中國機械工程學刊第四十二卷第五期第 439~449 頁(民國一百一十年)
Journal of the Chinese Society of Mechanical Engineers, Vol.42, No.5, pp. 439~449 (2021)

Estimation Method and Experimental Verification of the Least Cutting Passes for Fabrication of a Nanochannel Trapezium Groove on Single-Crystal Silicon with Changed Downward Force at a Fixed Cutting Depth

Zone-Ching Lin*, Shih-Hung Ma** and Zhi-Rong Chen**

Keywords: atomic force microscope (AFM), silicon expected depth, nanochannel, least cutting passes

ABSTRACT

Employing the concept of specific down force energy (SDFE), the paper establishes a method to estimate the least cutting passes for optimal step-by-step approximation to objective convergence function of the expected depth of nanochannel trapezium groove. This method is a two cutting passes offset fabrication method. For this method, a fixed downward force is set at the 1st cutting pass on each cutting layer is set to use. At the 2nd cutting pass, downward force is changed to achieve the same cutting depth as the one at the first cutting pass. Through simulated change of offset amount, the protruding height on the bottom of groove is smaller than the set convergence value. Then, regulating the downward force repeatedly can make the protruding height on botton of groove meet the range of convergence value being below 0.54nm as set by the paper. When a real AFM machine changes the downward force, additional time and efforts have to be spent on changing the downward force. But this paper, for acquisition of the least fabrication lead time during actual application, applies SDFE theoretical model to further estimate the least cutting passes for reaching the expected depth of nanochannel trapezium groove. This method not only can estimate the least cutting passes, but also can make the number of changes of downward force become the least. Finally, the paper even conducts experiments for verification, proving that the above method can really make the fabrication lead time become the least.

Paper Received March, 2021. Revised June, 2021. Accepted August, 2021. Author for Correspondence: Zone-Ching Lin.

* *Professor, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan. email: zclin@mail.ntust.edu.tw.*

** *Graduated Student, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan. email: m10603217@mail.ntust.edu.tw m10903240@mail.ntust.edu.tw*

*** *Graduated Student, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: m10603217@mail.ntust.edu.tw*

INTRODUCTION

Atomic force microscope (AFM), invented by G. Bining et al. (1986), is a kind of scanning probe microscope (SPM) commonly applied to measurement and observation of the surface morphology of conductors and non-conductors. Therefore, many scholars successively studied the measurement and application of AFM. Nanjo et al. (2003) considered the sharp tip of TM-AFM probe as a perfect sphere to carry out simulated small-sphere scanning on an ideal plate under a fixed setpoint value. Lüben et al. (2004) saw probe tip as a perfect sphere, and used contact mode AFM to explore the probe deflection and vertical pressure on a quartz plate.

Nevertheless, using one-pass cutting seldom can exactly reach the desired cutting depth in practical fabrication. But using multi-pass cutting can reach the desired fabrication depth through step-by-step increase of the cut and removed volume of the workpiece. Therefore, in manufacturing industry multi-pass fabrication has been generally applied more extensively. However, in the process of multi-pass fabrication, if action force and the number of passes are inappropriately selected, fabrication time will be increased, and the fabrication depth will exceed the desired depth. Therefore, a suitable downward force of cutting and a suitable number of cutting passes are the important parameters of multi-pass fabrication. As to the studies about optimization methods of multi-pass fabrication parameters, Chen et al. (1996) considered the cutting depth of each cutting pass the same. Therefore, they divided the desired target depth by the cutting depth of each pass to achieve the desired number of cutting passes. Shunmugam et al. (2000) uses an optimization method of genetic algorithm approach to find the optimal number of fabrication passes. Satishkumar et al. (2006) studied the use of non-conventional optimization technologies, including genetic algorithm approach, simulated annealing and ant colony optimization, to solve the algorithmic problem of the optimal sub-division of the depth of cut for multi-pass cutting. Li et al. (2014) used CNC lathe to regulate the machine parameters, and further save the energy consumption and shorten the fabrication time of machine. Geng et al. (2013) established a mathematical model to predict the depth of AFM nanochannel trapezium groove. Keith et al. (2010) used 5-axis micro-tool machine and micro-probe for fabrication of scratches and analysis of the wearing of probe.

Nevertheless, none of the above literatures mentioned the use of different optimization algorithms, as proposed by this paper, to explore the problem of machining parameter optimization of multi-pass fabrication. Under the related constraints, step-by-step regulation of parameters is employed to develop an innovative method by approximating the objective function and calculate the least cutting passes for reaching the objective cutting depth for nanoscale multi-pass cutting.

EXPERIMENTAL EQUIPMENT AND SPECIFIC DOWN FORCE ENERGY AND EXPERIMENTAL METHOD

Introduction of Experimental Equipment

The AFM machine used in the study is Veeco Instruments Inc.'s AFM at Dimension 3100 (D3100), which is equipped at the laboratory of Tungnan University; and the material used in the paper's experiments is single-crystal silicon substrate with diameter 2 inches and thickness 254-304μm, which was provided by Ample Gola International Co., Ltd. The paper uses AFM's diamond-coated probe as a tool for the cutting experiment of straight-line groove on single-crystal silicon substrate and for observation. The paper also uses AFM equipment to carry out nanocutting fabrication and measurement of surface morphology before and after fabrication.

The probe used in experiments is the diamond-coated DT-NCHR probe produced by NanoSensors Inc. The thickness of its diamond coating is around 100nm, and the probe tip is like a semi-sphere with a spherical radius of around 150nm. Therefore, when this probe is used for fabrication of silicon wafer, the probe tip is just like a semispherical cutting tool. The spring constant of the probe provided by the manufacturer is 42 N/m, and its resonance frequency is 320 kHz. In order to obtain a more accurate spring constant k_r of probe, the paper firstly uses a computer-scanned AFM of tapping mode to find the actual resonance frequency f_r of probe for experiments. As known from the natural frequency equation $f^2= k/m$ in the mechanics of vibration, the square of resonance frequency of probe is positively proportional to the spring constant of the probe cantilever, with $k_r = (f_r^2 \times k_v)/f_v^2$. The actual spring constant k_r of probe in the experiments of the paper can be obtained from the resonance frequency f_v and spring constant k_v of probe provided by the manufacturer, as well as the actually measured resonance frequency f_r.

Measurement Method of The Downward Force of AFM Probe

In order to accurately measure the downward force during nanofabrication, the paper applies the measurement method of downward force in AFM contact mode. For the nanofabrication way by AFM of contact mode, the probe firstly presses down into the workpiece. Right now the probe will have deflection. Therefore, downward force is produced in Z axial direction between the probe and the sample. After that, the paper controls the probe to move on the XY plane, and nanofabrication can thus be produced. Focusing on the measurement way of downward force of probe onto the workpiece to be fabricated, the paper uses force-distance curve for measurement. The force-distance curve explains the relationship between the setpoint value and offset amount of the probe cantilever.

According to the description on Dimension 3100 Manual printed by Veeco Digital Instruments Inc. (2000) through change of setting of the setpoint value, the feedback loop kept by the cantilever deflection voltage can be regulated. Under the force calibration mode, the parameter of setpoint is defined as a horizontal midline in the force-distance diagram. Changing the setpoint value would also make the force-distance curve in the diagram move up and down on the plane. This is because the horizontal midline in the diagram would always be equal to the setpoint value.

Therefore, the measurement method of downward force is to let the probe move to and fro on the sample in vertical direction for one time, and then keep the record of relationship between the offset amount of probe and the displacement of Z axis, with the distance from A to D corresponds to lowering of the probe, and the distance from D to F corresponds to lifting of the probe. The setpoint value set for scanning intersects at point D on the force-distance curve.

When the probe of AFM takes contact mode to carry out nanocutting fabrication, the probe would, according to the set setpoint value, make the probe cantilever take a fixed deflection amount to produce a fixed downward force to press down into the workpiece in Z axial direction. Then, after controlling the probe's straight-line movement on XY plane, nanocutting fabrication can be produced. The size of downward force during nanocutting fabrication is set by different setpoint values of AFM machine. Therefore, the paper intends to find the relationship between the setpoint value and the positive downward force of AFM probe on single-crystal silicon substrate. To find it out, the paper, before experiment is performed, firstly sets different setpoint values for the AFM machine of contact model, and the offset amount (*d*) of the probe cantilever measured by different setpoint values. Then, the paper substitute the offset amount of the probe cantilever in equation (1) in order to find the corresponding downward force value of this setpoint. The distance from point D to point F is *d* (nm). The distance *d* is just the offset amount of the cantilever when the probe bears positive downward force. After the distance *d* multiplies the positive elasticity coefficient k_r of the probe, the downward force F_d can be obtained as follows:

$$F_d=k_r d \quad (1)$$

Experiment and Calculation of SDFE Value of Single-Crystal Silicon

The paper considers that in the actual nanofabrication process, the workpiece bears sufficient downward force from the cutting tool of AFM probe, which presses downward to the workpiece and produces downward force energy to carry out fabrication of cutting. For the mechanism that the workpiece is fabricated, the atomic particles are moved and removed; and this is a model of volume change. Therefore, in order to meet the physical phenomenon more closely, the paper uses the concept of specific down force energy (SDFE) to predict the cutting depth of cutting pass on different cutting layers at a fixed downward force.

Therefore, the SDFE in this paper is defined as follows: Let the downward force of applied by the cutting tool of probe onto the cutted workpiece multiply the power of the increased cutting depth to produce energy; and then divide such energy by the volume removed from workpiece by the cutting tool of probe due to downward force, resulting the SDFE. The equation of SDFE is shown in equation (2) [Lin and Hsu, 2012]

$$\text{SDFE(specific down force energy)} = \frac{F_d \times \Delta d_n}{\Delta V_n} \quad (2)$$

Here, F_d denotes the downward force applied by cutting tool onto the workpiece; Δd_n denotes the increased cutting depth at the n^{th} cutting pass; and ΔV_n denotes the volume removed from the workpiece at the n^{th} cutting pass. Since the volume removed from the workpiece by downward force changes with the increase of cutting depth, ΔV_n is the function of cutting depth Δd_n.

The paper supposes that with the same workpiece material at different downward forces and different cutting passes, the SDFE value of nanoscale cutting inclines to be a fixed value. Besides, since the AFM probe tip is like a semispherical cutting tool, the volume removed from the workpiece by cutting tool at the 1st cutting pass can be obtained by the geometric equation of sphere.

The cutting at each cutting pass is just like a semispherical cutting tool pressing into the workpiece to carry out straight-line moving and fabrication. As observed from the cross-section morphology of groove depth in cutting direction after the cutting experiment, the cutting tool of probe initially presses into a shallower depth (d_i). As the cutting tool moves, the cutting depth gradually increases from a shallow depth to a fixed value (d_1) in the middle area. The removed volume also increases with the deepening of the cutting depth. This phenomenon is the same as the model simulated by the paper using a solid model being actually constructed by CATIA CAD software. Therefore, the way that the paper measures and calculates the average cutting depth, and takes the position of middle area of the fabricated groove as the cutting depth, meets the actual cutting situation.

Therefore, the downward-press removal volume at the 1st cutting pass initially forms a spherical cap at a shallower downward-press depth. From moving of the cutting tool to fabrication of groove, the depth in the middle area gradually inclines to be at a fixed cutting depth. As to the volume removed by downward force after moving of cutting tool, due to fabrication in the abovementioned process, the volume of the distance of the radius R behind the cap of the workpiece being cutted in by the probe in advancing direction has been removed. Therefore, at this moment, the removed volume is half of the cap volume under the cutting depth, and the removed volume ΔV_1 is shown as equation(3):

$$\Delta V_1 = \frac{1}{2}\pi \Delta d_1{}^2 \left(R - \frac{\Delta d_1}{3} \right) \quad (3)$$

where R denotes the radius of the tip of the cutting tool of probe; and Δd_1 denotes the cutting depth at the 1st cutting pass.

As to the volume removed by downward force at over two cutting pass, since the groove is removed at the previous cutting pass, the removed volume is just like a wedge of an arc. And this geometric shape has to go through the complicated integral before achieving such a removal volume.

Therefore, for the geometric shape of cutting tool and the cutting depth valued, the paper uses CATIA's CAD software to make a solid model in order to carry out simulation and calculation of cutting removed volume. The simulation and calculation concepts proposed by the paper are that for the cutting removed volume of the probe at the $(i+1)^{th}$ position under SDFE, it is supposed that the AFM probe moves from the i^{th} position for a distance of cap radius of the probe cutting into the workpiece under SDFE. Then CAD software is used to construct and calculate such a removed volume. This paper, using the cutting removed volume of the probe at the $(i+1)^{th}$ position under SDFE, supposes that the AFM probe moves from the i^{th} position for a distance of tip cap radius of the cutting into the workpiece. CAD software is also used to calculate this cutting removed volume.

Therefore, the paper applies a certain fixed downward force to put action on the workpiece. The paper also uses the radius of curvature of the probe tip and the depth being cut out to calculate the volume removed from the workpiece at the stable depth during the 1st cutting pass, and employs CAD for simulation and calculation of the volume removed from the workpiece after cutting for multiple cutting passes. The downward force energy produced by the downward force of probe on the workpiece when cutting reaches such a fixed depth is divided by this removed volume, thus achieving the SDFE value of the paper.

The straight-line cutting experiments are made at different downward forces of 32.79μN, 38.5μN and 47.31μN respectively at the 1st cutting pass. CAD software is ued to calculate the removed volume at this cutting depth. When the concept of SDFE is used for calculation, it can be found that the SDFE inclines to be a fixed constant 0.01775($\mu N \cdot \mathrm{nm} / nm^3$).

USE OF THE THEORY OF SDFE TO ESTABLISH AN ESTIMATION METHOD OF THE LEAST CUTTING PASSES FOR REACHING THE EXPECTED DEPTH BY USING TWO CUTTING PASSES OFFSET FABRICATION METHOD AT A FIXED CUTTING DEPTH

The paper employs the concept of SDFE to establish an two cutting passes offset fabrication method at a fixed cutting depth and changed downward force to fabricate a nanochannel trapezium groove on single-crystal silicon substrate to the expected depth. This method is that the paper firstly sets a fixed downward force at the 1st cutting pass on each cutting layer. At the 2nd cutting pass, downward force is changed to make it reach the same cutting depth as the one at the first cutting pass. And on the previous layer before reaching the expected depth of nanochannel trapezium groove, the paper changes the downward force at the 1st cutting pass on the last cutting layer, further reaching the expected depth of the fabricated nanochannel trapezium groove. However, in actual practice, when the machine is changing the downward force, additional time needs to be spent on setting the downward force. In order to use less fabrication lead time for reaching the expected depth of the fabricated nanochannel trapezium groove, the number of changes of downward force has to be decreased. The paper repeats regulation of downward force until a suitable downward force, the least cutting passes and the least fabrication lead time can be used for reaching the expected depth of the nanochannel trapezium groove.

Use of the Theory of SDFE to Establish an Two Cutting Passes Offset Fabrication Method at Changed Downward Force and a Fixed Cutting Depth

In order to converge the offset amount within a range, the paper sets that under a fixed cutting depth on each cutting layer, cutting for one cutting pass is firstly made. After that, the probe is offset rightwards for fabrication. In this way, between the shape of the fabricated cross-section before probe offset and the shape of the fabricated cross-section after probe offset, there is a protruding height on the bottom of nanochannel trapezium groove. If this protruding height on the bottom of nanochannel trapezium groove exceeds the set convergence value of protruding height, the probe should be offset step by step to carry out fabrication. If step-by-step offset of the probe is made, the protruding height on the bottom of nanochannel trapezium groove at the two re-fabricated cross-sections would converge to be within a range. In order to make the straight-line nanochannel groove's bottom have a result closer to a plane after fabrication at the bottom, this paper sets the range of numerical value of the protruding height on the bottom of nanochannel trapezium groove to be at a numerical value of the surface roughness of single-crystal silicon substrate at below 0.54nm. Right now, it is supposed that the probe offset amount required for fabrication of groove has been reached.

Then the paper uses SDFE value for step-by-step inverse induction of the required downward force for fabrication of groove after the probe offsets. The above theoretical model is that after the cutting tool of probe offsets laterally at the same cutting depth being set, the concept of SDFE is employed to simulate the downward force that needs to be changed for lateral offset. If it is required to simulate a cutting pass with the groove having a greater depth after the 2nd cutting layer, the removed volume is just like an arc wedge after the 2^{nd} cutting layer. And this geometric shape has to go through the complicated integral before achieving such a removed volume. Therefore, the paper uses CAD software to calculate this removed volume. Through the concept of SDFE, it is found that if it is required to approximate the SDFE value set by this paper, the downward force right now would be decreased. Therefore, the paper takes this concept to establish simulation of the required downward force at the same cutting depth.

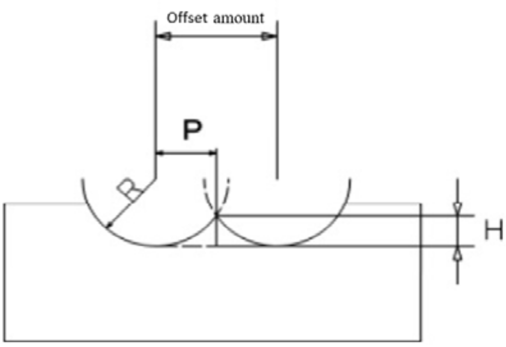

Fig. 1. Schematic diagram of protruding height on the bottom of nanochannel trapezium groove

Fig 1 is the schematic diagram of protruding height on the bottom of nanochannel trapezium groove between two cutting passes. Here, an equation can be used to estimate the protruding height value of this offset amount. If the offset amount can be used for reaching this expected cutting depth, and the protruding height value can be met, then the two cutting passes offset fabrication method can be established.

As shown in Figure 1, H is the protruding height produced on the bottom of nanochannel trapezium groove between two cutting passes,R is the radius of probe tip and P is the half of offset amount between two cutting passes. From Figure 1, the following relational equation can be derived:

$$H = R - \sqrt{R^2 - P^2} \tag{4}$$

The simulation steps of the entire simulation process of the theoretical model for fabrication of a nanochannel trapezium groove by using two cutting passes offset fabrication method with changed downward force are further explained as follows:

1. First of all, the cutting depth of V-shaped groove at the 1st cutting pass is the depth for simulated fabrication of a nanochannel trapezium groove at the 1st cutting pass.
2. After cutting of the 1st cutting pass is completed, lift up the cutting tool of probe and make it leave the surface of substrate, preventing it from contacting the substrate during offset.
3. Set the offset amount of the probe that gives the same cutting depth as the 1st cutting pass. Offset the probe rightwards to cut for the 2nd cutting pass.
4. As shown in Figure 1, observe the protruding height value on the bottom of nanochannel trapezium groove at the two cutting passes.
5. If such protruding height value on the bottom of nanochannel trapezium groove exceeds the set convergence value, with the convergence value of protruding height set by the paper to be 0.54nm, then step by step decrease the rightward offset amount.
6. In order to give a range for offset amount, the paper makes the offset amount converge to be within a range. Right now, if the protruding height value on the bottom of nanochannel trapezium groove exceeds the set convergence value, step by step offset the probe, and then carry out fabrication. If the probe is step by step offset, let the protruding height value on the bottom of nanochannel trapezium groove converge to be within a range. Right now, supposed that the offset amount of probe required for fabrication of the nanochannel trapezium groove has been reached.
7. Use CAD software to calculate the removed volume by downward force at the 2nd cutting pass after offset.
8. Use SDFE value to step by step induce inversely the required downward force at the 2nd cutting pass for fabrication of nanochannel trapezium groove after the probe offsets.
9. If it is required to increase the width of the nanochannel trapezium groove with the same cutting depth, refer to the steps aforesaid and use the same offset amount to increase the number of times of offset. Furthermore, increase the cutting passes, and use the same downward force at the 2nd cutting pass. Then the required nanochannel trapezium groove can be achieved.

Estimation Method of The Least Cutting Passes for Reaching The Expected Depth in Two Cutting Passes Offset Fabrication Methed with Changed Downward Force at a Fixed Cutting Depth

This paper innovatively introduces the use of a greater downward force to make the protruding height on the less than the set convergence value, and establishes a method to estimate the least cutting passes and the least fabrication time for reaching the expected depth of nanochannel trapezium groove. In order to avoid creation of destruction to the probe at multiple passes, the paper firstly sets a fabrication safety factor for downward force of the probe and obtains a greater downward force value to carry out cutting and fabrication of nanochannel. First of all, the paper sets a fixed downward force for the 1st cutting pass on each cutting layer, and then changes the downward force at the 2nd cutting pass in order to make it reach the same cutting depth as the one at the 1st cutting pass. And on the previous layer before reaching the expected depth of nanochannel trapezium groove, the paper changes the downward force at the 1st cutting pass on the last cutting layer, further reaching the expected depth of the fabricated nanochannel trapezium groove.

However, in actual practice, when the AFM machine changes the downward force, additional time needs to be spent on setting the downward force. In order to use less fabrication lead time for reaching the expected depth of the fabricated nanochannel trapezium groove, the number of changes of downward force has to be decreased. Through simulation, the offset amount can be changed to make the protruding height on the bottom of nanochannel trapezium groove less than the set convergence value, and then repeated regulation of downward force can be made. It is calculated that gradual deepening can be made at a fixed downward force from the 1st cutting layer to the last cutting layer at the 1st cutting pass, and make it reach the expected depth of the fabricated nanochannel trapezium groove.

The paper establishes a mathematical model for the objective function and constraints of the least cutting passes of the changed downward force for reaching the expected cutting depth when carrying out cutting of single-crystal silicon substrate by the cutting tool of AFM probe within a range of useable downward force, and develops a method to step by step regulate the cutting depth to approximate the set objective cutting depth and achieve the least changes of downward force. The objective function established by the paper is to be able to find the least cutting passes and the least changes of downward force at a suitable downward force in reaching the expected depth within a range of useable downward force. The related objective function and constraint equation are shown below.

For the optimization objective of multi-pass nanocutting, the paper mainly estimates the least cutting passes and the least changes of downward force at a suitable downward force in reaching the expected depth of nanochannel trapezium groove within the range of useable downward force. Therefore, the objective function and constraint are defined and expressed as follows.

Suppose N is the sum of the number of times n of cutting passes and the number of changes of downward force T_{cf}, then:

$$N=n+T_{cf} \tag{5}$$

Objective function:

$$N_{min.} = \text{Minimum } N \tag{6}$$

Then, the constraint are:

Subject to：

1.Fixed size of radius of AFM probe tip: R_{tip} (nm)

2.Range of working downward force of the probe: $F_{d\,min} < F_d < F_{d\,max}$ (7)

3. Protruding height on the bottom of nanochannel trapezium groove between two cutting passes < 0.54 nm

4. $\left| d_f - d_{objective} \right| \le \varepsilon_{depth}$ (8)

where F_{dmin} denotes the least downward force of probe for fabrication; $F_{d\,max}$ denotes the maximum downward force the probe can bear; d_f denotes the predicted depth obtained from calculation; $d_{objective}$ denotes the expected objective depth; ε_{depth} denotes the difference in convergence value between the predicted depth obtained from calculation and the expected objective depth.

In this paper, it is supposed that ε_{depth}= 0.05 nm. The calculation steps of the related objective function and the constraint equation are further explained below.

Within the range of permissible downward force of the AFM probe used by the paper, and when the shape of probe is known, the paper step by step regulates the increment of cutting depth in order to search the least cutting passes for reaching the expected objective depth in offset fabrication of two cutting passes at a suitable downward force. To know the number of cutting passes for reaching the expected depth, the paper has to meet the condition that the difference between the predicted depth and the expected objective depth of the nanochannel trapezium groove at the 1st and the 2nd cutting passes on the last cutting layer both reach the convergence value of in depth.

If the same cutting pass under the actions of different downward forces can be used to reach the approximated objective depth, and can meet the range of difference for equation (8) of difference in expected depth, the paper can further compare the ε_{depth} of different downward forces, and select a downward force being closest to the objective depth that is expected to reach, and take it as an optimal downward-forces for cutting in finding a more accurate cutting result.

As known from the above, the paper intends to use the least cutting passes under a certain suitable downward force to reach the expected objective depth. Therefore, in the calculation process, the paper firstly supposes that a smaller downward force being within a range the probe can fabricate is the initial downward force value, and then uses an optimization calculation method of step-by-step approximation method to calculate the expected depth to be close to the expected objective depth. Using step-by-step approximation method, the paper obtains the required cutting passes that meet the predicted depth calculated by equation (8) at this downward force. Then, gradually increasing the downward force value, the paper can decrease the cutting passes of fabrication to make the depth close to the objective depth. Finally, the paper calculates the downward force of the 1st cutting pass and the downward force of the 2nd cutting pass under the constraints that the objective function N of the sum of the least number of cutting passes and the least number of changes of downward force is met.

SIMULATION AND EXPERIMENTAL VERIFICATION

Simulation Results of Straight-Line Nanochannel Trapezium Groove by Two Cutting Passes Offset Method at a Fixed Cutting Depth and Changed Downward

Force

In order to avoid any damage caused to the probe during multi-pass cutting, the paper firstly sets the maximum downward force under the safety factor of the probe's downward force to carry out offset method of two cutting passes in order to achieve the number of cutting layers and cutting passes for reaching the expected objective depth. The paper firstly sets the maximum range 137μN for the machine test. In order to avoid any damage caused to the probe during multi-pass cutting, the paper firstly takes a safety factor n=1.5 to calculate the maximum downward force 91.3μN for the test. The paper firstly uses this downward force to carry out simulation test.

For the offset method of two cutting passes, a downward force is firstly fixed to conduct fabrication at the 1st cutting pass on each cutting layer; and the downward force at the 2nd cutting pass is then changed, making the cutting depth be the same as the one at the 1st cutting pass. After that, when cutting proceeds to the 1st cutting pass and the 2nd cutting pass on the cutting layer right before the expected objective depth is almost reached, the downward force is changed in order to make the expected objective depth reached on the last cutting layer. When using the maximum downward force under the safety factor to perform the above fabrication method, the paper can calculate the number of cutting layers and cutting passes. For the offset method of two cutting passes at a fixed cutting depth and changed downward force as set by the paper, the expected objective depth is 80nm, and has to converge at below the convergence value of depth ε_{depth} (ε_{depth} = 0.05nm). Using the simulation results, the paper takes the offset amount 24.5nm and the protruding height value 0.501nm on the bottom of nanochannel trapezium groove to conduct simulation.

The paper firstly uses a fixed downward force 91.3μN at the 1st cutting pass to simulate the results on the 7th layer. At the 1st cutting pass, the downward force is all fixed at 91.3μN for simulation up to the 7th layer. The simulated depth reaches 84.652nm, which exceeds the expected objective depth 80nm, and also exceeds the convergence value 0.05nm of depth from equation (6). As seen in Table 1, when the simulated depth on the 6th cutting layer has reached 77.088nm, but the downward force at the 1st cutting pass on the last cutting layer is changed to be 9.062μN, and the downward force at the 2nd cutting pass is changed to be 5.166μN, so that the number of changes of downward force on the same cutting layer is made to be increased for one more time. But when the machine actually changes the downward force, additional time has to be spent on changing the downward force. From the measurement in the experiment, the paper finds that the time for change of downward force for one time is around 7 minutes.

The paper intends not only to calculate the least cutting layers and the least cutting passes, but also to make the number of changes of downward force become the least, so as to make it spend the least fabrication lead time. The paper introduces step by step search of an optimal downward force through simulation, and makes calculation that the depth can be gradually deepened at the 1st cutting pass from the 1st cutting layer to the last cutting layer. And at the 2nd cutting pass on each cutting layer, the downward force is changed in order to make the cutting depth at the 2nd cutting pass be the same as the one at the 1st cutting pass. In this way, when the above method is used for calculation of the least number of cutting layers and the least number of cutting passes, the least number of changes of downward force and the least fabrication lead time can both be obtained as well.

Table 1. Simulation results on the last cutting layer at a fixed cutting depth and a fixed downward force 91.3μN

	Cutting pass	Downward force (μN)	Offset amount of cutting tool (nm)	Protruding height on the bottom calculated by CAD (nm)	Simulated depth (nm)	Removed volume (nm^3)	Width of opening (nm)	SDFE value ($\mu N \cdot nm / nm^3$)
1st cutting layer	1st cutting pass	91.3			23.006	118332.115		0.01775
	2nd cutting pass	23.259	24.5	0.501	23.006	30146.213	184.156	0.01775
2nd cutting layer	1st cutting pass	91.3			36.957	71759.228		0.01775
	2nd cutting pass	30.848	24.5	0.501	36.957	25245.281	221.693	0.01775
3rd cutting layer	1st cutting pass	91.3			49.746	65782.293		0.01775
	2nd cutting pass	31.184	24.5	0.501	49.746	22468.365	247.651	0.01775
4th cutting layer	1st cutting pass	91.3			59.887	52161.876		0.01775
	2nd cutting pass	31.549	24.5	0.501	59.887	18924.609	264.330	0.01775
5th cutting layer	1st cutting pass	91.3			68.792	45804.310		0.01775
	2nd cutting pass	31.985	24.5	0.501	68.792	17646.587	276.732	0.01775
6th cutting layer	1st cutting pass	91.3			77.088	42671.820		0.01775
	2nd cutting pass	32.514	24.5	0.501	77.088	15896.267	286.674	0.01775
7th cutting layer	1st cutting pass	9.062			80.000	10268.664		0.01775

The paper takes the downward force calculated by safety factor as the basis for repeated regulation of downward forces for approximation to a suitable downward force. Hence, the paper also takes n = 1.6 as another safety factor for calculation of downward force 85.625μN so as to conduct simulation of the offset method of two cutting passe. It is found that the simulated depth of the 7th cutting layer is 77.809nm, which has not reached the expected objective depth yet. When simulation proceeds to the 8th cutting layer,the simulated depth is 83.861nm, which has exceeded the convergence value of depth. Comparing to the simulation result at downward force 91.3μN, the downward force of this simulation is rather small.

Hence, not until the 8th cutting layer can the expected objective depth be reached. Therefore, in the next step, the downward force would be regulated to be greater to make the cutting passes become the least.

Using the abovementioned calculation method of cutting passes and regulation method of downward force, the downward forces required for calculation and simulation by the paper under the regulated n=1.55 and n=1.57 are 88.387μN and 87.261μN respectively. The paper uses these two downward forces to conduct simulation of offset method of two cutting passes. It is found that the simulated depth on the 7th cutting layer at the downward force 88.387μN is 80.952nm, and the convergence value of its depth reaches 0.952nm. The simulated cutting depth on the 7th cutting layer at the downward force 87.261μN is 80.15nm, and the convergence value of its depth reaches 0.15nm. This is quite close to the convergence value 0.05nm of depth as set by the paper.

Through the above method, the paper step by step reduces the interval of downward force. Therefore, the paper further takes the safety factor n=1.572 to calculate the downward force 87.15μN, and uses this downward force to simulate the offset method of two cutting passes. In Table 2, it can be seen that the simulated depth on the 7th cutting layer at this downward force is 80.027nm, which has reached the expected objective depth and also reached the convergence value of depth to be below 0.05 nm. Therefore, the simulation results of this time are successful. From the simulation results of the offset method of two cutting passes aforesaid, and through repeated regulation of downward force, the paper finally obtains the downward force 87.15μN, which is taken as a suitable downward force for reaching the expected objective depth.

Table 2. Simulation results of the 1st cutting pass at a fixed cutting depth and a fixed downward force 87.15μN

n=1.572	Cutting pass	Downward force (μN)	Offset amount of cutting tool (nm)	Protruding height on the bottom calculated by CAD (nm)	Simulated depth (nm)	Removed volume (nm³)	Width of opening (nm)	SDFE value (μN·nm/nm³)
1st cutting layer	1st cutting pass	87.15			21.904	107544.106		0.01775
	2nd cutting pass	22.709	24.5	0.501	21.904	28023.429	180.595	0.01775
2nd cutting layer	1st cutting pass	87.15			35.162	65094.913		0.01775
	2nd cutting pass	29.060	24.5	0.501	35.162	21705.746	217.501	0.01775
3rd cutting layer	1st cutting pass	87.15			47.263	50414.206		0.01775
	2nd cutting pass	29.141	24.5	0.501	47.263	19866.512	243.087	0.01775
4th cutting layer	1st cutting pass	87.15			56.825	46948.073		0.01775
	2nd cutting pass	29.362	24.5	0.501	56.825	15817.554	259.604	0.01775
5th cutting layer	1st cutting pass	87.15			65.601	43088.924		0.01775
	2nd cutting pass	30.033	24.5	0.501	65.601	14848.983	272.507	0.01775
6th cutting layer	1st cutting pass	87.15			73.104	36838.673		0.01775
	2nd cutting pass	30.592	24.5	0.501	73.104	12931.220	282.081	0.01775
7th cutting layer	1st cutting pass	87.15			80.027	33990.955		0.01775
	2nd cutting pass	30.905	24.5	0.501	80.027	12053.841	289.858	0.01775

Analysis on Experimental Results of Straight-Line Nanochannel Trapezium Groove by Offset Method of Two Cutting Passes at a Fixed Cutting Depth and Changed Downward Force

In order to prove that the paper's offset method of two cutting passes at a fixed cutting depth and changed downward force is feasible, the paper conducts on AFM fabrication experiment of straight-line nanochannel trapezium groove on single-crystal silicon substrate. Not only acquisition of the least cutting passes, the paper also needs to obtain the least fabrication lead time. The paper firstly uses the simulation result of the most suitable downward force 87.15μN obtained from AFM machine to conduct the offset method of two cutting passes at a fixed cutting depth and changed downward force. In the experiment, the offset amount is regulated to be the same as the one set in the simulation, i.e. 24.5nm.

The experimental measurement results of the individual morphology of the middle cross-section of the pattern of the fabricated nanochannel trapezium groove, and its depth, open width and protruding height on the buttom of nanochannel trapezium groove are shown in Figure 2. Since there are too many experimental layers, based on the experimental measurement data and simulation results of 7th cutting layer, the paper conducts analysis.

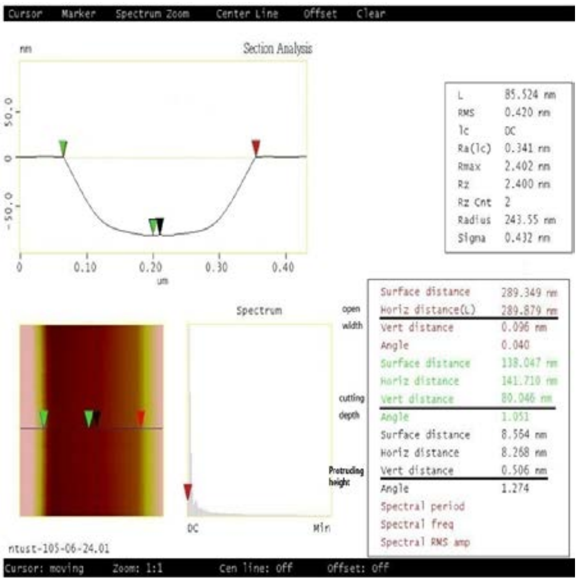

Fig. 2. Experimental measurement of depth,open width and protruding height on the bottom of nanochannel trapezium groove on the 7th cutting layer at the force 87.15μN

When fabrication at the downward force 87.15μN proceeds up to the 7th cutting layer. The depth of the nanochannel trapezium groove in the experiment is 80.046nm, which is quite close to the simulation result of the depth 80.027nm of the nanochannel trapezium groove. Both of them are quite close, and have both reached at below the convergence value of depth.

In order to prove that the simulation and experimental result of the downward force 87.15μN requires the least cutting passes, the paper keeps on using other simulation results to conduct experiments respectively. From the simulation results, the paper takes a greater downward force 88.387μN and a smaller downward force 86.625μN to carry out experimental fabrication. The experimental results for the part at the downward force 88.387μN show that on the 7th cutting layer the depth is 80.952nm which has exceeded the convergence value 0.54nm of depth; and the experimental protruding height values on the bottom of nanochannel trapezium groove are all 0.506nm, being the same as the simulation results.

Besides, a smaller downward force 86.625μN is also used to carry out experimental fabrication. The experimental results and the simulation results are the same. Cutting has to proceed up to the 8th layer can the expected cutting depth be exceeded. The experimental cutting depth is 83.924nm, which is quite close to the simulation result 83.861nm. Therefore, it is proved that at the downward force 86.625μN, the required cutting passes are not the least.

Comparison Between Estimated Simulation Results And Experimental Results Of The Least Cutting Passes And The Least Number Of Changes Of Downward Force For The Offset Cycle Method Of Two Cutting Passes At A Fixed Downward-Press Depth And Changed Downward Force To Reach The Expected Depth

Within the range of downward force for fabrication by AFM probe, the paper regulates the size of the required downward force in order to estimate the least cutting passes for reaching the expected objective depth. The paper sets the expected objective depth to be 80nm, and lets the depth on the last cutting layer converge at 0.05 nm. Within the working range of AFM probe in terms of downward force, and under the constraints that the shape of probe is known and the SDFE value is $0.01775\left(\mu N \cdot nm \big/ nm^3\right)$, the paper sets the offset amount to be 24.5nm. The paper uses the abovementioned constraint equations and calculation steps of less cutting passes and less number of changes of downward force for reaching the expected objective cutting depth, and then searches the depth of each cutting pass at different downward forces as well as the number of changes of downward force. The calculation and searched results of depths at different downward forces and various cutting layers are shown in Table 3.

As known in Table 3, according to the abovementioned calculation steps and the calculation results of step-by-step approximation search method, the paper finds that when cutting to the 7th layer at the downward force 87.15μN, it is estimated that the calculated depth is 80.027 nm, which forms a difference of 0.027nm from the expected objective depth 80nm. Comparing to other downward forces, on the cutting layers at other smaller downward forces, less number of cutting passes can be used to reach the expected depth. And at a cutting depth with a greater downward force at the same cutting pass, the expected objective depth would be exceeded. It is also seen in Table 3 that when downward force is 87.15 μN, the number of changes of downward forces is also the least. Therefore, the downward force 87.15μN is a suitable downward force that the least number of cutting passes and the least number of changes of downward force can be achieved by the paper for reaching the expected objective depth.

From the measurement in the experiment, the paper finds that the time for change of downward force for one time is around 7 minutes. Therefore, the fabrication lead time of the method of using a fixed downward force at the 1st cutting pass for reaching the expected depth is around 7 minutes less than the originally set method of changing the downward force for two times on the last cutting layer. Based on the change of downward force for one time on each cutting layer, and the change of downward force for 7 times, around 12.5% of time for changing the downward force can be saved. Therefore, the method of using a fixed downward force at the 1st cutting pass for reaching the expected depth is quite feasible.

Table 3. Difference in cutting depth and its objective depth (80nm) of the 1st and 2nd cutting passes on each cutting layer at different downward forces searched by the method of achieving the least cutting passes and the least number of changes of downward force by the offset method of two passes at a fixed cutting depth and changed downward force for reaching the expected objective depth, as well as the experimental depth at the downward force 87.15μN

Downward force (μN)	Number of cutting layers	Number of changes of downward force	Calculated depth on the cutting layer at the 1st and 2nd cutting passes d_f(nm)	$d_f - d_{objective}$ (nm)	Depth measured in experiment (nm)
86.625	7	7	77.809	-2.191	
	8	8	83.861	3.861	
87.15	7	7	80.027	0.027	80.046
87.261	7	7	80.15	0.15	
88.387	7	7	80.952	0.952	
91.3	7	7	84.652	4.652	

In order to prove the paper's method of finding the least cutting passes and the least number of changes of downward force by the offset method of two passes at a fixed cutting depth and changed downward force for reaching the expected objective depth, the paper uses the results obtained from the above calculation to perform offset cutting of two cutting passes at the downward force 87.15μN as well as a measurement experiment of cutting depth and width of opening. It can be seen in Table 3 that the depth at the 1st and 2nd cutting passes on the 7^{th} cutting layer measured in the experiment is 80.046nm, whereas the experimental result of depth as seen in Figure 2 is 80.046nm. It is quite close to the expected objective depth 80nm, and reaches below the convergence value 0.05nm of depth.

Therefore, it is proved that the paper's offset method of two cutting passes at a fixed cutting depth and changed downward force for reaching the expected objective depth as well as the paper's constraint equations and calculation steps of the least cutting passes and the least number of changes of downward force for reaching the expected objective depth within the range of useable downward force are feasible.

CONCLUSION

The paper uses the concept of SDFE to establish an offset method of two cutting passes at a fixed cutting depth and changed downward force. After setting the constraints, the paper uses the offset method of two cutting passes to carry out simulation. The paper intends not only to calculate the least number of cutting layers and the least number of cutting passes, but also to achieve the least number of changes of downward force, so as to make it spend the least fabrication lead time.

The paper introduces step by step search of an optimal downward force through simulation, and makes calculation that the depth can be gradually deepened at the 1st cutting pass at a fixed downward force from the 1st cutting layer to the last cutting layer until the expected depth of nanochannel trapezium groove is reached at the 1st cutting pass on the last cutting layer. And at the 2nd pass on each cutting layer, the downward force is changed in order to make the cutting depth at the 2nd cutting pass be the same as the one at the 1st cutting pass. When the above method is used for calculation of the least number of cutting layers and the least number of cutting passes, the least number of changes of downward force and the least fabrication lead time can both be obtained as well. And from the difference between the experimental and simulation results, this method is proved to be feasible.

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預定深度之單晶矽奈米流道梯型凹槽固定下壓深度及改變下壓力之加工到最少切削道次估算方法及實驗驗證

林榮慶 馬士閎 陳致榮
國立台灣科技大學 機械工程系

摘要

本文利用比下壓能觀念，建立最佳化之逐步逼近到預定之奈米流道梯形凹槽深度之目標收斂函數的最少切削道次之估算方法。其方法為兩切削道次偏移循環加工方法，此方法在每一切削層第一切削道次皆設定一固定下壓力，第二切削道次則改變下壓力取得與第一切削道次之相同切削深度，而經由模擬改變偏移量使凸起高度小於設定之收斂值後再反覆調整下壓力，使得凸起高度滿足本文中所設定之收斂值 0.54nm 範圍內;實際 AFM 機台在改變下壓力時，需額外耗費工時來改變下壓力，而本文為了在實際應用上取得最少加工前置時間，則應用比下壓能理論模式進一步估算出可達到預定奈米流道梯形凹槽深度之最少切削道次估算方法，在估算出最少切削道次之外，也使得變換下壓力次數達到最少，本文最後還進行了實驗來驗證，證實了確實可使加工前置時間為最少。