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Simulation Model Establishment and Experimental Verification for Cutting of Trapezium Groove on Single-Crystal Silicon Nanochannel to Expected Depth and Expected Width

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Keywords: atomic force microscopy(AFM),silicon substrate, trapezium groove on nanochannel,width, depth

ABSTRACT

The paper uses specific down force energy (SDFE) equation and two-pass offset cycle cutting method to further derive the required equations of total offset amount of probe for cutting of trapezium groove on nanochannel to expected depth and expected width, probe offset amount of two adjacent cutting passes, number of cutting passes and upward height value at the bottom. Finally, the paper establishes a method for simulation of cutting of trapezium groove on nanochannel to expected depth and expected width. The paper also uses atomic force microscopy (AFM) to carry out experimental verification of nanocutting. The paper uses the total offset amount of probe to estimate the number of cutting passes on each cutting layer, and then substitutes the probe offset amount of the adjacent mutual cutting passes in the calculation equation of upward height at the bottom of trapezium groove, thus achieving the upward height value at the bottom of trapezium groove The paper also proposes that the upward height value at the bottom should be converged at below the set objective convergence value. If the upward height value at the bottom calculated from the estimated two adjacent cutting passes exceeds the objective convergence value, one more cutting pass should be added until the upward height value at the bottom below the objective convergence value ,then the probe offset amount of the two adjacent cutting passes and the number of cutting passes on the cutting layer are obtained by calculation. In order to prevent the probe from being broken during cutting for multiple times, we set a safety coefficient for the maximum permissible downward force of AFM probe. The maximum downward force under the safety coefficient is just the maximum downward force that the paper permits to use. Finally, experimental verification is employed to prove that the theoretical model and simulation method developed by the paper for cutting of trapezium groove on nanochannel to expected depth and expected width are reasonable.

INTRODUCTION

In recent years the related scholars have proved that atomic force microscopy (AFM) can be used to carry out cutting of nano-microstructures on a surfaces. AFM was invented by G. Bining et al. (1986), and is a kind of scanning probe microscope (SPM). AFM is generally used to measure and observe the surface pattern of conductor and non-conductor. Therefore, the related scholars perform exploration of the measurement and application of AFM. Nanjo et al. (2003)considered the 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. Lübben 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.AFM is not only a tool that can be used to directly observe the microscopic appearance of a substance's surface, but also an equipment for cutting of tiny parts and microstructures. The main reason for the use of AFM probe tip to conduct mechanical cutting was that due to the change of action force between probe tip and sample, applying sufficient downward force on the probe tip could make the probe tip press down onto the surface of object. With the movement of the probe tip, cutting was carried out. As a result, specific geometric patterns were formed, and thus specific nanostructure was machined. Therefore, for cutting of nanoscale microstructures, not only the high-cost

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electronic beam or ionic beam cutting method can be used, AFM can also be applied to nanolithography and nanoscale cutting. It was proved by the related scholars that applying AFM probe as a cutting tool to carry out mechanical cutting was a quite useful technique in cutting of nano-microstructures, such as semiconductor, optoelectronic components and metallic surface (2008). Fang et al. (2000) used AFM probe to conduct nano-scratching experiments of silicon (Si) substrate coated with crystal-free aluminum (Al.) film. Experimental results showed that scratch depth deepened with the increase of probe tip load and scribing cycles. Besides, the effects of downward force of the cutting tool of probe were most obvious. And for multiple-pass cutting, the depth of the cut groove would be deepened with the increase of scribing cycles.Schumacher et al. (2000) used AFM to carry out mechanical cutting on the surface of heterogeneous structures of GaAs/AlGaAs, and then a single-electron transistor was fabricated. Yan et al. (2007) directly used AFM to construct a system similar to computer numerical control (CNC) cutting system, and took AFM probe as a cutting tool to carry out scratching of micro-nanostructures on the surface of silicon wafer deposited with copper film. Wang et al. (2010) used AFM to cut nanochannel on the surface of silicon oxide, and explored through experiments how downward force was related to cutting speed and cutting depth. The experiment of scratching Si wafer by AFM cutting tool of probe done by Tseng (2010) also showed that the depth and width of the scratched groove increased with the increase of downward force and scratch cycles of probe. After regression from the experimental data, it was found that the dimensions of nanogroove cut by AFM probe and the downward force of probe were of logarithmic function relationship, whereas the former and scratch cycles were of power-law function relationship. Lin and Hsu (2012) proposed a calculation method for the fewest cutting passes by using AFM to cut sapphire substrate at a certain depth. None of the above literature mentioned the paper's cutting method that cuts trapezium groove on straight-line nanochannel of single-crystal silicon substrate to expected depth and expected width.

EXPERIMENTAL EQUIPMENT AND SPECIFIC DOWN FORCE ENERGY (SDFE) EQUATION 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 of the paper's experiments is 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 to carry out cutting experiment of straight-line groove on silicon substrate and for observation. The paper also uses AFM equipment to carry out nanocutting and measurement of surface morphology before and after cutting.

The probe used in experiments is the diamond-coated DT-NCHR probe produced by Nanosensors Inc. The probe tip is like a semi-sphere with a spherical radius of around 150nm. Therefore, when this probe is used for cutting of silicon wafer, the probe tip is just like a semispherical cutting tool. The spring constant k_v of the probe provided by the manufacturer is 42 N/m, and its resonance frequency f_v is 320 kHz. In order to obtain a more accurate spring constant k_r of probe, the paper firstly uses tapping mode AFM to find the actual resonance frequency f_r of probe for experiments. Besides, since the spring constant k_r of probe in the experiments can be obtained from the equation $k_r = (f_r^2 \times k_v)/f_v^2$, the actual spring constant k_r of probe in the experiments can be acquired from the resonance frequency f_v and spring constant k_v of probe provided by the manufacturer, as shown in Table 1, and the actually measured resonance frequency f_r.

Table 1 Resonance frequency f_r. and spring constant k_v of probe provided by the manufacturer, and the actually measured resonance frequency f_r. and spring constant k_r of probe

f_r (measured resonance frequency)	385 kHz	k_r (actual probe spring constant)	60.8 N/m
f_v (measured resonance frequency)	320 kHz	k_v (manufacturer-provided probe spring constant)	42.0 N/m

Measurement method of downward force fo AFM probe

In order to accurately measure the downward force during nanocutting, the paper applies the measurement method of downward force in AFM contact mode. For the nanocutting way by AFM contact mode, the probe firstly presses down to the workpiece. During this time 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 nanocutting can thus be produced. Focusing on the measurement way of downward force of probe onto the workpiece to be cut, the paper uses force-distance curve for measurement. The force-distance curve explains the relationship between setpoint value and offset amount of the probe cantilever. Before conducting the experiment, the paper firstly sets different setpoint values for AFM machine under the contact model, and uses different setpoint values to measure the offset amount d of probe cantilever, and then substitutes the offset amount of probe cantilever in equation (1) to acquire the corresponding downward force value F_d of this setpoint (2012). In equation (1), k_r is the spring constant of probe.

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

SDFE theoretical model and SDFE calculation method

During the development process of the cutting method of trapezium groove on straight-line nanochannel of single-crystal silicon substrate to expected depth and expected width, the paper applies specific down force energy (SDFE) as the fixed value, and uses AFM experiment to calculate the SDFE value of the cut single-crystal silicon substrate. The paper considers that in the actual nanocutting process, the workpiece is under sufficient downward force from the cutting tool of probe. As down force energy is produced from pressing downward into the workpiece for a certain depth, cutting is carried out in cutting direction. The mechanism that the workpiece is being cut is just the moving and removal of atomic particles, and this is a volume change mode. SDFE is defined as follows: let the downward force applied by the cutting tool of probe onto the workpiece multiply the energy produced from the depth of downward press, and then divide such quotient by the volume removed from workpiece by the cutting tool due to downward press. The equation of SDFE is shown in equation (2) (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 for cutting at the cutting pass on the nth cutting layer; and ΔV_n denotes the volume removed from workpiece by downward press of the nth cutting pass. Since the volume removed from workpiece by downward press changes with the increase of cutting depth, ΔV_n is the function of cutting depth Δd_n

The paper supposes that under the same workpiece material, 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 workpiece by cutting tool at the 1st cutting pass on the 1st cutting layer can be obtained by the geometric equation of sphere. The cutting at each cutting pass on the 1st cutting layer is just like a semispherical cutting tool pressing into the workpiece to carry out straight-line moving and cutting. As observed, after the cutting experiment, from the cross-section morphology of groove depth in cutting direction, the cutting tool of probe initially presses into a shallower depth (Δd_i). As the cutting tool moves, the cutting depth gradually increases from a shallow depth to a fixed value (Δd_1) in the middle area. The removed volume also increases with the deepening of the depth of downward press. This phenomenon is the same as the model simulated by the paper using the solid model actually constructed by CATIA CAD software. Therefore, the way that the paper measures and calculates the average depth, and takes the position of middle area of the cut groove as the cutting depth, meets the actual cutting situation..

From the moving of cutting tool to the cutting 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 cutting in the abovementioned process, the volume of the distance of the radius R behind the cap of workpiece being cutted in by the probe in advancing direction has been removed.

Therefore, at this moment, the removed volume at the 1st cutting pass on the 1st cutting layer is half of the spherical cap volume under the cutting depth (Δd_1, and the removed volume ΔV_1 is shown as follows:

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

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

As to the volume removed by downward force at the 1st cutting pass on the 2nd cutting layer, since the groove is removed at the 1st cutting pass on the 1st cutting layer, the removed volume is just like an arc wedge. Therefore, for the geometric shape of cutting tool and the cutting depth, the paper uses CATIA's CAD software to make a solid model in order to carry out simulation and calculation of the volume removed by the downward force at 1st cutting pass on the 2nd cutting layer.

The simulation and calculation concepts proposed by the paper are that for the down-press removed volume of SDFE with the probe at the (i+1)th position, it is supposed that the AFM probe moves from the ith position for a distance of cap radius with the probe pressing down into the workpiece. The paper uses CAD software to construct and calculate such a down-press removed volume. The paper applies an important concept that for the down-press removed volume of SDFE with the probe at the (i+1)th position, it is supposed that the AFM probe moves from the ith position for a distance of cap radius of the probe tip pressing down into the workpiece. CAD software is also used to calculate this down-press removed volume (2012). Therefore, the paper applies a certain downward force to have action on workpiece. The paper also uses the curvature radius of probe tip and the depth of cutting to calculate the volume removed from workpiece at the stable depth during the 1st cutting pass on the 1st cutting layer, and employs CAD software for simulation and calculation of the volume removed from workpiece during multiple cutting passes on multiple cutting layers.

Table 2 shows the related data of straight-line cutting of groove at the 1st cutting pass on the 1st cutting layer using different downward forces. From the result of the cutting depth Δd1 at the 1st cutting pass on the 1st cutting layer obtained from the AFM experiment as shown in Table 2, CAD software is used to calculate the removed volume $\Delta V1$ at such cutting depth. When using SDFE concept to carry out calculation, it can be found that SDFE value inclines to be a fixed constant 0.01775($^{\mu N \cdot \mathrm{nm}}/_{nm^3}$).

Table 2 Related data of straight-line cutting at the 1st cutting pass on the 1st cutting layer under different downward forces

Downward force Fd(μN)	cutting depth at the 1st cutting pass on the 1st cutting layer obtained from AFM experimental measurement △d1(nm)	Removed material volume calculated by CAD △V1(nm³)	Removed material volume calculated by equation △V(nm3)	SDFEreaction value calculated by CAD simulation ($\mu N \cdot nm / nm^3$)	SDFEreaction value calculated by theoretical model ($\mu N \cdot nm / nm^3$)
30.23	7.353	12524.63	12524.63	0.01775	0.01775
40.21	9.833	22272.45	22272.45	0.01775	0.01775

TWO-PASS OFFSET CYCLE CUTTING METHOD OF TRAPEZIUM GROOVE ON NANOCHANNEL

The two-pass offset cycle cutting method of trapezium groove on nanochannel is explained as follows: First of all, it is set that under a fixed cutting depth on each cutting layer, the cutting depth at the 1st cutting pass is firstly cut. After that, the probe is offset rightwards to cut the workpiece at the 2nd cutting pass on this cutting layer. During this time the cutting depth at the 2nd cutting pass on this cutting layer has the same cutting depth as the 1st cutting pass. In this way, between the shape of the cut cross-section before probe offset and the shape of the cut cross-section of trapezium groove bottom at the two cutting passes after probe offset, there is an upward height value H at the bottom, as shown in Figure 1.

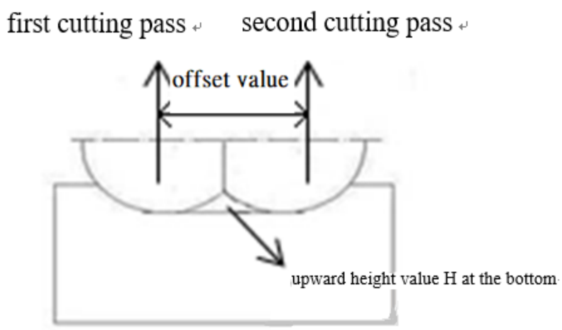

Fig. 1. Schematic diagram of upward height H at the bottom of trapezium groove between two cutting passes

If this upward height value H at the bottom of trapezium groove exceeds the set convergence value of upward height at the bottom, the probe should be offset step by step to carry out . After step-by-step offset of the probe, the upward height value H at the bottom at the two cutting passes of cutting is made to converge to within a range. In order to make the trapezium groove's bottom on straight-line nanochannel have a result closer to a plane after cutting at the bottom, the paper sets the range of numerical value of the upward height at the bottom to be a numerical value with the surface roughness of single-crystal silicon substrate at below 0.54nm. Right then, it is supposed that the probe offset amount required for cutting of trapezium groove on nanochannel has been achieved.

During this time, after the probe is offset, substitute the SDFE value obtained from AFM experiment in SDFE equation (2). Since ΔVn in equation (2) is the function of Δdn, which is the same cutting depth at the 1st cutting pass on this layer. Since the radius of AFM probe has been known, CAD software can be used to find ΔVn. After inverse induction from equation (2), the required downward force for cutting trapezium groove at the 2nd cutting pass on this cutting layer after probe offset can be acquired. The above theoretical model is that after the cutting tool of probe offsets laterally on this cutting layer, which is set to have the same cutting depth, SDFE concept is employed to calculate the downward force of the laterally offset probe that needs to be changed during probe cutting of workpiece at the 2nd cutting pass on this cutting layer.

If it is required to simulate the trapezium groove on nanochannel that uses a greater depth after the 2nd cutting layer, then under the preset cutting depth on the 2nd cutting layer, volume is removed during cutting on the 1st cutting layer, and the removed volume is just like an arc wedge. Therefore, the paper uses CAD software to calculate the removed volume. Similarly, using SDFE equation (2) can obtain the downward force required for the cutting pass on the 2nd cutting layer. Therefore, the paper takes this concept to establish this cutting layer that has the same cutting depth, and to calculate the required downward force of each cutting pass on each cutting layer.

The above shows the entire simulation process of the theoretical model of two-pass offset cycle cutting method of trapezium groove on nanochannel on this cutting layer that has the same cutting depth. The paper further explains the simulation steps as follows:

1. First of all, the cutting depth of V-shaped groove at the 1st cutting pass on this cutting layer is the cutting depth for simulated cutting of trapezium groove pattern at the 1st cutting pass.
2. After cutting of the 1st cutting pass on the 1st cutting layer 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 cutting depth of the 2nd cutting pass on this cutting layer be the same cutting depth at the 1st cutting pass on this cutting layer. Offset the probe rightwards to cut the 2nd cutting pass on this cutting layer.
4. As shown in Figure 1, observe the upward heights value H at the bottom of trapezium groove on the cross-section before and after probe offset at the two cutting passes on this cutting layer.

5. If the upward height value H at the bottom of trapezium groove exceeds the set convergence value 0.54nm of upward height at the bottom set by the paper, conduct step-by-step decrease of rightward offset amount at the 2nd cutting pass on this cutting layer. After step-by-step offset of probe in this way, if the upward height value H at the bottom of the cross-section at the two cutting passes on this cutting layer converges to below 0.54nm as set by the paper, at this moment it is supposed that the probe offset amount required for the two adjacent cutting passes in the cutting of trapezium groove on straight-line nanochannel has been achieved.
6. Use CAD software to calculate the volume removed by cutting at the 2nd cutting pass on this cutting layer after probe offset at two adjacent cutting passes.
7. Use SDFE equation to inversely induce the required downward force at the 2nd cutting pass on this cutting layer after offset of probe.
8. If it is required to increase the width of trapezium groove on straight-line nanochannel with the same cutting depth on this cutting layer, then use the same probe offset amount of the two adjacent cutting passes on this cutting layer. Offset the probe rightwards, and calculate the required downward force. Then the trapezium groove pattern on nanochannel required on this cutting layer that has 3 cutting passes can be simulated. If necessary, this cutting layer can be increased with the 4th cutting pass so as to increase the width of trapezium groove on nanochannel. This practice is just the same as the previous practice that increases the 3rd cutting pass on this cutting layer.

ESTABLISHMENT OF CUTTING METHOD OF TRAPEZIUM GROOVE ON NANOCHANNEL TO EXPECTED DEPTH AND EXPECTED WIDTH

The paper uses the above two-pass offset cycle cutting method. The geometric shape of probe tip can be seen as a sphere. The cross-section at different cutting passes at the same cutting depth can be used to take their shapes as intersecting circles. During this time, the radius of probe has a depending relationship with the cutting depth and width. Therefore, the paper further establishes the cutting method of trapezium groove on nanochannel to expected depth and expected width. According to the method innovatively established by the paper, we can decide the required number of cutting passes n for cutting of trapezium groove on nanochannel to expected depth and expected width, total offset amount Ptotal of probe between cutting passes, probe offset amount Pn between two adjacent cutting passes, and the upward height value H at the bottom produced between two adjacent cutting passes. Focusing on the paper's innovative cutting method of trapezium groove on nanochannel to expected depth and expected width, the paper establishes derivation of the following equations.

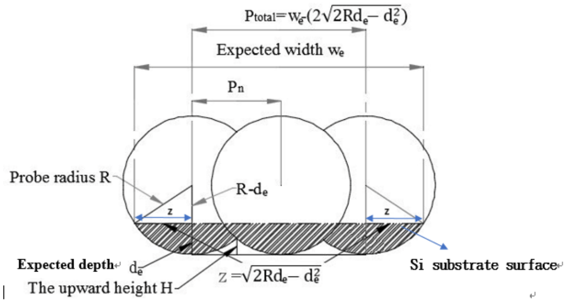

Fig. 2. Schematic diagram of geometric relationship in cutting of trapezium groove on nanochannel to expected depth and expected width (3 cutting passes)

First of all, set the numerical values of expected depth and expected width for cutting to the last cutting layer, as shown in Figure 2. In Figure 2, d_e denotes the expected depth for cutting to the last trapezium groove on nanochannel; w_e denotes the expected width for cutting to the last trapezium groove on nanochannel; P_{total} denotes the total offset amount of probe; P_n denotes the probe offset amount at two adjacent cutting passes; H denotes the upward height at the bottom; and z denotes the horizontal distance from the center of probe to the connected place between probe and the edge of trapezium groove. The probe tip radius R is known to be 150nm. Using Pythagorean theorem, the equation of z in Figure 2 can be derived as follows:

$$\because z^2 + (R - d_e)^2 = R^2$$

$$\therefore z = \sqrt{2Rd - d_e^{\,2}} \tag{4}$$

From Figure 2, it can be seen that there is z by both the left and right sides at the farthest cutting pass, so that $2z=2\sqrt{2Rd_e - d_e^{\,2}}$. In order to obtain the required total offset amount of probe, equation (5) of total offset amount of probe can be derived from Figure 2 as follows:

$$P_{total}= w_e-(2\sqrt{2Rd_e - d_e^{\,2}}) \tag{5}$$

As seen from equation (5), when the last expected depth and expected width of trapezium groove on nanochannel have been known, the total offset amount of probe can be acquired from equation (5). During this time we further find that after calculation of total offset amount of probe, the probe offset amount Pn at two adjacent cutting passes is the main key point affecting the upward height H of trapezium groove. And from simulation, it is known that if the cutting passes in the middle of total offset amount of probe is more, the upward height H at the bottom will be smaller; and if the cutting passes in the middle of total offset amount of probe is less, the upward height H at the bottom will be greater. When the cutting depth of each cutting layer has been decided, SDFE equation can be used to find the predicted required downward force for the cutting depth on this cutting layer, and then we can decide how much downward force is required when this cutting depth is achieved.

Besides, if downward force has been set, the cutting depth on each simulated cutting layer can also be obtained from SDFE equation. If the maximum permissible downward force of AFM probe is used to cut trapezium groove, we cannot instantly achieve the expected depth of trapezium groove on the 1st cutting layer. Right then, the method of increasing cutting layer has to be used to cut downwards continuously. SDFE equation should also be used to calculate the cutting depth on each cutting layer at the set downward force, as well as the downward force required to be set for different cutting passes at the same cutting depth on each cutting layer. As cutting continues until reaching the cutting depth on the last cutting layer, the total depth of the cut trapezium groove on nanochannel has to reach the expected depth.

The above theoretical equation can be used to derive the required total offset amount of probe. However, how many cutting passes and how much probe offset amount Pn at the two adjacent cutting passes should be used are the key questions. If a smaller probe offset amount can be used to achieve the expected depth and expected width of trapezium groove, not only the upward height at the bottom can be obtained, a smaller number of cutting passes can also be achieved. Therefore, focusing on this point, the paper derives the equation of probe offset amount Pn at two adjacent cutting passes and the equation of upward height H at the bottom between two adjacent cutting passes, as shown in equation (6) and equation (7) respectively as follows:

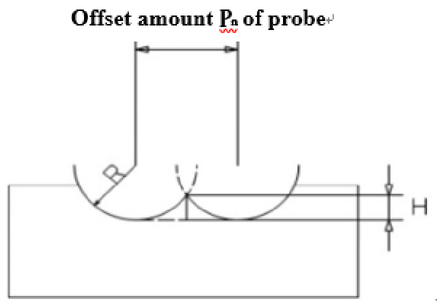

Fig. 3. Schematic diagram of probe offset amount Pn at two adjacent cutting passes and upward height H at the bottom

As known from Figure 2 and Figure 3, H is the upward height at the bottom of trapezium groove produced between two adjacent cutting passes; P_n is the probe offset amount between two adjacent cutting passes; and the n in P_n represents the number of cutting passes on each cutting layer. If there are two cutting passes only, the n in P_n is 2, and $P_{total} = P_2$. Therefore, from Figure 2 and Figure 3, P_n and H equations can be derived and expressed as equations (6) and (7) as follows:

$$P_n=\frac{P_{total}}{n-1} \qquad (6)$$

$$H = R - \sqrt{R^2 - (\frac{P_n}{2})^2} \qquad (7)$$

From equation (5), we can calculate the required total offset amount Ptotal of probe for cutting of trapezium groove on nanochannel to expected depth and expected width. If each cutting layer is divided into n cutting passes for cutting, equation (5) can be used to calculate the total offset amount Ptotal. According to equation (6), Ptotal is divided by (n-1), and then we can calculate the probe offset amount Pn of two adjacent cutting passes required to reach the expected depth and expected width of trapezium groove. After we have obtained the probe offset amount Pn of two adjacent cutting passes on each cutting layer, we also have to substitute this Pn value in equation (7) to calculate the upward height value H at the bottom, and then observe the selected number of cutting passes, and check whether the upward height value H at the bottom has exceeded the convergence value 0.54nm. If the calculated upward height value H at the bottom has exceeded the convergence value 0.54nm, we can increase one more cutting pass, and substitute the number of cutting passes n, with a cutting pass additionally increased, in equation (6).

Calculate the required probe offset amount Pn, and then observe again whether the upward height value H at the bottom still exceeds 0.54nm. If the upward height value H at the bottom has not exceeded the convergence value 0.54nm, the number of cutting times n set for the new cutting pass is the required number of cutting passes on each cutting layer. Figure 4 shows the schematic diagram showing how the expected depth and expected width of trapezium groove on nanochannel have geometric relationship with existence of 4 cutting passes on each cutting layer. The central part in Figure 4 is divided into probe offset amounts Pn at two adjacent cutting passes for 3 times. Suppose that the figure of suitable number of cutting passes on each cutting layer has been finally found. Then SDFE equation can be used to calculate the cutting depth at each cutting pass with set downward force on each cutting layer. As cutting continues until reaching the cutting depth on the last cutting layer, the accumulated total depth and total width of trapezium groove being simulated are close to the expected depth and expected width of trapezium groove on nanochannel.

The above related calculation equations concerning cutting of trapezium groove on nanochannel to expected depth and expected width merely belong to relationships of geometric shapes. They are unrelated to the cutting force required for cutting by AFM machine, and also have no involvement in the number of cutting layers for cutting to expected depth. Therefore, when using the above equations and simulation method, the last depth and last width for simulation of trapezium groove are the total depth and total width for cutting of the last trapezium groove on the last cutting layer.

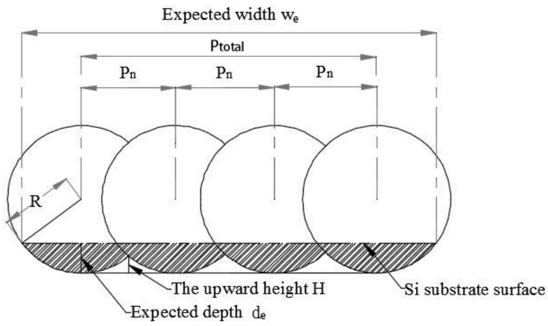

Fig. 4. Schematic diagram showing how the expected depth and expected width of trapezium groove on nanochannel have geometric relationship with existence of 4 cutting passes on each cutting layer

PLANNING AND EXPLORATION OF PATHS FOR DIFFERENT STRAIGHT-LINE CUTTING PASSES

As seen from simulation of the paper, , if the probe carries out cutting, with probe offsetting rightwards, on the same cutting layer in the same direction, the downward force after the 2nd cutting pass needs to be adjusted for one time only. This is because the removed volume after the 3rd cutting pass equals to the removed volume after the 2nd cutting pass. In this way, the number times of adjustment of downward forces and the time spent can both be saved.

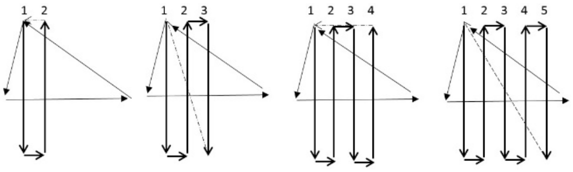

Fig. 5. The schematic diagram showing cutting paths on a certain cutting layer. From the left to the right are the cutting paths of 2 cutting passes, 3 cutting passes, 4 cutting passes and 5 cutting passes. Of them, the black solid line is the cutting path; the dotted line is the path after the cutting of the entire offset cycle is completed and the probe returns to the starting point; and the black fine line is the path that scans the cross-section.

As shown in Figure 5, on a certain cutting layer, the paper mainly lists out the above 4 cutting paths with cutting passes, and takes them for example. Of them, the black solid lines show the cutting paths of different cutting passes, and the dotted lines show the paths after having cut the entire offset cycle and returned to the position at the starting point 1. The figure is the schematic diagram of 4 cutting paths with 2 cutting passes, 3 cutting passes, 4 cutting passes and 5 cutting passes respectively, which are properly shown from the left to the right. After the probe starts pressing downwards at the origin and cuts for the 1st cutting pass, the probe is lifted up and offset rightwards. With the downward force changed, the probe presses downwards again to cut for the 2nd cutting pass. Then cutting rightwards continues, and so on and so forth. If cutting is completed, and cutting on the next cutting layer is going to be carried out, lift up the probe once again, and let the probe follow the path of dotted line and go back to position 1. After that, move the probe to the position of the black fine line path, and switch to the cross-section scanning model. After the entire cross-section has been scanned, the probe will automatically return to position 1 so as to proceed with the same cutting cycle on the next cutting layer.

SIMULATION OF CUTTING OF TRAPEZIUM GROOVE ON NANOCHANNEL TO EXPECTED DEPTH AND WIDTH AND EXPERIMENTAL VERIFICATION

The abovementioned theoretical equations concerning cutting of trapezium groove on nanochannel to expected depth and expected width merely belong to calculation by geometric equations, so they are unrelated to downward force and the number of cutting layers. Calculation is simply made by direct cutting of trapezium groove on nanochannel to expected depth and expected width. Therefore, the paper has to further consider to carry out simulation of downward force and make experimental verification in order to prove that the abovementioned theoretical equations and simulation method established by the paper for cutting of trapezium groove on nanochannel to expected depth and expected width are reasonable.

Simulation of cutting of trapezium groove on nanochannel to expected depth and width

First of all, the paper explores the part of single cutting layer. The paper considers that on a single cutting layer, the expected depth 20nm for cutting of trapezium groove on straight-line nanochannel is the cutting depth on the 1st cutting layer. Therefore, the cutting depth (Δd_1) on the 1st cutting layer is 20nm. Using SDFE equation, the downward force at the 1st cutting pass on the 1st cutting layer can be calculated as 80.02μN. The widths expected to be reached by the trapezium groove on nanochannel contain two widths, namely 202nm and 250nm. As seen from the simulation results in Table 3 and Table 4 below, when the expected depth and width of trapezium groove on nanochannel are 20nm and 202nm respectively, the upward height value H at the bottom for 3 cutting passes is 0.572nm, exceeding the set convergence value 0.54nm of upward height H at the bottom. Thus, when adding one more cutting pass according to the method of the paper, the 1st cutting layer is changed to have 4 cutting passes for simulation.

During this time, the upward height value H at the bottom immediately decreases to be 0.254nm, being smaller than the convergence value 0.54nm. Therefore, the quantity of 4 cutting passes is regarded as a better number of cutting passes for cutting. Besides, as seen from the simulation results in Table 4, for cutting with only one cutting layer, the cutting depth is 20.024nm and the width of opening is 202.07nm, which respectively have less difference from the expected depth 20nm and expected width 202nm of trapezium groove. Therefore, the simulation results are acceptable.

Table 3 Simulation data for cutting of trapezium groove on straight-line nanochannel to expected depth 20nm and expected width 202nm on the 1st cutting layer having 3 cutting passes

No. of cutting layers	Downward force (μN)	Cutting pass	Simulated cutting depth (nm)	Probe offset amount P_n (nm)	Upward height value at the bottom calculated by CAD (nm)	SDFE value ($\mu N \cdot nm / nm^3$)	Removed volume (nm^3)	Width of opening (nm)	Safety Coefficient
1st cutting layer	80.02	1st cutting pass	20.024	26.17	0.572	0.01775	90271.576	202.09	1.5
	23.17	2nd cutting pass	20.024	26.17		0.01775	26139.290		
		3rd cutting pass	20.024			0.01775	26139.290		

Table 4 Simulation data for cutting of trapezium groove on straight-line nanochannel to expected depth 20nm and expected width 202nm on the 1st cutting layer having 4 cutting passes

No. of cutting layers	Downward force(μN)	Cutting pass	Simulated cutting depth (nm)	Probe offset amount Pn (nm)	Upward height value at the bottom calculated by CAD (nm)	SDFE value ($\mu N \cdot nm / nm^3$)	Removed volume (nm3)	Width of opening (nm)	Safety Coefficient
1st cutting layer	80.02	1st cutting pass	20.024	17.44	0.254	0.01775	90271.576	202.07	1.5
	15.57	2nd cutting pass	20.024	17.44		0.01775	17563.328		
		3rd cutting pass	20.024	17.44		0.01775	17563.328		
		4th cutting pass	20.024			0.01775	17563.328		

Table 5 Simulation data for cutting of trapezium groove on straight-line nanochannel to expected depth 20nm and expected width 250nm on the 1st cutting layer having 4 cutting passes

No. of cutting layers	Downward force(μN)	Cutting pass	Simulated cutting depth (nm)	Probe offset amount Pn (nm)	Upward height value at the bottom calculated by CAD (nm)	SDFE value ($\mu N \cdot nm / nm^3$)	Removed volume (nm3)	Width of opening (nm)	Safety Coefficient
1st cutting layer	80.02	1st cutting pass	20.024	33.44	0.935	0.01775	90271.576	250.07	1.5
	29.33	2nd cutting pass	20.024	33.44		0.01775	33088.364		
		3rd cutting pass	20.024	33.44		0.01775	33088.364		
		4th cutting pass	20.024			0.01775	33088.364		

Table 6 Simulation data for cutting of trapezium groove on straight-line nanochannel to expected depth 20nm and expected width 250nm on the 1st cutting layer having 5 cutting passes

No. of cutting layers	Downward force(μN)	Cutting pass	Simulated cutting depth (nm)	Probe offset amount Pn (nm)	Upward height value at the bottom calculated by CAD (nm)	SDFE value ($\mu N \cdot nm / nm^3$)	Removed volume (nm3)	Width of opening (nm)	Safety Coefficient
1st cutting layer	80.02	1st cutting pass	20.024	25.08	0.525	0.01775	90272.93	250.07	1.5
	22.23	2nd cutting pass	20.024	25.08		0.01775	25080.85		
		3rd cutting pass	20.024	25.08		0.01775	25080.85		
		4th cutting pass	20.024	25.08		0.01775	25080.85		
		5th cutting pass	20.024			0.01775	25080.85		

When the expected depth and expected width of trapezium groove are 20nm and 250nm respectively, as seen from the simulation results in Table 5 and Table 6, the upward height value H at the bottom on the 1st cutting layer having 4 cutting passes is 0.935nm, which exceeds the set convergence value 0.54nm of upward height at the bottom. Thus, when adding one more cutting pass according to the method of the paper, the 1st cutting layer is changed to have 5 cutting passes for simulation. During this time, the upward height value H at the bottom immediately decreases to be 0.525nm, being smaller than the convergence value 0.54nm. Therefore, the quantity of 5 cutting passes is regarded as a better number of cutting passes for cutting. Besides, as seen from the simulation results on the 1st cutting layer, the cutting depth is 20.024nm and the width of opening is 250.07nm, which respectively have rather small difference from the expected depth 20nm and expected width 250nm of trapezium groove. Therefore, the simulation results are acceptable.

Experimental verification of cutting of trapezium groove on nanochannel to expected depth and width

Using the abovementioned theoretical equation and method for simulation of cutting of trapezium groove on nanochannel to expected depth and expected width, we can calculate the total offset amount Ptotal of probe, number of cutting passes n on each cutting layer, probe offset amount Pn of two adjacent cutting passes, and upward height value H at the bottom; and then simulate cutting of trapezium groove on nanochannel to expected depth 30nm and expected width 202nm. In Table 7, the probe offset amount Pn of two adjacent cutting passes calculated by the paper is 22nm; the number of cutting passes is two cutting passes; and the upward height value H at the bottom is 0.404nm, which is smaller than the convergence value 0.54nm of the upward height at the bottom. Since the paper uses AFM machine, it is known that the maximum permissible downward force of probe is 137μN. Here, in order to prevent the probe from being broken during cutting for multiple times, we preset a minimum safety coefficient 1.5. When the maximum permissible downward force of AFM probe is 137μN, and the safety coefficient is 1.5, the permissible maximum downward force of probe is calculated to be 91.33μN.

Therefore, the downward force used for the 1st cutting pass on the 1st cutting layer is 91.33μN. As known from the simulation results in Table 7, the cutting depth at the 1st cutting pass on the 1st cutting layer is 23.014nm only, being smaller than the expected depth 30nm. Thus, the paper increases one more cutting layer. Through the simulation results, the downward force at the 1st cutting pass on the 2nd cutting layer is 34.95μN; the downward force at the 2nd cutting pass is 19.88μN; the simulated total depth of trapezium groove is 30.011nm; the total width of opening is 202.029nm; the probe offset amount Pn of two adjacent cutting passes is 22nm; and the upward height value H at the bottom is 0.404nm. Figure 6 below is the diagram of experimental measurement result of upward height value H at the bottom in the

AFM cutting experiment of two cutting passes on the 2nd cutting layer when the expected depth of trapezium groove on straight-line nanochannel is 30nm and the expected width is 202nm; and Figure 7 is the diagram of experimental measurement results of AFM experimental total depth and AFM experimental total width of trapezium groove on straight-line nanochannel.

Table 7 Comparison of experimental and simulation results of cutting of trapezium groove on nanochannel to expected depth 30nm and expected width 202nm on two cutting layers and for two cutting passes

No. of cutting layers	Downward force (μN)	Cutting pass	Experimental depth (nm)	Simulated depth (nm)	Probe offset amount P_n(nm)	Experimental upward height value at the bottom (nm)	Simulated upward height value at the bottom (nm)	SDFE value ($\mu N \cdot nm / nm^3$)	Experimental width of opening (nm)	Simulated width of opening (nm)
1st cutting layer	91.33	1st cutting pass	23.027	23.014	22.00	0.393	0.404	0.01775	181.696	181.682
	20.94	2nd cutting pass	23.027	23.014				0.01775		
2nd cutting layer	34.95	1st cutting pass	30.023	30.011	22.00	0.394	0.404	0.01775	202.041	202.029
	19.88	2nd cutting pass	30.023	30.011				0.01775		

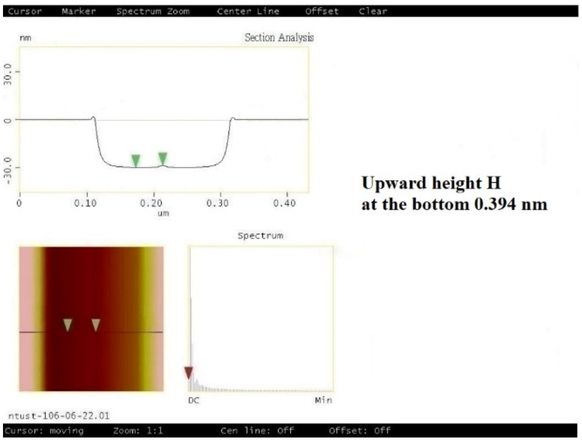

Fig. 6. Experimental measurement result of upward height value H at the bottom in the AFM experiment of cutting of trapezium groove on straight-line nanochannel on the 2nd cutting layer having two cutting passes when the trapezium groove on straight-line nanochannel has expected depth 30nm and expected width 202nm.

As seen from Figure 6 and Figure 7, the upward height value H at the bottom of AFM experiment at two adjacent cutting passes is 0.394nm, which is proved to be smaller than the convergence value 0.54nm of upward height at the bottom. Besides, the total experimental depth of trapezium groove on nanochannel is 30.023nm, and the total experimental width of opening is 202.041nm. As seen from the comparison of simulation and experimental results in Table 7, the experimental upward height value at the bottom of two adjacent passes on the 2nd cutting layer is 0.394nm, and the simulated upward height value at the bottom is 0.404nm, having a small difference in between, and both being smaller than the convergence value 0.54nm of upward height at the bottom. As known from Table 7, the difference in total depth and total width of opening of trapezium groove between experimental and simulation results is 0.040% and 0.006% respectively.

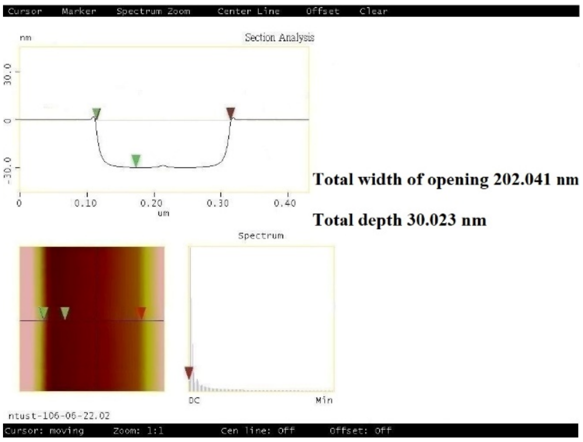

Fig. 7. Experimental measurement results of AFM experimental total depth and experimental total width of opening for the trapezium groove on straight-line nanochannel on the 2nd cutting layer having two cutting passes when the trapezium groove on straight-line nanochannel has expected depth 30nm and expected width 202nm.

Both of them have a difference of less than 0.1%, having a very small difference indeed. Besides, the simulated and experimental total depths and total widths of trapezium groove on straight-line nanochannel are also very close to the expected depth and expected width of trapezium groove. Hence, from the AFM experimental results, it is proved that the theoretical equation and method established by the paper for simulation of trapezium groove on nanochannel to expected depth and expected width are reasonable.

CONCLUSION

The paper has derived the equations of total offset amount required for cutting of trapezium groove on nanochannel to expected depth and expected width, offset amount of two adjacent cutting passes, number of cutting passes on each cutting layer, and upward height at the bottom. The paper also establishes the cutting method of trapezium groove on straight-line nanochannel to expected depth and expected width. Furthermore, the paper proposes that the upward height value at the bottom at two cutting passes should be converged at the set convergence value. If the calculated upward height value at the bottom at the two adjacent cutting passes exceed the convergence value, one more cutting pass should be increased on each cutting layer until the calculated upward height value at the bottom at two adjacent cutting passes can be converged at below the convergence value.

Besides, the maximum permissible downward force of AFM probe is known. In order to prevent the probe from being broken during cutting for multiple times, we preset a minimum safety coefficient. When the probe is under maximum permissible downward force and safety coefficient, the permissible maximum downward force of probe used in this study can be calculated. Finally, a comparison is made between simulation results and AFM experimental results of cutting of trapezium groove on straight-line nanochannel to expected depth and expected width. As seen from the simulation results and experimental results, the difference in depth and width of trapezium groove on straight-line nanochannel is very small, and these results of total depth and total width of opening are also only slightly different from the expected depth and expected width of trapezium groove on nanochannel.

Besides, the experimental and simulation results of upward height value at the bottom of two adjacent cutting passes are both smaller than the convergence value. Therefore, it is proved that the theoretical equations and method established by the paper for simulation of cutting of trapezium groove on single-crystal silicon nanochannel to expected depth and expected width are reasonable.

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加工單晶矽奈米流道梯形凹槽到預定深度及寬度之模擬模式建立及實驗驗證

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摘要

本文用比下壓能公式及兩道次偏移循環加工法，進一步推導出加工奈米流道梯形凹槽到預定深度與預定寬度所需的探針總偏移量，相鄰兩切削道次的探針偏移量，切削道次數目及底部凸起的公式。最後建立加工奈米流道梯形凹槽到預定深度及預定寬度的模擬方法，並用原子力顯微鏡進行奈米切削實驗驗證。本文用探針總偏移量來估算每一切削層的切削道次，再將其相鄰相切削道次的探針偏移量代入梯形凹槽底部突起的底部上凸值計算公式，得出梯形凹槽底部突起的底部上凸值。本文並提出底部上凸值應收斂在所設定之目標收斂值內。假如估算之相鄰兩切削道次所計算出的底部上凸值超出目標收斂值，則再多加一切削道次，直到由計算所得之相鄰兩切削道次的探針偏移量及切削道次數目，進一步計算出的梯形凹槽底部上凸值可收斂在目標收斂值內，即可得出所需的每一切削層的相鄰兩切削道次的探針偏移量及切削道次數目。我們為了避免探針在切削多次時產生斷裂，因此我們在 AFM 探針的最大容許下壓力設了安全係數，在安全係數下之最大下壓力為本文可允許允許使用的最大下壓力。最後利用實驗驗證來證實本文所建立的加工奈米流道梯形凹槽到預定深度及預定寬度的理論模式及模擬方法為合理的。