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# Estimation of resist profile for line/space patterns using layer-based exposure modeling in electron-beam lithography

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ABSTRACT

One of the essential tasks in the dose control for fabrication of 2-D and 3-D patterns using electron-beam lithography is estimation of remaining resist profiles after development. A conventional approach is to compute the exposure distribution for a target pattern through convolution with the point spread function (PSF) and then obtain the resist profile via simulation of the development process based on the exposure distribution. A new approach which does not require calculation of the exposure distribution and simulation of the resist development is proposed. It utilizes a set of experimental results on which estimation of the resist profile is based, and has a good potential to provide an alternative to the conventional approaches. In this paper, the proposed approach is described in detail along with the results obtained from an extensive simulation and also experiments.

## 1. Introduction

The electron-beam (e-beam) lithographic process consists of selectively exposing the resist by e-beam and subsequently developing it for pattern transfer. For applications such as predicting the remaining resist profile (just resist profile hereafter) in grayscale lithography [1,2] and proximity effect correction [3–5], both steps are often simulated. In the first step, the exposure (energy deposited in the resist) distribution is computed by convolution between a circuit pattern (dose distribution) and a point spread function (PSF) which depicts the exposure distribution when a single point is exposed [6]. PSF's are usually obtained by theoretical modeling such as a double-Gaussian function or a Monte Carlo simulation [7]. In the second step, the developing rate at each point in the resist is computed based on the exposure at the point and developing conditions, and an iterative procedure is employed to derive the remaining resist profile [8]. While such simulations are widely used, it is not unusual that the estimated profile of the remaining resist is substantially different from the actual profile obtained in experiment. The reasons for this deviation may include (i) the actual parameters such as beam diameter are different from those in the system specifications, (ii) certain effects may not be considered in simulation, and (iii) the actual remaining resist profile varies with the developing condition. Also, such simulations are very time-consuming. Hence, it is worthwhile to develop a new method which does not require exposure calculation and development simulation, in order to provide an alternative to the conventional simulation-based methods.

Resist profiles obtained in experiments reflect all effects and actual parameters involved in the e-beam lithographic process. Therefore, an experiment-based method has a potential to generate an estimated profile close to the actual one. A new method is proposed for estimating the resist profiles using a set of experimental results without the exposure estimation and development simulation. This new method should be distinguished from the conventional approaches, such as PROSIM [9], where the exposure distribution and/or resist profile is obtained through simulation. The idea of the method is to adopt the concept of "base patterns." The resist profiles of the base patterns are obtained through experiments and are used in estimating the resist profile of a given pattern consisting of the base patterns. In this paper, an implementation of the method which utilizes the base pattern of line to estimate resist profiles of $L/S$ (line/space) patterns is presented to demonstrate the feasibility of the method through computer simulation and experiments.

The rest of the paper is organized as follows. The conventional estimation method is briefly reviewed in Section 2. The proposed approach is described in Section 3. Details of the estimation

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method are presented in Section 4. Simulation and experimental results are discussed in Section 5, followed by a summary in Section 6.

## 2. Conventional estimation method

### 2.1. Exposure model

The substrate system consists of a substrate and a certain type of resist with initial thickness of $H$ on top of the substrate, as illustrated in Fig. 1. The 3-D point spread function is denoted by $psf(x,y,z)$, which describes the exposure distribution in the resist when a point on the $X$–$Y$ plane is exposed. The resist depth is along the $Z$-dimension. Let $f(x,y,0)$ represent the e-beam dose (energy given) to the point $(x,y,0)$ at the surface of the resist for writing a circuit feature (refer to Fig. 1):

$$f(x,y,0)=\begin{cases} D & \text{if } (x,y,0) \text{ is within a feature} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

where $D$ is a constant dose.

Let $e(x,y,z)$ denote the exposure distribution at the point $(x,y,z)$ in the resist. Then, the 3-D spatial distribution of exposure can be derived by the following convolution:

$$e(x,y,z)=\int\int f(x-x',y-y',0)psf(x',y',z)dx'dy' \tag{2}$$

From Eq. (2), it can be seen that the exposure distribution at a certain depth $z_0$ can be computed by the 2-D convolution between $f(x,y,0)$ and $psf(x,y,z_0)$ in the corresponding plane $z=z_0$, i.e., $e(x,y,z)$ may be estimated layer by layer. Note that the PSF, $psf(x,y,z)$, reflects all the effects affecting energy deposition including the e-beam blur.

### 2.2. Development model

Although the 3D exposure model provides complete information on how electron energy is distributed in the resist, it does not directly depict the remaining resist profile after development. Therefore, it is required to take the resist development process also into account. In this study, a simplified version of the resist development method ("cell removal method"), PEACE, [8] is used to derive the remaining resist profiles for comparison purpose. In this model, the resist is partitioned into rectangular cells, and the exposure is estimated at each cell. Then the developing rate $r(x,y,z)$ of each cell is calculated from its exposure $e(x,y,z)$ through a nonlinear mapping of ($e$-to-$r$) conversion formula which is experimentally determined. The conversion formula derived in our experiment is given by:

$$r(x)=F[e(x)]=3700\cdot e^{-\left(\frac{e(x)-1.0e11}{5.6e10}\right)^2}-152.5 \tag{3}$$

where $r(x)$ is in nm/minute and $e(x)$ in $eV/\mu^2$.

Through iterations, the remaining time for complete development of each of the exposed cells is updated. Simulation continues for a specified developing time to obtain the final remaining resist profile. Accuracy of this approach is entirely dependent on how accurate and realistic the exposure estimation, conversion formula and development simulation process are.

## 3. Proposed approach

### 3.1. Base patterns

The proposed method is based on the approach where a minimal set of experiments is carried out in order to extract a sufficient amount of information on the resist development process in a certain experimental set-up. The patterns employed in these experiments are referred to as *base patterns*, which are long rectangles (lines) in this study. Through these experiments, the dose and width of rectangle are varied to collect the data needed for estimation of the remaining resist profile of a target pattern. The more data are collected, the more accurate estimation is possible. However, the number of experiments is to be minimized from the viewpoint of practicality. Therefore, it is required to sample a limited number of base patterns to collect enough data for the estimation. It is assumed that a base pattern is sufficiently long along the $Y$-dimension such that any variation along the $Y$-dimension can be ignored, or only the cross-section of resist perpendicular to the $Y$-axis can be considered (refer to Fig. 2). In the cross-section, $e(x,y,z)$ and $r(x,y,z)$ are replaced by $e(x,z)$ and $r(x,z)$, respectively.

### 3.2. 2-D exposure model

In an earlier effort [10], a method which takes the proposed approach to estimation of remaining resist profiles was developed, but based on a 2-D exposure model. This method, to be referred to as "2-D Mod," is briefly described below, to which the new estimation method is to be compared. In the 2-D exposure model, the exposure is assumed not to change along the depth dimension ($Z$-dimension), i.e., $e(x,z)$ in the cross-section is averaged over $0\leqslant z\leqslant H$ (see Fig. 1), resulting in $e(x)$.

Suppose that the target pattern consists of two identical lines and the center-to-center distance between the two lines is $I$. The

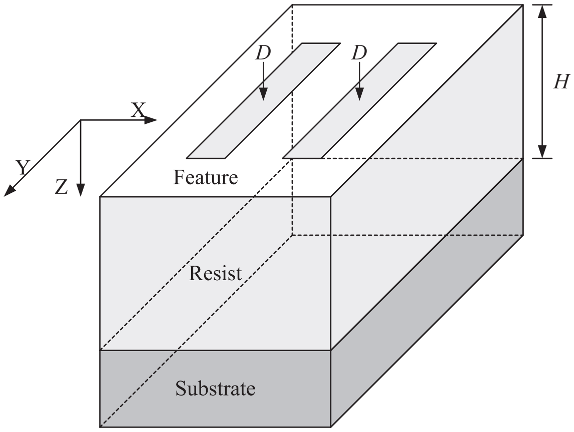


**Fig. 1.** Coordinates of the substrate system where $H$ is the initial thickness of resist and $D$ is the dose given to each feature.

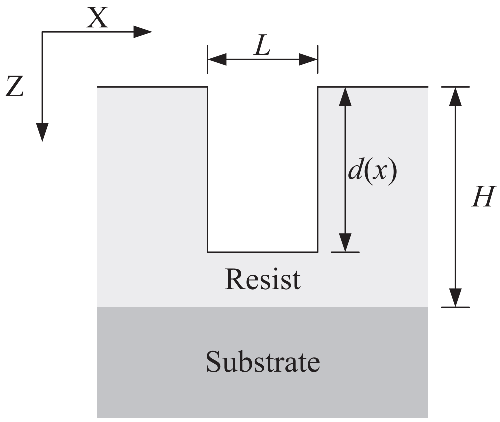


**Fig. 2.** Cross-section of the resist profile of a base pattern.

base pattern for estimating the resist profile of the target pattern is a single line. Let the resist (depth) profile of the base pattern be represented by $d_1(x)$. The resist profile of the target pattern, $d_2(x)$, is estimated from $d_1(x)$ as follows. The developing rate is estimated as $r_1(x) = \frac{d_1(x)}{T}$ where $T$ is the developing time, and the exposure distribution for the base pattern is computed by $e_1(x) = F^{-1}[r_1(x)]$ (refer to Eq. (3)). Then, noting the linearity of exposure, the developing rate distribution for the target pattern can be obtained as:

$$r_2(x) = F[e_2(x)] = F[e_1(x) + e_1(x - l)] \tag{4}$$

Finally, the resist profile of the target pattern is estimated to be:

$$d_2(x) = r_2(x) \cdot T \tag{5}$$

A fundamental problem of this method is that the exposure variation along the depth dimension is not taken into account, which can lead to a significant estimation error [11–13]. Also, the lateral development of resist is not explicitly considered in the estimation procedure though $d_1(x)$ itself includes the lateral component of resist development. Therefore, in this paper, an estimation method which employs a 3-D exposure model and explicitly accounts for the lateral development is presented.

### 3.3. Layer-based exposure model

The new estimation method adopts the idea of layer-based exposure modeling in order to improve the estimation accuracy. The resist is modeled as a stack of layers parameterized by $z$. By analyzing the simulation results for several base patterns on different substrate systems, it is shown that the exposure distribution with respect to $z$ (over layers) given $x_i$, i.e., $e(x_i, z)$, is similar to $e(x_j, z)$, where $x_i$ and $x_j$ are any two points within the exposed area, as shown in Fig. 3a. Therefore, $e(x, z)$ can be modeled using a family of normalized decreasing functions of $z$ with parameters including the resist thickness, the feature size (width of exposed area), and the distance from $x$ to the center of a feature. In this way, given a certain point $x_0$ within the feature, a normalized distribution curve of $e(x_0, z)$ can be modeled, which is denoted by $N(x_0, z)$. That is,

$$e(x_0, z) = e(x_0) \cdot N(x_0, z) \tag{6}$$

where $e(x_0)$ is initialized as follows:

$$e(x_0) = F^{-1}[r(x_0)] = F^{-1}\left[\frac{d(x_0)}{T}\right] \tag{7}$$

Then, for the developing time $T$, the depth $d'(x_0)$ is estimated to satisfy:

$$\int_0^{d'(x_0)/d_0} \frac{d_0}{F[e(x_0, z)]} dz = T \tag{8}$$

where $d_0$ is the thickness of a layer of the resist defined in the model.

In general, a smaller $d_0$, i.e., a higher resolution in the resist-depth dimension, leads to a higher estimation accuracy. The (fractional) depth error in the estimation is defined as

$$\Delta d(x_0) = \frac{d'(x_0) - d(x_0)}{d(x_0)} \tag{9}$$

The above estimation procedure is iterated until the depth error converges to a sufficiently small value. In each iteration, $r(x_0)$ or equivalently $e(x_0)$ is adjusted according to $\Delta d(x_0)$ and $e(x_0, z)$ is

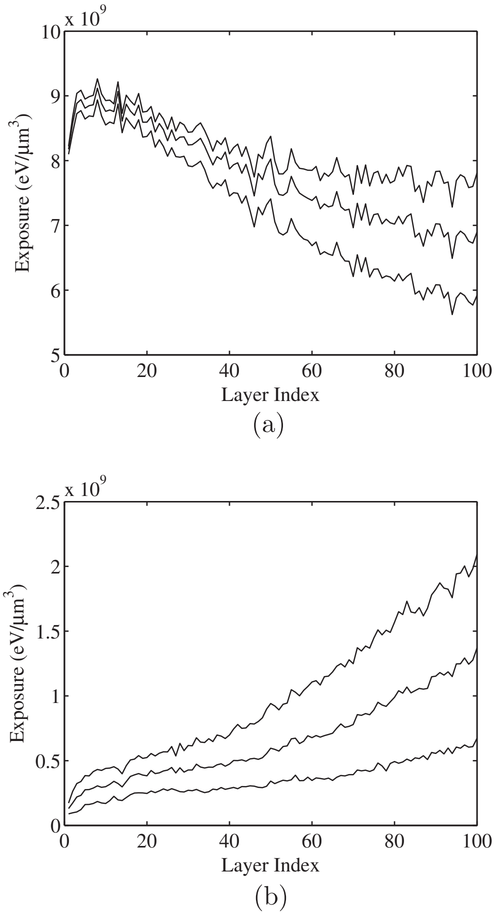


**Fig. 3.** Exposure distribution along the resist-depth dimension for three arbitrary points in (a) the exposed area and (b) the unexposed area on the substrate system of 500 nm PMMA on Si. The curves were obtained through computing the exposure with the 3-D model of 100 layers.

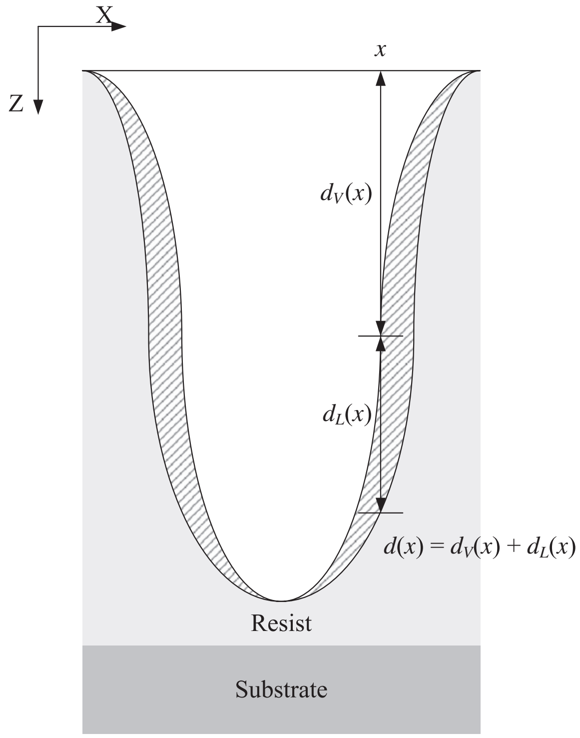


**Fig. 4.** Depth at $x$, $d(x)$, may be modeled as a combination of vertical component $d_V(x)$ and lateral component $d_L(x)$. The white area in the profile corresponds to the resist developed vertically and the area marked by slanted lines corresponds to the resist developed laterally.

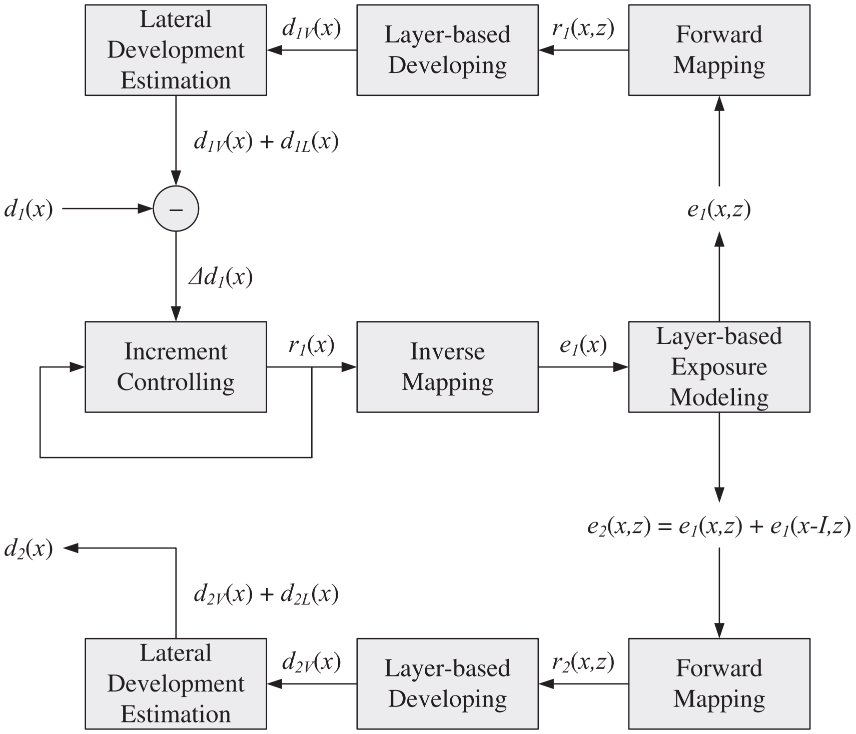


**Fig. 5.** Flowchart of the proposed estimation method.

recomputed. Through these iterations, $e(x_0, z)$ can be modeled accurately enough to avoid either underestimation or overestimation.

From the analysis of 3-D exposure distribution, it is also found that the distribution of $e(x,z)$ along the $Z$-dimension changes abruptly when crossing the boundary between the exposed and unexposed areas without a gradual transition region. The $e(x,z)'s$ for different $x$ in the unexposed area are different from those in the exposed area, but similar among themselves, as shown in Fig. 3b. Therefore, the same approach to modeling $e(x,z)$ (as the one described above for the exposed area) can be taken also for the points in the unexposed area, i.e., outside features. This layer-based modeling is essential to the proposed estimation method, and is proved to be effective.

## 4. Estimation method

In Section 3, it is implied that $d(x_0)$ is only dependent on $r(x_0, z)$. However, the resist developing process is isotropic and progresses in all possible directions. Therefore, $d(x_0)$ depends on not only $r(x_0, z)$ but also $r(x, z)$ within the domain which can be specified by:

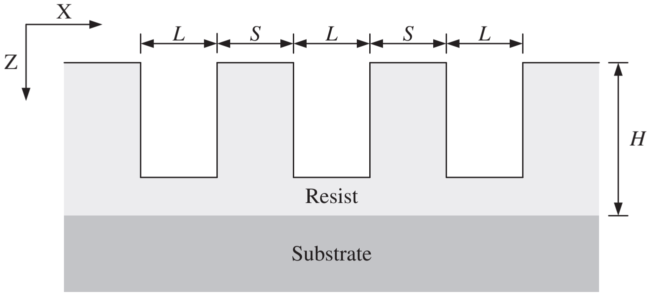


**Fig. 6.** An illustration of line and space pattern used in simulation.

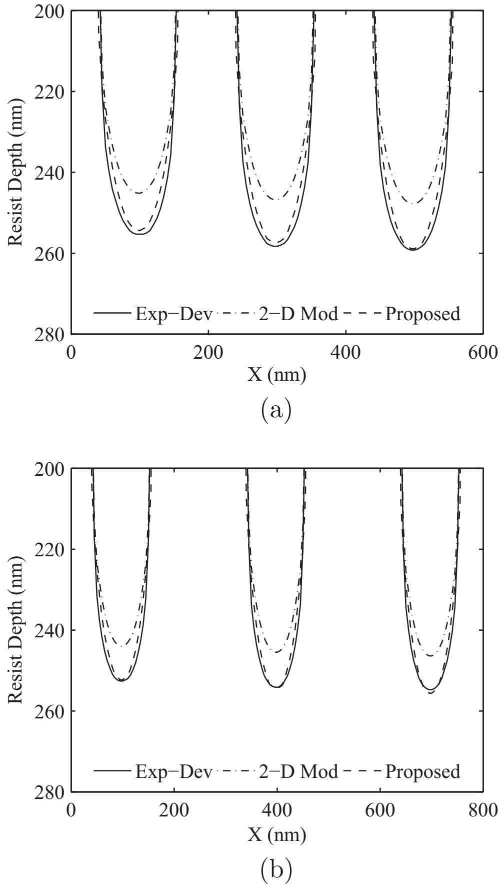
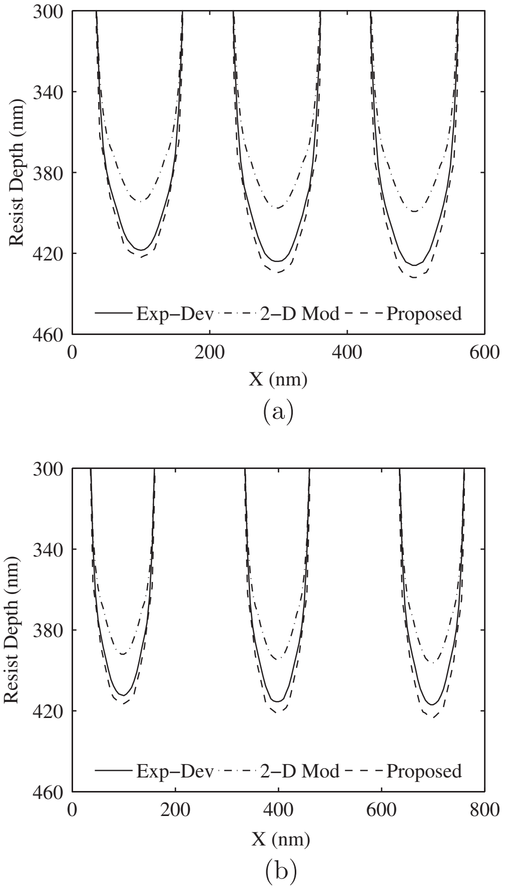


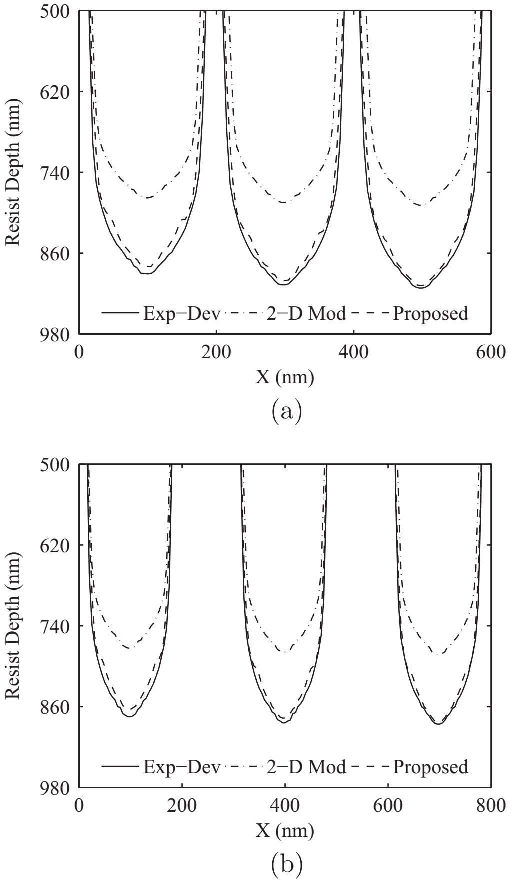
**Fig. 7.** Remaining resist profiles of an 8-line pattern with (a) $L$ = 100 nm/$S$ = 100 nm and (b) $L$ = 100 nm/$S$ = 200 nm on the substrate system of 300 nm PMMA on Si. Only the first 3 lines are shown.



(a)

(b)

**Fig. 8.** Remaining resist profiles of an 8-line pattern with (a) $L = 100$ nm/$S = 100$ nm and (b) $L = 100$ nm/$S = 200$ nm on the substrate system of 500 nm PMMA on Si. Only the first 3 lines are shown.



(a)

(b)

**Fig. 9.** Remaining resist profiles of an 8-line pattern with (a) $L = 100$ nm/$S = 100$ nm and (b) $L = 100$ nm/$S = 200$ nm on the substrate system of 1000 nm PMMA on Si. Only the first 3 lines are shown.

$$\{r(x,z)|0 < |x - x_0| \leqslant w\} \tag{10}$$

where $w$ is a certain width within which the resist development interacts laterally.

Though the resist is developed in all possible directions, $d(x)$ may be modeled as a combination of vertical component $d_V(x)$ (defined as the depth increment due to vertical development) and lateral component $d_L(x)$ (defined as the depth increment due to lateral development) as illustrated in Fig. 4. Note that the increased width due to lateral development makes the depth larger and $d_L(x)$ refers to this depth increment. For a feature with a uniform dose, the exposure is always highest at the center and decreases monotonically toward the edges, which indicates the lateral development is non-existent at the center. Hence, the exposure at the center of feature can be estimated considering the vertical development only (without the lateral development). For any other point in the exposed and unexposed areas, its exposure is estimated by additionally considering its lateral development due to the exposures or equivalently rates of all the points from the center point to the point itself. In the current implementation, an iterative procedure is employed where the estimation of the lateral development may be expressed by:

$$d_L(x_i) = G[T, r(x_k)|k = 0, 1, 2, \cdots, i] \tag{11}$$

where $G_L[\cdot]$ represents the process of estimating lateral development.

For simplicity, the estimation method is described for a target pattern consisting of two lines sufficiently long along the $Y$-dimension and separated by distance $I$. In this case, the base pattern is a single line of which remaining resist profile obtained through experiment is denoted by $d_1(x)$. As discussed above, $d_1(x)$ is composed of vertical component $d_{1V}(x)$ and lateral component $d_{1L}(x)$. The remaining resist profile of the target pattern, which is to be estimated, is denoted by $d_2(x)$. The developing rate distributions of the base and target patterns are denoted by $r_1(x,z)$ and $r_2(x,z)$, respectively. The estimation steps are depicted below (also refer to the flowchart in Fig. 5).

*Step 0:* Measure the depth profile, i.e., $d_1(x)$ from the experimental result of a base pattern.

*Step 1:* For the base pattern, set an initial value for its exposure $e_1(x)$ (without considering the variation along the depth dimension), i.e., $e_1(x) = F^{-1}[r_1(x)] = F^{-1}[\frac{d_1(x)}{T}]$.

*Step 2:* Compute the layer-based exposure $e_1(x,z)$ based on $e_1(x)$ using Eq. (6), and convert it into developing rate $r_1(x,z)$ using the conversion formula in Eq. (3).

*Step 3:* Compute the vertical component $d_{1V}(x)$ using Eq. (8), and then compute the lateral component $d_{1L}(x)$ using Eq. (11).

*Step 4:* Evaluate the depth error $\Delta d_1(x) = \frac{d_{1V}(x)+d_{1L}(x)-d_1(x)}{d_1(x)}$. If it is smaller than a certain threshold, proceed to *Step 5*. Otherwise, adjust $r_1(x)$, or equivalently $e_1(x)$, and go back to *Step 2*.

*Step 5:* Compute the layer-based exposure $e_2(x,z)$, i.e., $e_2(x,z) = e_1(x,z) + e_1(x - I, z)$, and convert it into developing rate $r_2(x,z)$ using the conversion formula in Eq. (3).

*Step 6:* Compute the vertical component $d_{2V}(x)$ using Eq. (8), and then compute the lateral component $d_{2L}(x)$ using Eq. (11).

*Step 7:* Derive the final depth profile $d_2(x)$ by taking both vertical and lateral components into account, i.e., $d_2(x) = d_{2V}(x) + d_{2L}(x)$.

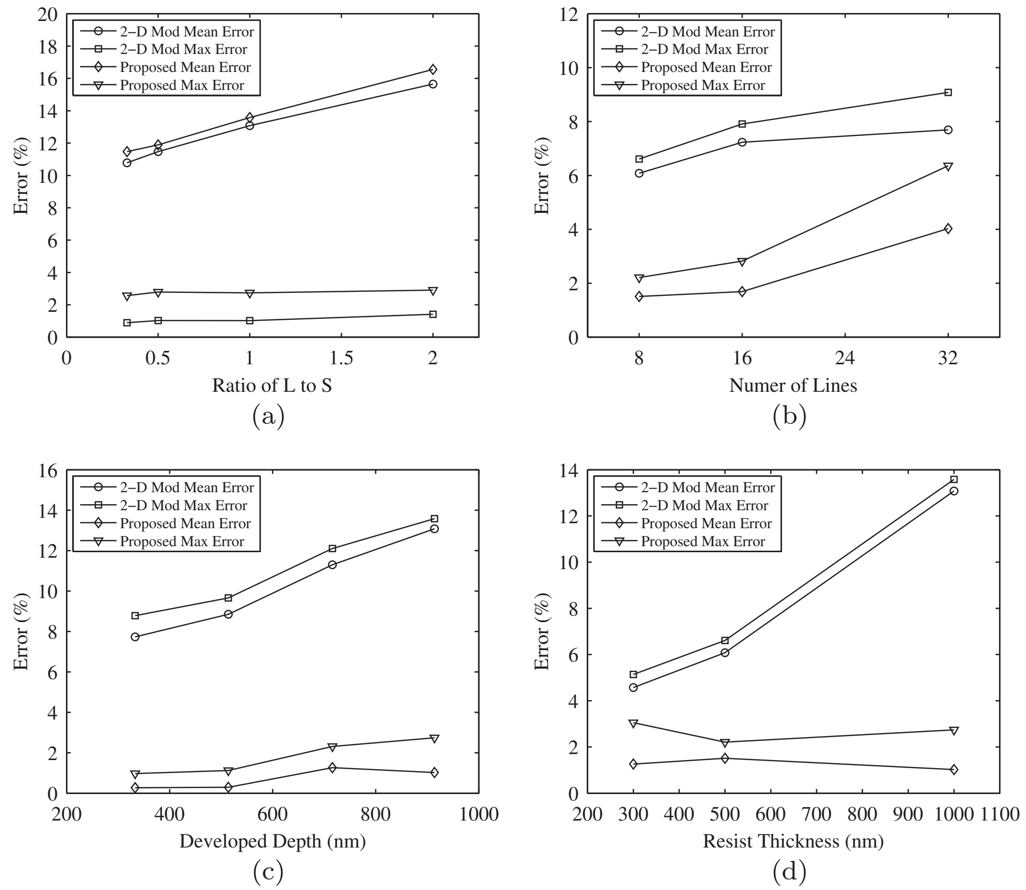


**Fig. 10.** Percent depth error (mean and maximum) with respect to (a) the ratio of $L$ to $S$ with $N = 8$ on the substrate system of 1000 nm PMMA on Si; (b) the number of lines with $L = 100$ nm/$S = 100$ nm on the substrate system of 500 nm PMMA on Si; (c) the developed depth (controlled by the developing time) with $L = 100$ nm/$S = 100$ nm and $N = 8$ on the substrate system of 1000 nm PMMA on Si; (d) the resist thickness (300 nm/500 nm/1000 nm) with $L = 100$ nm/$S = 100$ nm and $N = 8$.

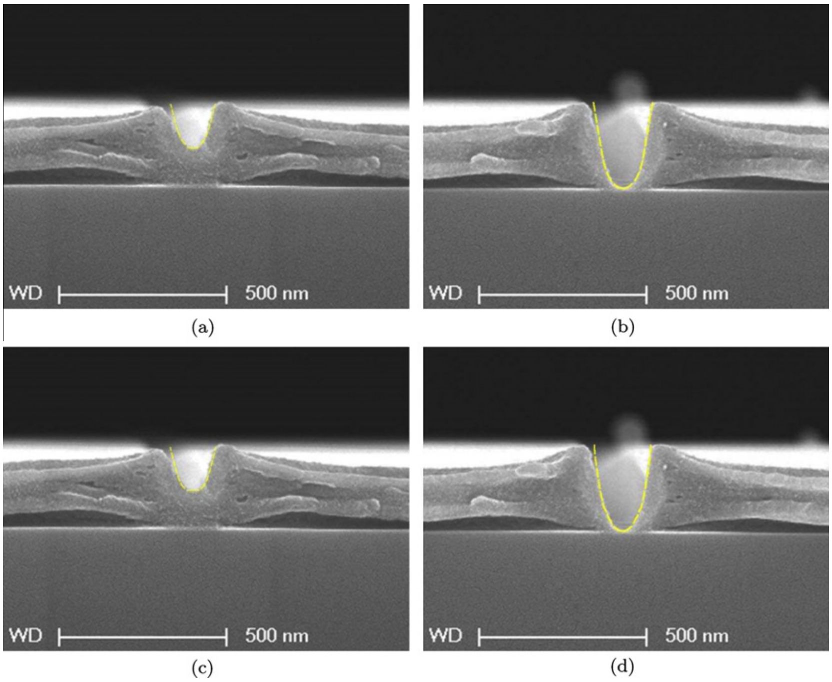


**Fig. 11.** Measured and estimated resist profiles (yellow curves): (a) measured $d_1(x)$, (b) measured $d_1(x)$, (c) estimated from the measured profile $d_1(x)$ in (b), and (d) estimated from the measured profile $d_1(x)$ in (a). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

It should be clear that the above estimation procedure can be easily generalized for $N$-line target patterns where $N > 2$. In *Step 0*, the measurement of $d_1(x)$ may be done from the cross-section SEM image of the resist profile or using the AFM. In any case, the measurement error must be minimized since the estimation result depends on the measured depth profile.

## 5. Results and discussion

The performance of the proposed estimation method has been evaluated through both simulation and experiment.

### 5.1. Simulation results

An extensive simulation has been carried out with multi-line patterns and different substrate systems. The line width ($L$), space between lines ($S$) and the number of lines ($N$) are varied (refer to Fig. 6). The substrate system is composed of PMMA on Si where the three different thicknesses of PMMA, 300, 500, and 1000 nm, are considered. In the current model, the resist consists of 100 layers.

The proposed estimation method and the 2-D Mod method (Section 3.2) have been compared to the conventional method (Exp–Dev, Section 2) which requires the exposure computation and resist-development simulation. A set of typical remaining resist profiles estimated by the three methods is provided in Figs. 7–9. Compared to the 2-D Mod method, it can be seen that the proposed method can achieve the remaining resist profiles much closer to those by the Exp–Dev method in most cases. However, it should be noticed that the 2-D Mod method never overestimates remaining resist profiles since it employs the 2-D exposure model while the proposed method leads to a slight overestimation in some cases.

The two methods (2-D Mod and the proposed) are compared in terms of the percent depth error (mean and maximum), which is defined at each point $x$ by:

$$\text{Percent depth error} = \frac{d_{est} - d_{org}}{d_{org}} \times 100\% \tag{12}$$

where $d_{est}$ denotes the depth estimated by the 2-D Mod or proposed method, and $d_{org}$ denotes the depth estimated by the Exp–Dev method, respectively. This percent depth error is defined for general resist profiles (binary or grayscale lithography). But, for binary lithography where the feature width is of main concern, a percent width error may be adopted. In Fig. 10, the percent mean and maximum depth errors are plotted with respect to the ratio of $L$ to $S$, the number of lines, the developed depth (controlled by the developing time), and the resist thickness. The results show that the proposed method outperforms the 2-D Mod method by reducing the mean error up to about 14.24%. And the reduction of the maximum error is about 13.65%.

From the above plots of errors, it is observed that as each of the ratio of $L$ to $S$, the number of lines, the developed depth (controlled by the developing time), and the resist thickness increases, the advantage of the proposed method becomes more and more visible. For a larger ratio of $L$ to $S$ or a larger number of lines, the interaction among lines increases and therefore the less accurate estimation method, 2-D Mod, suffers more. For a thicker resist, the exposure variation along the depth dimension is larger which makes the 2-D Mod cause larger errors since it ignores the exposure variation.

### 5.2. Experimental results

The proposed estimation scheme has been tested also via experiment. Si wafer was spin-coated with 300 nm PMMA and soft-baked at 160 °C for 1 min. Two long lines of 100 nm wide, separated by a sufficiently long distance to ignore any interaction (proximity effect), were exposed with different doses ($200\ \mu C/cm^2$ and $225\ \mu C/cm^2$) using ELIONIX ELS-7000 e-beam lithography system (50 KeV) and the sample was developed in MIBK:IPA = 1:2 for 40 s. The cross-section SEM images of the two resist profiles are provided in Fig. 11a and b. The depth profile was measured from each SEM image (see the yellow curve) and used as $d_1(x)$, i.e., the depth profile of a base pattern. Then, from each measured profile $d_1(x)$, the other resist profile (as a target pattern) was estimated by the proposed estimation method. The estimated resist profiles (yellow curves) of the target patterns are overlaid in the corresponding SEM images in Fig. 11c and d. The mean percentage errors between the measured and estimated resist profiles are 5.25% (Fig. 11c) and 3.81% (Fig. 11d), demonstrating high accuracy of the proposed estimation method.

In practice, the measured $d_1(x)$ may include an error. In order to examine the effect of the measurement error on the estimation result, a "measurement error" of 5% was added to or subtracted from the base pattern profiles, $d_1(x)$, in Fig. 11a and b. Then, the resist profiles of the target patterns were estimated from the error-added $d_1(x)$. The average estimation error turns out to be 6.68%, compared to 4.53% without the added error. The proposed estimation method does not appear to be very sensitive to the measurement error, i.e., does not amplify the measurement error.

## 6. Summary

In this paper, a method for estimating remaining resist profiles of $L/S$ patterns, which does not require the exposure calculation and resist-development simulation, is proposed. By analyzing the simulation results from a set of base patterns on different substrate systems, a layer-based model is formulated. An adaptive procedure is employed in estimation of the lateral development in remaining resist profiles. Through an extensive simulation, it has been shown that the proposed method estimates almost the same resist profiles as those by a typical conventional (3-D) method like the Exp–Dev method in most cases, and outperforms the 2-D Mod method by further reducing the estimation error. Also, it has been demonstrated experimentally for a single-line target pattern that the estimated resist profile closely matches the actual profile. Therefore, the proposed method has a good potential to provide an alternative way for estimation of resist profiles where the conventional methods are not applicable and/or too time-consuming. The future study will include further experimental verification for the multi-line target patterns, and extension to general patterns with a spatially varying dose distribution and the grayscale lithography.

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