate feature depth with machining parameters, which also demonstrate good prediction capability.

5.1 Semi-empirical Model for Feature Depth Prediction

In this study, we tried to understand and model the effect of process parameters on the machined feature dimension. It is well known from the indentation process that applied force is related to the contact area of the sample and the indenter. If the geometry of the indenter is known, the depth of the indentation can be correlated to the applied force. 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 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 we proposed a model structure considering the machining mechanism, and identify the model coefficients through experiments. Further experiments were performed to validate the results from the semi-empirical model,

In nano-indentation and nano-scratching, 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. The threshold contact force F_{tc} can be considered as the minimum applied normal force 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: $\frac{1}{E_c} = \frac{1-\nu_t^2}{E_t} + \frac{1-\nu_s^2}{E_s}$, here E_t , ν_t and E_s , ν_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 (Carpick, 1997), the relationship between contact area and applied force can be derived as:

$$\sigma_c = 1.5 \frac{F_c}{A_c}, \text{ and } F_c = \frac{2\sigma_c A_c}{3} = \frac{4\pi^3 R^2 \sigma_c^3}{3E_c^2} \quad (1)$$

As observed from Equation 1, 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 directly scratch process for polymer films like PGMA [18]. In our vibration-assisted nanomachining process, the geometry of tip-sample contact is very complicated, which is related to both depth and width of the machined features. Inspired by the force model for the indentation and nano-scratching process, a similar model structure can be developed for our nanomachining process as:

$$F_{set} = k \frac{A_c^m}{V_{xy}^n} - b \quad (2)$$

$$A_c = A(\text{Depth}, \text{width}) \quad (3)$$

In this mode, the tip-sample contact area is related to the applied force on the tip with power terms m and n , and coefficients k and b . Since the force and the contact area are directly related to the vibrational amplitude of the tip (V_{xy}), we specifically put this factor in the model. The tip-sample contact area is a nonlinear function of feature depth and width, as shown in Eq. 3. If the coefficients can be identified properly, Equation 2 and 3 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 2 and 3. We can start with a trial value of feature depth, then the contact area can be calculated from Eq. 3 and setpoint force can be derived from Eq. 2. If the derived setpoint force is different 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.

For Equation 3, it is difficult to express the tip-sample contact area analytically from the feature depth and width. A numerical method was developed to estimate the contact area between the tip and the sample [19]. We first discretized the AFM tip and the sample nearby into voxels, and found the contact area between AFM tip and sample surface for each angle of the tip rotation, as described in our previous work [19]. The contact area is a single layer of voxels between AFM tip and sample surface. If the dimension of each voxel is small enough, the contact area between one voxel and the sample surface is very close to the area of side surface of this voxel, so the total contact area between AFM tip

Figure 5. (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.

and sample surface can be estimated by calculating the sum of side surface area of all contacted voxels.

The power terms m and n , and coefficients k and b in the semi-empirical model shown in Eq. 2 can be optimally fitted from experiments. From the experiments as shown in Figure 3 and 4, for each machining test, the feature depth and width for each given setpoint force and XY-vibration amplitude were measured by AFM. Using these 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 2 and 3. The final model is given as:

$$F_{set} = 58.86 \frac{A_c^{0.56}}{V_{xy}^{0.51}} + 47.7 \quad (4)$$

With the fitted semi-empirical model by Equation 4, the feature depth can be calculated for a given setpoint force by Newtonian Iteration Method by combining Equations 3 and 4, as discussed before. Using this method, we plot the predicted and measured feature depth and the relative prediction error in Figure 5. In general, good model prediction can be obtained. The maximum relative error is about $\pm 20\%$. 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.

5.2 Regression Models for Feature Depth Prediction

The semi-empirical model can give very good prediction of the feature depth. However, it is computationally intensive and relatively complex to implement for process planning. Therefore, we also studied the regression models for fast, efficient feature depth estimation. The regression models were built to reflect the impact of setpoint force, XY vibration amplitude, and feed rate on the machined feature dimensions. Linear and non-linear regression models were explored.

From the analysis of Table 4, all the process parameters (i.e. setpoint force, XY vibration amplitude, and feed rate) and the interaction 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 5:

$$\text{Depth} = -9.49 + 0.101 * F_{set} + 0.17 * V_{xy} - 4.13 * \text{Feed} - 0.07 * (F_{set} - 160) * (\text{Feed} - 1) \quad (5)$$

The R^2 for the linear model is 0.9245, indicating a very good fit. The results from model prediction and the experimental results are shown in Figure 6 (with the red dots are the predicted depth,

Figure 6. (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.

the blue dots are measured depth, and sequence number is the number of trench corresponding to Table 3). For most machining conditions, the depths from the model prediction fit very well to the measured ones with relative error mostly below 20%. Considering the large process variability and the measurement error in nanometer scale, the linear model also provides good prediction of feature dimensions.

The linear model provides a good fit without considering much physical meaning of the process. From our understanding of the tip-based nano machining 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 3 and Figure 3-4, the feature depth increases with setpoint force and XY vibration amplitude, and decreases with larger feed rate. We select a nonlinear expression to describe this relationship as shown in as Equation 6:

$$D_p = k_1 \frac{F_{set}^a * V_{xy}^b}{Feed^c} \quad (6)$$

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

Figure 7. (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.

Figure 8. (a) The measured depth (blue) and predicted depth (red) of the semi-empirical model for experiments from the verification group. (b) The relative error of the model prediction.

decreases with the increasing of feed rate.

Using the least square method, we determine all the parameters k_1 and a, b, c in the equation 7:

$$Depth = 0.000126 \frac{F_{set}^{1.576} * V_{xy}^{0.857}}{Feed^{0.348}} \quad (7)$$

The results from nonlinear model prediction and the experimental results are shown in Figure 7 (with the red dots are the predicted depth, the blue dots are measured depth, and sequence number is the number of trench corresponding to Table 3). For most machining conditions, the depths from the nonlinear model fit very well to the measured ones with relative error mostly below 20%.

5.3 Model Verification and Comparison

The previous results from three different models (the semi-empirical model and regression models) show good fitting between the model and experiments. 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 $\mu\text{m/s}$ to 1.3 $\mu\text{m/s}$) to test and compare the effectiveness of three models. For the semi-empirical model, we plotted the predicted depth and experimentally measured depth in Figure 8 (a), and the relative error between the model prediction and experimental results in Figure 8 (b). The values of predicted depth from the semi-empirical model are very close to the experimentally measured depth from the verification group. Under most machining conditions, the relative error is below $\pm 20\%$. These linear and nonlinear regression models also give the similar prediction capability for the verification experimental results.

The three different models were compared by calculating their corresponding root of mean square error (RMSE) as shown in Table 5. From Table 5, we can find that all three models have a relatively small RMSE and provide good prediction capability. Further refinement of the semi-empirical mechanical model and numerical methods for contact area estimation should further decrease the RMSE. 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 sample surface. This can be the reason that linear regression model provides similar prediction to the nonlinear model. For the nonlinear model, the format is easy to understand and, the relationships between machining parameters and feature depth are clearly shown. Both linear and nonlinear model are computationally efficient and very easy to be implemented in process planning.

Table 5. RMSE for all of three predictive models

	Linear statistical model	Nonlinear statistical model	Semi-empirical mechanical model
RMSE	0.151	0.153	0.159

6. Conclusions

In this paper, we have investigated the relationship between feature dimension (width and depth) with respect to the machining parameters (setpoint force, XY vibration amplitude and feed rate) for the tip-based vibration-assisted nanomachining process. Experiments with different machining conditions were conducted, and the results were analyzed using statistical methods to determine the significant factors. Feature width was predominately affected by XY vibration amplitude while feature depth was affected by setpoint force, XY vibration amplitude and feed rate. A semi-empirical model was developed to describe the relationship between feature depth and setpoint force as well as XY vibration amplitude. Both linear and nonlinear regression models were developed to correlate feature depth with machining parameters. All the models show good fit between predicted feature depth and measured feature depth for most machining conditions, which provide good potentials in process planning for implementation of the nanomachining process.

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