Process simulation of nano-channel forming by thin film deposition

Jian Jin¹, Si Di²*, Wang Hao³, Xiaojun Li¹, Xudi Wang⁵*, Xuetong Sun⁶

¹Shenzhen Institutes of Advanced Technology Shenzhen, China
¹Hefei University of Technology HeFei, China
²Shenzhen Institutes of Advanced Technology Shenzhen, China
²Guangzhou Institute of Advanced Technology, Chinese Academy of Sciences Guangzhou, China
³Hefei University of Technology Hefei, China
⁴Hefei University of Technology Hefei, China
⁵Hefei University of Technology Hefei, China
⁶Guangzhou Institute of Advanced Technology, Chinese Academy of Sciences Guangzhou, China

* Corresponding author: si.di@giat.ac.cn
* Corresponding author: wxudi@hfut.edu.cn

Abstract—In the traditional fabrication process of micro/nano-fluidic chips, thermal bonding is usually used for channel sealing, but it is easy to cause channel blockage, especially when the channel size is nanometer. The film deposition is a better way to seal the nano channel, and by controlling the deposition angle, the shape and size of the sealed channel can also be controlled. In order to understand the channel formation process of thin film deposition more intuitively, based on the COMSOL software, a free molecular flow module is used to simulate the film deposition process. The growth of the film is characterized by the post-processing of geometric deformation, so as to predict the channel shape. By comparing the simulation results with the experimental results, it can be seen that this simulation can explain the process of forming channels by angle-deposited films to a certain extent, and predict the channel size. In addition, the simulation results, in turn, can guide the film deposition process, so as to control the size of nano channel.

1. INTRODUCTION
The core of the fabrication of micro/nano-fluidic chips is the fabrication of micro/nano-fluidic channels [1-2]. The common processing method is to first use nano-imprinting [3], lithography [4], electron beam lithography [5] and other technologies to make nano groove structure, and then combine the thermal bonding technology [6-8] to seal the channel. However, during the bonding process, the bonding materials in the molten state will inevitably flow into the channel groove structure. With the decrease of the channel size, especially when the channel size reaches nanometer level, the bonding
method can easily lead to channel blocking, which has a negative impact on the precise control of channel size and process reliability. Therefore, the bonding sealing method is mainly used for the fabricating of channels with micron size and above.

From the previous paper [9], we know that angle film deposition can be used to seal channels, so as to solve the channel blockage problem of channel sealing. In addition, by controlling the deposition angle, the shape of the sealed channel can be controlled. In order to understand the channel formation process more intuitively, the free molecular flow module of COMSOL software is used to simulate the film deposition process. The growth of the film is characterized by the post-processing of geometric deformation, so as to predict the channel shape. By comparing the simulation results with the experimental results, it can be seen that this simulation can explain the process of forming channels by angle-deposited films to a certain extent, and predict the channel size. In addition, the simulation results, in turn, can guide the film deposition process, so as to control the size of nano channel.

2. FILM DEPOSITION SIMULATION

2.1 The Simulation Principle
In the process of film deposition, the air pressure in the vacuum chamber is below $10^{-1}$ Pa. In this environment, the average free path of the particles is very large, and the collision between the particles and the wall has replaced the internal collision of particles as the main form of motion. Under this condition, the particle motion state belongs to the free molecular flow. Therefore, this simulation is based on the COMSOL molecular flow module, through the angle coefficient method, to calculate the distribution of the film after deposition in the groove substrate.

Meanwhile, in the result post-processing, the accumulated film thickness in the X, Y direction is added to the "deformation" command. With this command, the geometric deformation of the substrate in the X, Y direction is controlled, and the growth of the film at the groove can be visualized, and the shape of the formed channel can be predicted.

2.2 Model Building
In the actual film deposition experiment, the target material in the cavity is bombarded by ion beam, and the target particles are splashed out and then spread to the substrate. In order to achieve different angle film deposition, we put wedge block with different angle under the substrate. For simulation modeling, first we set a vacuum chamber, as shown in Figure 1, and set the emission source at the top right. The nano groove structure is arranged at the bottom. The height and width of the nano-groove are both 200 nm, which is consistent with the actual experiment. In addition, in order to save calculation times, the groove is set at different positions of the bottom to simulate the film deposition process at different angles.

![Figure 1. Model Building](image-url)
Different from the traditional molecular dynamics simulation to calculate the flow field distribution, the motion state of particles in this simulation belongs to molecular flow. When particles are emitted from the emission source, their velocity value and direction have been determined. Because the impact of the collision between the particles on the deposition is small, the collision between the particles is not considered.

In order to more accurately simulate the film deposition process, we use an independent random function variable (rand) to characterize the velocity and direction of the particles released from the target material. For constraining the angle of particles deposited on the substrate, a collimator is set up above the nanogroove. During the flight of the particles, the energy of the particles is not lost. When the particle touches the wall surface and the nano-groove, we will set it to "frozen". The desorption probability and secondary electron effect are not considered in the simulation.

2.3 Meshing
The size and shape of the mesh will affect the calculation time and the accuracy of the results. Larger grids may achieve faster calculation speeds, but accuracy cannot be guaranteed. A grid that is too small may greatly reduce the calculation efficiency. Therefore, the size of the grid needs to be set according to the actual problem. In this paper, the entire model is divided into free triangle meshes. For the part of the grooved substrate, it is necessary to accurately calculate the film deposition at this location, therefore, a denser grid is needed. We set the grid size of this part to be equal to the particle diameter, that is, 0.2 nm. For other areas, we do a roughening process to reduce the amount of calculation. The model diagram after meshing is shown in the Figure 2.

![Meshing](image)

Figure 2. Meshing

2.4 Post-Processing
In the post-treatment, we calculate the deformation in X, Y direction according to the thickness of the deposited film on the substrate surface. As the number of "frozen" particles increases, the groove wall continues to deform until the sum of the deformations of the two sidewalls is equal to the channel width, that is, the groove substrate is closed and the channel structure is formed, then the calculation stops. The maximum width D of the channel can be read by software.
2.5 Simulation Results
We set up three groups of different inclination angles (35°, 25°, and 10°) to simulate the film deposition. The simulation results are shown in Figures 3, 4, and 5. It can be seen from the results that the channel structure is formed by the film growth, and the channel size gradually decreases as the incident angle becomes smaller.

![Figure 3. Simulated deposition result at 35°](image1)

![Figure 4. Simulated deposition result at 25°](image2)
3. Angled Film Deposition to Seal Nanochannels

3.1 Experimental Process

The process of angle film deposition and sealing of nanochannels mainly includes three steps. First, the fabrication of imprint template. Second, the replication of the nanogrooves structure. Third, the angle-deposited film to seals the channel.

(1) Fabricating of imprinting template

The original imprinting template is made by laser holographic lithography. The minimum linewidth of the template is 200 nm. The main steps are: first, the photoresist AZ1350 is spin-coated on a cleaned and dried quartz substrate. Secondly, through laser holographic lithography technology, patterned photoresist. After development, the remaining photoresist is as the etching mask. Finally, silicon was etched by reactive ion etching to obtain nano-groove structure. The etching plasma is a mixture of Ar and CHF3 gas.

(2) Replication of nano-groove structure

Through nano-imprinting technology, the groove structure on the imprinting template is transferred to SU-8. The main steps are as follows: first, SU-8 photoresist is spin coated on the silicon substrate. Secondly, cover the template on the photoresist and transfer the graphics under certain pressure. Finally, after UV exposure, Post-baking and demolding, the pattern reproduction is completed.

The specific steps refer to our previous work [10].

(3) Sealing of the channel

After the SU-8 nano-groove structure is fabricated, the channel is sealed by angle film deposition. The process is shown in Figure 6. Through the coating machine, the SiO2 film is deposited into the groove at a certain angle and the channel is sealed. When the angle of incidence is different, the size of the channel formed will also change accordingly. This method can effectively control the channel size without re-creating the template. The coating angles (θ) selected in this paper are 35°, 25°, and 10° [9].
3.2 Experimental Results
As shown in Fig. 7, Fig. 8, and Fig. 9, the channel size is 127 nm when the inclination is 35°, the channel size is 110 nm when the inclination is 25°, and the channel size is 44.5 nm when the inclination is 10°.
4. RESULTS COMPARISON AND DISCUSSION

This article uses COMSOL software, using free molecular flow combined with deformed geometric post-processing method to simulate the process of film growth and channel formation on the groove-shaped substrate. It is the same as the film deposition angle selected in the experiment. The simulation also selected three deposition angles of 35°, 25°, and 10°. Through the calculation of the deformed geometry by COMSOL post-processing, the widest dimensions of the channels obtained by the simulation are 168nm, 130nm and 60nm, respectively, as shown in Figures 3, 4 and 5. Compared with the experimental results (127nm, 110nm, 44.5nm), the simulation results are generally larger (as shown in Figures 7, 8, and 9). However, the trend still has a certain reference value, that is, by changing the film deposition angle, the shape and width of the channel can be changed. Especially when the inclination angle is reduced, such as 10°, the simulated channel shape and size are closer to the experimental results.

The main reason for the simulation error is that when the COMSOL software starts to calculate, although the deposition caused the deformation of the groove wall, the subsequent deposition did not recognize the deformation. As a result, the subsequent film deposition can only accumulate on the original groove wall. The actual situation is that the film layer will continue to grow on the basis of the deposited film layer. Another reason is that in the actual experimental measurement process, the place we measured is the place with the largest width observed by the naked eye, and this may not be the place with the largest channel width. So, the actual measured width is smaller than the simulated data.

5. SUMMARY AND FUTURE WORK

In this paper, a nano-groove structure was fabricated by holographic lithography and nano-imprinting, and nano-channel structures of different sizes were obtained by depositing films at different angles. In order to visually describe the process of forming nanochannels by angle thin film deposition, this paper calculated the film deposition by the COMSOL software molecular flow module, and obtained the shape and size of the formed channel by post-processing. By comparing the simulation results with the experimental results, it can be seen that the simulation results are similar to actual experimental results. It can be seen that this simulation can explain the process of forming channels by angle-deposited films to a certain extent, and predict the channel size. Thus, the simulation results, in turn, can guide the film deposition process, so as to control the size of nano channel.

The current simulation method still has shortcomings and it cannot accumulate film on the deformed boundary. To achieve this, bidirectional coupling of deposition and deformation is needed. This is where the simulation needs to be improved in the future.
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