Process Simulation of Moving Mask Deep X-Ray Lithography

Yoshikazu Hirai[1], Sadik Hafizovic[2], Naoki Matsuzuka[3]
Jan G. Korvink[4], and Osamu Tabata[1]

Abstract

This paper presents a newly developed 3-Dimensional (3D) simulation system for Moving Mask Deep X-ray Lithography (M^2DXL) process, and its validation. The simulation system named X-ray Lithography Simulation System for 3-Dimensional Fabrication (X3D) is tailored to simulate a fabrication process of 3D microstructures by M^2DXL. X3D consists of three modules: mask generation, exposure and development. The exposure module calculates a dose distribution in resist using a generated X-ray mask pattern and its movement trajectory. The dose is then converted to a resist dissolution rate. The development module adopted the "Fast Marching Method" technique to calculate the 3D dissolution process and resultant 3D microstructures. This technique takes into account resist dissolution direction that is necessary for accurate 3D X-ray lithography simulation. The comparison between simulation results and measurements of "stairs-like" dose deposition pattern by M^2DXL showed that X3D correctly predicts the 3D dissolution process of exposed PMMA.

[1]*Graduate School of Engineering, Kyoto University, Yoshida-Honmachi, Sakyo-ku, Kyoto 606-8501, Japan*

[2]*Physical Electronics Laboratory, ETH Zurich, Hoenggerberg HPT-H4.2, Wolfgang-Pauli-Strasse 16, 8093 Zurich, Switzerland*

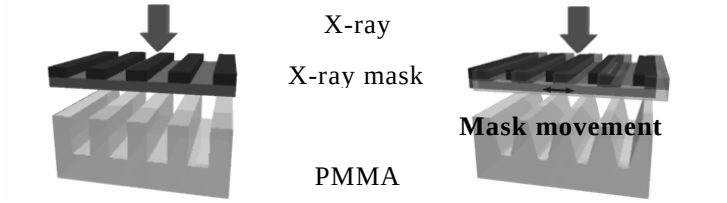
[3]*Graduate School of Science and Engineering, Ritsumeikan University, Noji-Higashi, Kusatsu, Shiga 525-8577, Japan*

[4]*IMTEK-Institute of Microsystem Technology, University of Freiburg, Georges-Koehler-Allee 102, D-79110 Freiburg, Germany*

1. INTRODUCTION

The LIGA process employs **D**eep **X**-**R**ay **L**ithography (DXRL) to produce metal or plastic microstructures that feature sizes down to 1 μm or less. In order to realize such a microstructure, a thick resist is first exposed to Synchrotron Radiation (SR) through an X-ray mask and the exposed resist is developed. By combining DXRL with subsequent electroplating and molding, replication of the fabricated microstructures in various materials such as plastics, metals and ceramics become possible. Conventional DXRL is good at fabricating microstructures with vertical sidewalls and high aspect ratio microstructures. However, this technique has very limited controllability of the cross-sectional shape of 3-dimensional (3D) microstructures. In order to apply DXRL to various fields such as micro-sensors, micro-actuators and MEMS devices, more flexible and precise controllability of the 3D microstructure is demanded. To address these requirements, several techniques have been proposed such as **M**oving **M**ask **D**eep **X**-ray **L**ithography (M^2DXL) technique [1], its extension [2] and inclined exposure technique [3]. M^2DXL technique shown in Fig. 1 is one of the highly promising 3D X-ray lithography techniques to realize 3D microstructures with free shaped and inclined walls [1, 4, 5]. In M^2DXL, the 3D microstructure is defined by an X-ray mask trajectory and the resultant dose distribution in resist.

On the other hand, very little attention has been paid to "3D" X-ray lithography simulation in these techniques. P. Meyer et al. [6] have focused on the determination of an optimal set of parameters for an X-ray lithography beamline and development condition. S. K. Griffiths et al. [7] have studied the dose distribution near an X-ray mask absorber edge due to photoelectron dose and the effects of this distribution on the 2D time series of development profile with analytical and numerical methods. Hagouel [8] models theoretically the development process of X-ray lithography and he solved the Hamilton-Jacobi equation by applying ray tracing techniques. However, there is little adaptability for 3D X-ray lithography techniques because these studies do not cover 3D geometrical aspects in the simulation. Another study on 3D



Conventional Deep X-Ray Lithography (DXRL)

Moving Mask X-ray Lithography (M^2DXL)

Fig. 1. Concept of M^2DXL.

development simulation developed by S. B. Bollepalli et al. [9] has targeted a thin resist geometry handling since this investigation was motivated by microelectronics manufacturing. Consequently, there has been no study of 3D simulation system that covers the complete process of 3D X-ray lithography technique including both X-ray exposure and development process of 3D microstructures as time series.

We have reported in previous work [10] that the dose distribution in resist and the resist dissolution direction are not sufficient to correctly calculate a 3D dissolution process and resultant 3D microstructures. Therefore, our target simulation system necessarily should take into account an X-ray exposure with M^2DXL technique and a development process. Based on this consideration, an X-ray lithography simulation system named **X**-ray Lithography Simulation System for **3**-**D**imensional Fabrication (X3D) was newly developed [11]. X3D calculates the propagation of the dissolution front and resist dissolution direction as required for 3D X-ray lithography simulation. Therefore, X3D enabled to simulate the 3D dissolution process and resultant 3D microstructures. In this respect, our simulation system differs from previously reported X-ray lithography simulation. From these viewpoints, X3D is tailored to simulate the fabrication process of 3D microstructures using M^2DXL and its capabilities are fundamental to put M^2DXL in practical use. Furthermore, the newly developed X3D enables us to fabricate rapid prototyping of 3D microstructures and greatly save time and cost for product development. This paper presents the structure of X3D, and the verification of simulation results for the first time.

2. DESCRIPTION OF X3D

2.1 ARCHITECTURE OF X3D

X3D for M^2DXL consists of three modules shown in Fig. 2: mask generation, exposure and development. The parameters of the SR source and the beamline, the X-ray mask layout data, the multiple stage system movement data, and experimental resist dissolution rate data are major inputs in this simulation system. The mask generation module can interface to multiple CAD database formats such as GDS-II and CIF. The exposure module models the X-ray lithography beamline components (filters and an X-ray mask), as well as X-ray mask movement on the multiple stage system. Here, transmission and absorption values of filter and X-ray mask materials required for dose calculation are retrieved from an optical properties database in X3D. To find out the resist dissolution rate at some location, X3D first calculates dose and then converts this dose to a rate by means of experimentally measured dose-dissolution rate relationship. The development module adopted the Fast Marching Method [12]

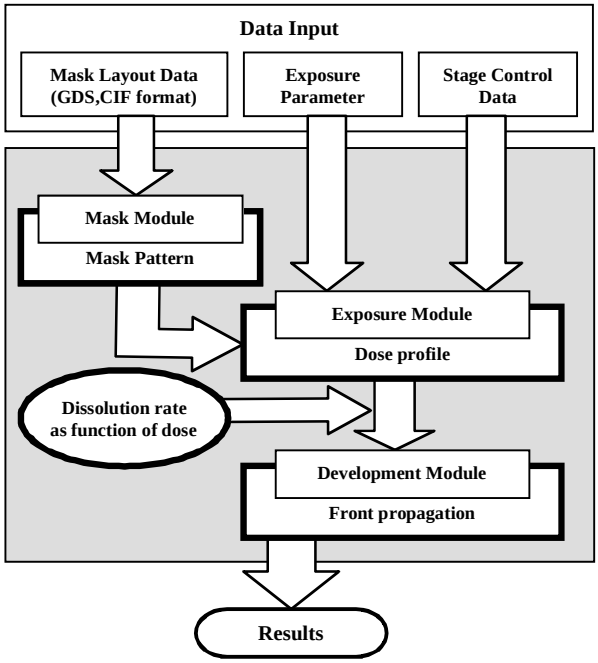


Fig. 2. Data flow in X3D.

to calculate the resultant 3D microstructure based on the experimental resist dissolution rate.

All of X3D's results, such as X-ray spectra in resist and dose distribution for any spatial region in the simulation domain are readable in *Mathematica*™ for further analysis. Additionally, geometrical data of a resultant 3D microstructure at an arbitrary time is extracted for visualization in graphical tool, e.g. *POV-Ray*.

2.2 EXPOSURE SIMULATION

The exposure simulation that calculates dose distribution in resist is composed of X-ray lithography components: the SR source, beamline filters, and the multiple stage system. The dose is defined as the amount of X-ray energy absorbed per unit volume and relates to the resist solubility into a developer [13, 14]. So the dose calculation should take into account the SR spectrum, X-ray transmission through filters and the X-ray mask membrane, photon absorption in resist, and also account for the X-ray mask movement on the multiple stage system.

Here, we introduce the plane corresponding to the initial resist surface as x-y plane, and the resist depth from the surface (z = 0) down to the bottom as z. In case of 3D X-ray lithography techniques including M^{2}DXL, dose has a variation not only in z direction but also in the x-y plane. Then at a specific point on the resist surface (x, y), the dose "*Dose* (x, y, z)" as a function of z can be expressed as [15, 16],

$$Dose(x, y, z) = T_E(x, y) I \int N(\lambda) B(\lambda) A(\lambda, z) T_F(\lambda) T_M(\lambda) d\lambda \qquad (1)$$

where λ is wavelength, T_E (x, y) is effective exposure time determined in accordance with X-ray mask trajectory, I is stored electron beam current, N (λ) is photon flux spectral distribution through per unit area, B (λ) is conversion factor from photon to energy units, A (λ, z) is absorption coefficient per unit length of the resist at depth z, T_F (λ) and T_M (λ) are transmission coefficients of filter T_F and X-ray mask membrane T_M. More accurate descriptions of the SR source, photon flux calculation, and the dose calculation will not be discussed in this paper.

2.3 DEVELOPMENT SIMULATION

The development simulation, calculates the resist dissolution process based on the results of exposure simulation, and relies on the Fast Marching Method. In order to calculate the 3D dissolution process only on the demanded simulation domain sizes, an "adaptive refinement" technique for Fast Marching Method was developed [11]. This technique allows us to overcome memory restrictions and improve computational speed. Thereby, X3D made it possible to simulate realistic MEMS devices of sizes in the order of mm on a standard engineering workstation, e.g. the simulation of a domain size of 10 mm x 5 mm x 0.2 mm = 10 mm^3 with a minimum detail size of 0.5 μm. The detailed discussion of X3D capability and framework are communicated in a separate publication [11].

3. MATHEMATICAL MODEL FOR DEVELOPMENT SIMULATION

3.1 PHYSICAL AND MATHEMATICAL PRINCIPLES

At any point of development time in the lithography development process, the interface between developer and undeveloped resist is defined as a boundary. The dose distribution is defined as a function of position by Eq. 1 and the resist dissolution rate is defined as a function of dose. From these relations, the dissolution rate is defined as a function of position and the developer-resist interface propagation is dominated by this dissolution rate. If there is a dose distribution only perpendicular to the surface (i.e. this is the case for conventional DXRL), the dissolution front moves perpendicularly only. On the other hand, if there is also a lateral dose gradient (i.e. in case of 3D X-ray lithography), the dissolution rate vector of the front is not perpendicular to the initial surface anymore; namely the dissolution front tends to move faster to the higher dose direction. The problem posed is how to model the propagation of the dissolution front and predict its profile and position at any moment

in the development process.

3.2 Level Set Method and Fast Marching Method

There are two numerical techniques to track a moving of 3D structures interface, “Level Set Method” and “Fast Marching Method”, introduced by J. A. Sethian [12]. These techniques cover a wide range of applications including problems of optics, seismology, path planning, robotic navigation, and fluid mechanics. Although they are fundamentally “different approaches” to address the problem of moving interface tracking, a common theory and numerical methodology are utilized in terms of moving interface tracking. The Level Set Method is developed for problems where an interface moves forwards in some places and backwards in others. The Fast Marching Method is designed for problems where an interface always moves in one direction, either forwards or backwards. Due to this constraint, the Fast Marching Method is significantly faster and computationally cheaper than the Level Set Method. Our resist dissolution problem has the property that the resist dissolution front always moves “one-way”. In other words, resist always dissolves and cannot be deposited. For this reason, the Fast Marching Method was applied to our problem.

4. System Validation and Discussion

4.1 Stairs-like Dose Deposition Pattern

To demonstrate a system validation of the developed X3D, a “stairs-like” dose deposition pattern shown in Fig. 3 was chosen. Despite of the dose deposition pattern’s geometrical simplicity, both necessity and validity of X3D which takes into account “local properties” discussed in 3.1, i.e. a dose distribution in resist and a resist dissolution direction, to calculate correctly the 3D dissolution process are clearly shown. The unique feature of the stairs-like pattern can be understood as follows. As shown in Fig. 4, the dissolution front moves faster in areas of high dose than in areas of low dose. Where the high and low dose regions meet, a step is formed. Since development is isotropic, the exposed sidewall is also subject to dissolution. This leads to rounding of corners and sidewall inclination. If a simulation system does not consider this local dissolution phenomenon, the obtained result becomes unreliable, i.e. the sidewall shape is vertical and the rounded off corner is not obtained.

The stairs-like pattern was deposited into the resist (PMMA: Poly-methylmethacrylate, CLAREX with 1.0 mm thickness commercialized by Nitto Jushi Kogyo Co., Ltd.) surface using an X-ray mask with a window width of 50 μm and a mask movement of 30 μm by M^2DXL. For the experiment and simulation, a

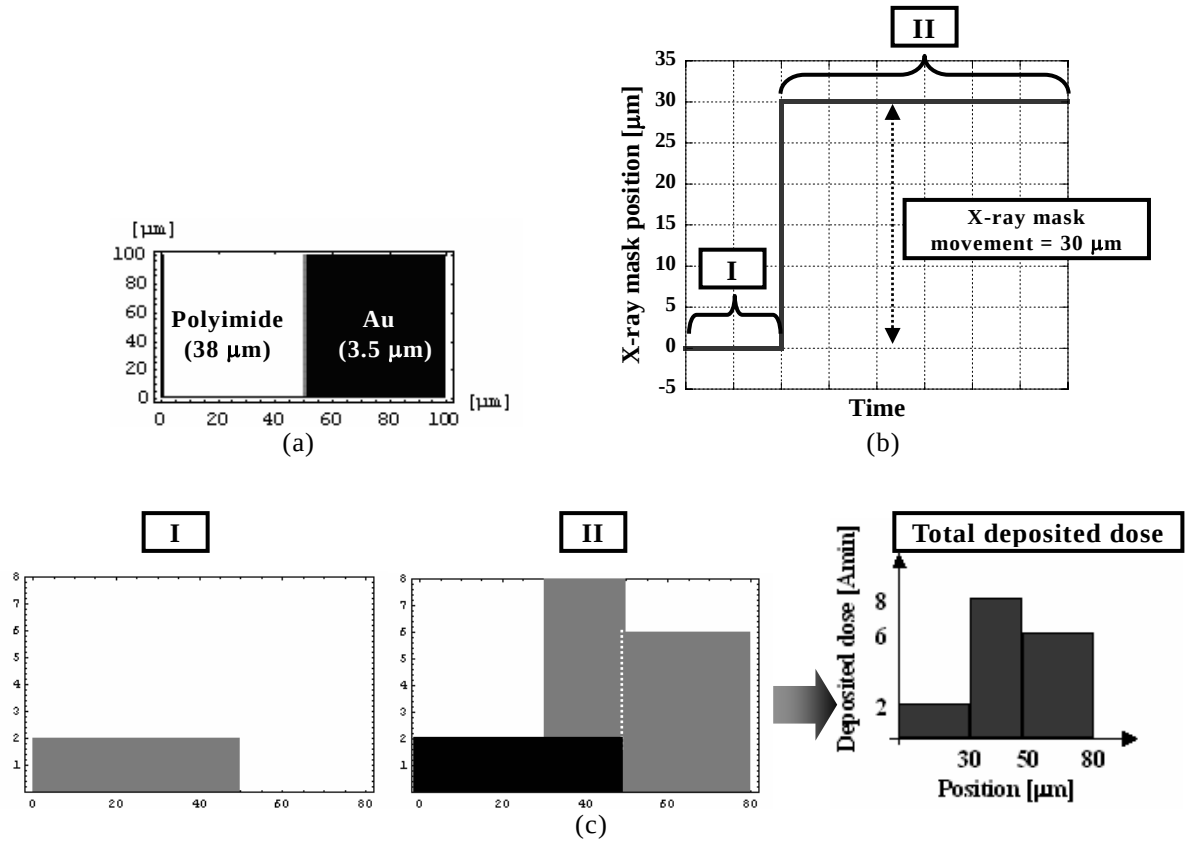


Fig. 3. (a) The X-ray mask pattern. (b) The X-ray mask movement pattern of the "stairs-like" dose deposition pattern. (c) The deposited dose given by M^2DXL. In Fig. 3 (c), I and II show the dose deposited by the coresponding phases I and II in Fig. 3 (b).

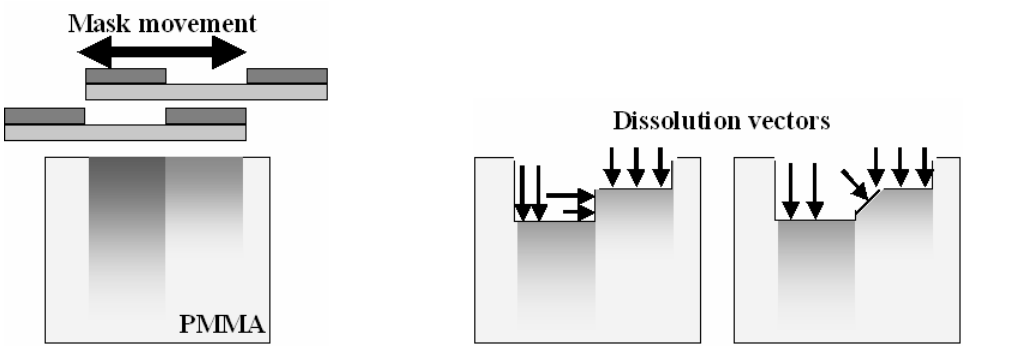


Fig. 4. (a) shows the dose profile deposited by M^2DXL and (b) shows the dissolution direction and rounded off edge. In this development process, the dissolution direction is affected by the dose distribution in resist.

dose of 1 A·min corresponding to a net X-ray dose of 9.61 J/cm^2 onto the PMMA was deposited. To develop exposed PMMA samples, GG-developer (15 vol% DI water, 60 vol % 2-(2-butoxyethoxy)ethanol, 20 vol % tetrahydro-1-4-oxazine and 5 vol % 2-aminoethanol) is used at a temperature of 39 ºC with a magnetic stirrer. The

Table 1. Simulation parameters

SR (AURORA)	Operating electron energy	ε	0.575 GeV
	Critical wave length	λ_c	1.5 nm
	Typical source size (vertical)	σ_y	0.14 mm
	Distance between source to mask	D	3.88 m
Exposure parameter	Filter (Be)		200 μm x 2
	Scan		20 mm
	X-ray mask movement		30 μm
X-ray mask	Absorber (Au)		3.5 μm
	Membrane (Polyimide)		38 μm
Development parameter	Developer		GG-developer
	Temperature		39 °C

following results and discussion are based on the simulation parameters summarized in

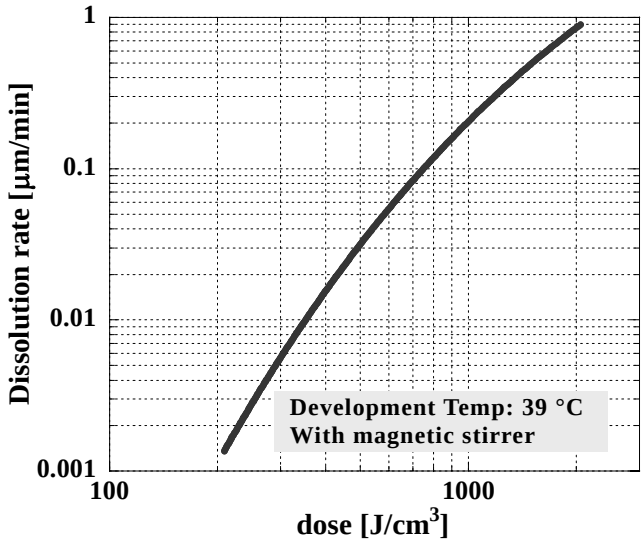


Fig. 5. Experimental dissolution rate as a function of dose.

Table 1. The experimental dissolution rate as a function of dose shown in Fig. 5 was used which was extracted in a dedicated experiment series [17, 18].

4.2 Simulation and Experimental Results

The exposure simulation results generated by X3D in Fig. 6 illustrate the dose profile in PMMA at three different locations on the sample with irradiation doses of 2.0, 6.0 and 8.0 A·min. Solid lines in Fig.6 represent the results directly derived from the Eq. 1. This indicates that X3D correctly calculates the beamline effects (windows, filters, scanning, and X-ray mask movement) and X-ray absorption in the resist. The calculated dose distributions are accurate. Figure 7 shows the development simulation result with development time of 120 min.

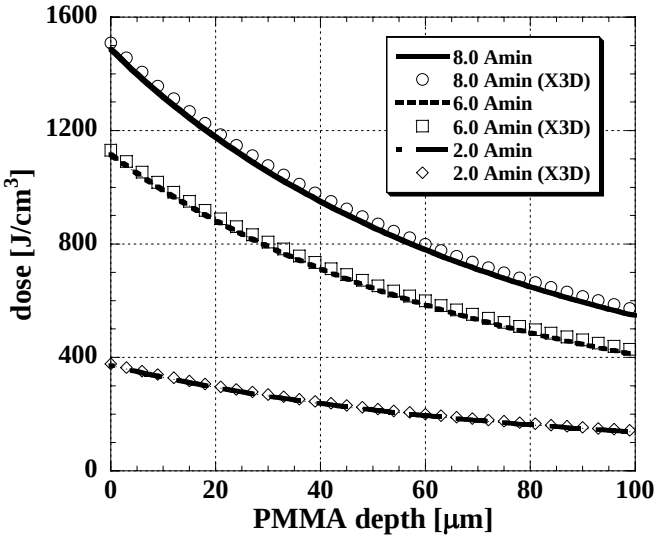


Fig. 6. Simulated dose profiles in PMMA with deposited dose of 2.0, 6.0 and 8.0 A·min. Continuous lines in figure represent the results derived from the equation (1).

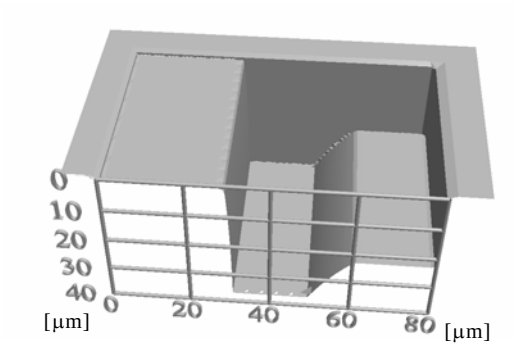


Fig. 7. Simulation result with a development time of 120 min.

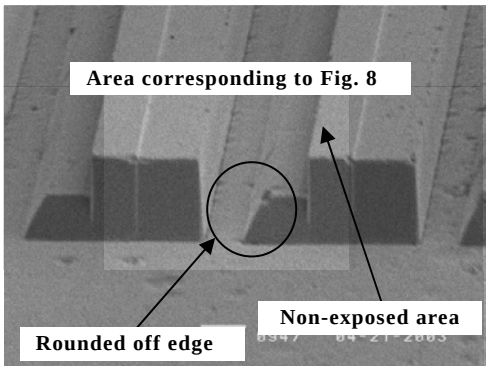


Fig. 8. Experimental result with a development time of 120 min.

Figure 8 shows the experimental result with a development time of 120 min. It should be emphasized that the sidewall shape was not vertical and the corner was rounded off in both Fig. 8 and Fig. 9. This result is attributed to the local dissolution phenomena. The simulation results were evaluated further by comparing with the measured development profiles. Figure 9 shows the measured results and the development profile extracted from the simulated data of X3D for a sequence of development times. As mentioned above, the same phenomenon of increase in edge roundness was observed both in the experiments and the simulation results. For the first time these 3D dissolution phenomena from both analytical simulation and experiments are demonstrated.

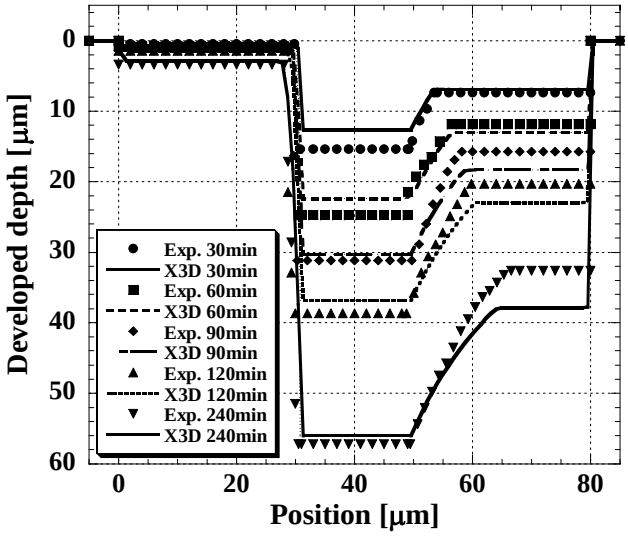


Fig. 10. Comparison of simulation results to measurements with development times of 30, 60, 90, 120 and 240 min.

5. CONCLUSIONS

We have developed a new simulation system covering the complete process of M^2DXL. From the comparison of simulation results to measurements of the stairs-like dose deposition pattern by M^2DXL, we confirmed the validity of our simulation tool X3D in predicting 3D microstructures. Although there is the slight disagreement with experiments on stairs-like pattern by M^2DXL, X3D reached a state where it can simulate 3D microstructures and complement difficult experimental work on M^2DXL technique.

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