Effective 3-D Process Modeling and Parameters Determination on Double Exposure in Deep X-ray Lithography

Yoshikazu Hirai, Naoki Matsuzuka and Osamu Tabata

Abstract

This paper describes a new analytical method to determine process parameters on Double Exposure in Deep X-Ray Lithography (D^2XRL). D^2XRL is a unique and promising technique for 3-dimensional (3-D) microfabrication among 3-D X-ray lithography techniques. By way of example, it was demonstrated that a micro-projection array with a very sharp tip is easily and successfully fabricated without any special apparatus. In order to advance the capabilities of D^2XRL to realize 3-D microstructures and MEMS devices, we have proposed the analytical method that is possible to calculate resist profiles of a 3-D microstructure fabricated by D^2XRL. The advantage of the newly proposed analytical method is that an effective relationship between resist profiles and process parameters on D^2XRL is derived directly from relational expressions. By the comparisons between resist profiles calculated by the analytical method and experimental results, it was successfully confirmed that this approach provides an easy way to realize the target micro-projection structures with an acceptable accuracy.
1. **INTRODUCTION**

Standard high-aspect-ratio Micro Electro Mechanical Systems (MEMS) are typically fabricated using LIGA (German acronym for Lithographie, Galvanoformung, Abformung) or other processes, e.g. Deep Reactive Ion Etching (DRIE), micro Electro-Discharge Machining (EDM), and UV lithography using SU-8®. The LIGA process is one of the most promising MEMS fabrication techniques, and this employs Deep X-Ray Lithography (DXRL) to produce plastic microstructures with feature sizes down to 0.1 µm. Conventional DXRL is good at fabricating high-aspect-ratio microstructures with vertical sidewalls. However, this technique has very limited controllability of the cross-sectional shape of 3-dimentional (3-D) microstructures. In order to apply DXRL to various fields such as MEMS devices and medical devices, several 3-D X-ray lithography techniques and its extension have been proposed by various research groups [1-3]. Compared with the previously reported 3-D X-ray lithography techniques, Double exposure in Deep X-Ray Lithography (D₂XRL) shown in Fig. 1 is a unique and promising technique for 3-D microfabrication. By way of an example, it was demonstrated that a micro-projection with the very sharp tip is easily and successfully fabricated without any special apparatus [4].

In order to advance the capabilities of D₂XRL to fabricate 3-D microstructures for MEMS devices, this study is aiming at an establishment of an effective analytical method of D₂XRL process which facilitates the realization of target 3-D microstructures precisely. The advantage of the newly proposed analytical method is, once “dissolution rate as a function of depth $z$” is determined, effective relationship

![Diagram](image.png)

**Fig. 1.** Schematic illustration of the process steps in D₂XRL (Step; (a) $\rightarrow$ (b) $\rightarrow$ (c)): (a) the normal exposure step; (b) the mask-less exposure step; (c) the image of fabricated structure by normal and mask-less exposures (i.e. D₂XRL); (d) the image of fabricated structure by normal exposure (i.e. DXRL).
between resist profiles and process parameters on $D^2XRL$ is derived directly from relational expressions. In this paper, a micro-projection was utilized as an example to demonstrate a validity of the analytical method and a verification of prediction accuracy through experiments is described.

2. DESCRIPTION OF 3-D PROCESS MODELING

2.1 PROCESS STEPS AND MECHANISM OF $D^2XRL$ [4, 5]

Figure 1 shows the process steps of the micro-projection structure by $D^2XRL$ using an X-ray mask with a circular absorber. If a poly-methylmethacrylate (PMMA), the most commonly used positive-tone thick photoresist in X-ray lithography, is developed after the exposure process (step: (a) $\rightarrow$ (d)), a cylindrical microstructure with the vertical sidewall is fabricated. In $D^2XRL$, a mask-less exposure as shown in Fig. 1 (b) is combined with a normal exposure before the development process. On $D^2XRL$ technique, the major process parameters are a combination of deposited dose on 1st and 2nd exposure steps and a development time as shown in Fig. 2. The tip angle tends to be sharpened when the ratio of the deposited dose on exposure (a) to the deposited dose on exposure (b) is higher. Figure 3 shows schematic of dose distribution in a PMMA depth direction given by $D^2XRL$ and a simplified development behavior. The development behavior to realize the micro-projection can be understood as follows. In the development process, the area A dissolves faster than area B because the dissolution rate increases exponentially to dose. Then, a step is formed at the boundary between area A and B regions. Since development is isotropic, the sidewalls of the steps are exposed to the developer and developed. This leads to rounding of corners and sidewall inclination. The theory for understanding these phenomena has been already confirmed in our previous experiments and simulation results [6, 7].

2.2 3-D PROCESS MODELING AND LITHOGRAPHY SIMULATION SYSTEM (X3D)

Development of a resist profile simulation tool and an analytical method to determine process parameter is a major interest among 3-D X-ray lithography research groups. One explanation for this interest is that there are a lot of complicated process parameters and difficulty in determining these parameters. In addition, the most important point of modeling 3-D X-ray lithography process accurately is that resist profile simulation tool should take into account a dissolution vector as well as the resultant dose distribution. In that case, the problem is how to model the propagation
of the dissolution front and calculate its profile at any development time. So far, the 3-D X-ray lithography simulation system (X3D) [7, 8], which adopted the Fast Marching Method [9] in development process simulation, has been the only approach to be able to handle this problem. Figure 4 (a) shows the simulated cross sectional view of a resist profiles for D²XRL using the Fast Marching Method. Figure 4 (b) shows more detail simulated results in three dimension by X3D. However trial and error is required to determine optimal process parameters. Therefore, a simple analytical method to determine the process parameters is required to advance the capabilities of D²XRL to fabricate MEMS devices.

<table>
<thead>
<tr>
<th>Development time [min]</th>
<th>Ratio of deposited dose “exposure (a) : exposure (b)”</th>
<th>1.0 : 2.2</th>
<th>2.1 : 1.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
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</tr>
<tr>
<td>120</td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 2. SEM images of micro-projection structures with different development time and deposited dose pattern. These structures were fabricated by the X-ray mask with an absorbers pattern of 15 µm in diameter. Deposited dose of “exposure (a)” and “exposure (b)” are corresponding to the exposure step in Fig. 1.

Fig. 3. Illustration of the development behaviors in D²XRL.
3. ANALYTICAL METHOD

3.1 CALCULATION OF RESIST PROFILES

A concept of the analytical method for the resist profile calculation is shown in Fig. 3. In this method, the resist profile is calculated by combining individually calculated vertical and lateral propagations of dissolution front [10]. A schematic of computational procedure is the follows.

1) Vertical Propagation of Interface: The relationship between the development time \( T \) and resist depth \( z \) is given by Eq. (1)

\[
T = V'(z) = \int_0^z R(z)^{-1} dz
\]

where \( R(z) \) is the dissolution rate as function of depth \( z \). Thus, the depth \( z \) is given by

\[
z = V^{-1}(T)
\]

Therefore, a resist profile that only takes into account the vertical propagation is calculated by substituting the dissolution rate \( R_A(z) \) and \( R_B(z) \), which indicate the dissolution rates for area A and B, respectively. Next, Eq. (2) is transformed to Eq. (3) by utilizing the position \( x \) and depth \( z \) as shown in Fig. 3 (c),

\[
z = V^{-1}(x, T)
\]

Fig. 4. Examples of resist profiles simulation tool for D²XRL: (a) Fast Marching Method; (b) X3D.
where

\[ T = V(x, z) \]

\[ = V_A(z) = \int_0^z R_A(z)^{-1} \, dz \quad \text{for } x \text{ at area A} \]

\[ = V_B(z) = \int_0^z R_B(z)^{-1} \, dz \quad \text{for } x \text{ at area B}. \]

2) **Lateral Propagation of Interface:** The propagating length \( x_p \) from the boundary between area A and B toward area B is given by

\[ x_p = L(z, T) = R_B(z)t(z) = R_B(z)(T - \int_0^z R_A(z)^{-1} \, dz) \]  \hspace{1cm} (4)

where \( t(z) \) is the lateral propagating time \( t \) which is given as a function of depth \( z \). Since \( x_p \) corresponds to a position along the \( x \)-axis, depth \( z \) at position \( x \) is given as

\[ z = L^{-1}(x,T). \]  \hspace{1cm} (5)

3) **Combined Propagations of the Procedure 1) and 2):** Based on results of Eqs. (3) and (5), the resist profiles are plotted. Please note that prior knowledge of the dissolution rate \( R_A(z) \) and \( R_B(z) \) is necessary to calculate resist profiles. This dissolution rate as a function of depth \( z \) is determined by a dedicated experimental method [4].

### 3.2 Experiments and Validation of Analytical Model

Experiments were carried out at BL-15 of “AURORA” at Ritsumeikan University. In the 1st exposure step (Fig. 1 (a)), PMMA (CLAREX commercialized by Nitto Jushi Kogyo Co., Ltd.) is exposed using the X-ray mask (fabricated by Optnics Precision Co., Ltd.) with an absorbers pattern of 10 µm in diameter. In the development process, the GG developer (60 vol% 2-(2-n-butoxyethoxy) ethanol, 20 vol% tetrahydro-1-4-oxazine, 15 vol% de-ionized water, and 5 vol% 2-aminoethanol) was used at a development temperature of 39.0 °C. The experimental conditions for the fabrication and a resist profiles simulation were summarized in Table 1.

Figure 5 shows the resist profiles of samples number 1 to 2 and 3 to 4. The depth zero corresponds to the original resist surface. The comparison between measurements, simulation results, and error is summarized in Table 2. From this result, it is confirmed that the structural shapes are calculated with acceptable accuracy. It is thought that the difference between the measurements and calculated resist profiles was caused by the measurement accuracy of the dissolution rate, and the experimental repeatability. The improvement of the experimental accuracy will enable us to calculate the resist profiles more accurately.
Table 1. Experimental conditions for the fabrication and the resist profile simulation of micro-projection: (a) setup parameters for exposure process at BL-15; (b) experimental parameters on sample number of micro-projection.

(a)

<table>
<thead>
<tr>
<th>SR (AURORA)</th>
<th>Operating electron energy $\varepsilon$</th>
<th>0.575 GeV</th>
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<tbody>
<tr>
<td></td>
<td>Critical wave length $\lambda_c$</td>
<td>1.5 nm</td>
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<tr>
<td></td>
<td>Typical source size (vertical) $\sigma_y$</td>
<td>0.14 mm</td>
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<tr>
<td></td>
<td>Distance between source to mask $D$</td>
<td>3.88 m</td>
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<table>
<thead>
<tr>
<th>Exposure parameter</th>
<th>Filter (Be)</th>
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</tr>
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<tbody>
<tr>
<td>Scan length</td>
<td>20 mm</td>
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</table>

<table>
<thead>
<tr>
<th>X-ray mask</th>
<th>Absorber (Au)</th>
<th>2.0 $\mu$m</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Membrane (Polyimide)</td>
<td>50 $\mu$m</td>
</tr>
</tbody>
</table>

(b)

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Deposited dose Mask [A·min]</th>
<th>Mask-less [A·min]</th>
<th>Development time [min]</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>3.0</td>
<td>2.0</td>
<td>30</td>
</tr>
<tr>
<td>2</td>
<td>3.0</td>
<td>2.0</td>
<td>60</td>
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<tr>
<td>3</td>
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<td>3.0</td>
<td>30</td>
</tr>
<tr>
<td>4</td>
<td>3.0</td>
<td>3.0</td>
<td>60</td>
</tr>
</tbody>
</table>

Fig. 5. Comparison between measurements and simulation results of resist profiles; (a) sample No. 1 to 2; (b) sample No. 3 to 4.

Table 2. Comparison between measurements, simulation results, and error.

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>(a) Measurement</th>
<th>(b) Simulation</th>
<th>(c) Difference</th>
<th>(d) Error</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>22.1</td>
<td>30.8</td>
<td>22.2</td>
<td>32.7</td>
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<tr>
<td>2</td>
<td>24.7</td>
<td>33.7</td>
<td>21.7</td>
<td>35.6</td>
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<tr>
<td>3</td>
<td>15.9</td>
<td>45.1</td>
<td>14.9</td>
<td>46.3</td>
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<tr>
<td>4</td>
<td>17.9</td>
<td>46.2</td>
<td>14.9</td>
<td>47.1</td>
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</table>
3.3 Determination of Process Parameters

The analytical method is useful to determine the process parameters for the target micro-projection. The advantage of this approach is that the relationship of the height and tip angle of micro-projection on development time can be derived directly from related equations. When the absorber pattern is a circle, the height and tip angle are given by Eqs. (6) and (7) respectively,

\[ H = V_A^{-1}(T) - L^{-1}(r, T) \quad \text{for} \quad L^{-1}(r, T) - V_B^{-1}(T) > 0 \]
\[ H = V_A^{-1}(T) - V_B^{-1}(T) \quad \text{for} \quad L^{-1}(r, T) - V_B^{-1}(T) \leq 0 \]

where \( r \) is the radius of the X-ray mask absorber pattern,

\[ \theta = -2 \arctan \left[ \frac{\partial}{\partial z} L(z, T) \right] \bigg|_{z=h} \quad \text{for} \quad L^{-1}(r, T) - V_B^{-1}(T) > 0 \]
\[ \theta = 180 \text{ [deg]} \quad \text{for} \quad L^{-1}(r, T) - V_B^{-1}(T) \leq 0 \]

where \( r = L(h, T) \). Figure 6 shows the dependences of the height and tip angle of the micro-projection on development time. The measurements of the tip angle show the small range from 30.8° to 46.2°. The tip angle tends to be sharpened by increasing the ratio of the deposited dose with the X-ray mask to the deposited dose without the X-ray mask. The same tendency was observed in the experimental results shown in Fig. 2. The minimum tip angle (i.e. the sharpest tip angle) confirmed by this method is 16.6° on the condition that the deposited dose with and without the X-ray mask are 6.0 A·min and 1.0 A·min, respectively, at the development time of 168 min. The maximum one is 84.54° on the condition that the deposited dose with and without the

![Fig. 6. The dependence of the height and tip angle of micro-projection on development time; (a) relationship between the development time and the height: (b) relationship between the development time and the tip angle.](image-url)
X-ray mask are 0.5 A·min and 4.0 A·min, respectively, at the development time of 144 min. From these results, the validity and efficiency of the analytical method to determine process parameters were confirmed.

4. CONCLUSION

The analytical method to determine the process parameters for D²XRL was successfully demonstrated with acceptable accuracy through the fabrication of micro-projection. By applying the analytical method, the parameters of micro-projection such as the height and tip angle were calculated easily and quickly. Consequently, the validity of the proposed approach was confirmed for determining the process parameters to realize the target 3-D microstructures. In future, good control of process parameters based on the proposed approach may lead to fabrication of MEMS devices.

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REFERENCES


