Step-width adjustment in fabrication of staircase structures*

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Three-dimensional structures increasingly find applications in various devices such as diffractive optical elements, photonic element, microelectromechanical systems, etc., and are often fabricated by e-beam lithography. Their performance is known to be highly sensitive to their dimensions. Therefore, it is critical to achieve high dimensional accuracy for the desired characteristics. However, as the feature size in three-dimensional structures decreases down to nanoscale, the lateral development of the resist and the proximity effect due to electron scattering can make dimensions of the written features in a device substantially different from the target dimensions. In this study, this issue is addressed for staircase structures; specifically, minimizing the difference between the target and the actual widths of each step. Through computer simulation and experiments, it has been shown that significant improvement in dimensional accuracy, especially the step widths of the staircase structures, can be achieved by the proposed practical width-adjustment scheme. © *2010 American Vacuum Society.* [DOI: 10.1116/1.3269794]

I. INTRODUCTION

An increasing number of devices require three-dimensional (3D) structures (for example, microelectromechanical systems, optical elements, etc.) and their dimensional fidelity is critical for their desired performance characteristics. Different methods have been employed in the fabrication of such 3D structures, including electron-beam (e-beam) grayscale lithography.[1–3] A dose (energy given to a point on the resist surface) control scheme that achieves the spatial exposure (energy deposited at a point) distribution resembling the shape of target 3D structure with discrete levels was developed.[4] Also, a staircase structure with the step height of 20 nm was successfully fabricated using e-beam grayscale lithography and reactive ion etching.[5]

In e-beam grayscale lithography, a 3D structure is transferred onto the resist or substrate using the remaining resist layer as a grayscale mask. The remaining resist profile, which resembles the 3D structure, is obtained by the e-beam lithographic process and the substrate is etched through the remaining resist. Therefore, it is essential to achieve the remaining resist profile required for accurate transfer of the 3D structure. In most cases, an empirical approach, which relies on the experimentally determined relationship between the e-beam dose or exposure and the remaining resist thickness, is used. However, such an approach takes into account neither the resist-development process nor possible variation in the feature size. The lateral development of the resist and the proximity effect due to electron scattering can cause substantial dimensional errors. In order to have an accurate control of the remaining resist profile, an analytic model, which considers the resist-development processes, in particular, lateral development, in addition to e-beam dose control, is required.

In this study, the issue of improving the dimensional accuracy of 3D structures fabricated by e-beam grayscale lithography is addressed for structures with discrete levels. Specifically, a step-width adjustment scheme is developed for accurately controlling the (remaining) resist profiles of the staircase structures. The goal of the scheme is to minimize the step-width error in the resist profile. The scheme is based on the 3D exposure and resist-development models. In the 3D exposure model,[6] the depth-dependent variation in exposure, as well as its lateral variation, is considered to generate a 3D exposure distribution in the resist. An exposure-to-developing rate-conversion formula is derived based on the experimental results. Then, a resist-development model with the rate-conversion formula is employed to estimate the resist profile through 3D simulation from which the amount of adjustment in step-width is determined. The performance of the step-width adjustment scheme has been analyzed through computer simulation and also experiments. It has been shown that this practical scheme is effective in reducing the step-width error.

This article is organized as follows. The exposure and developing rate models are described in Sec. II. The simulation method adopted for estimating the resist profile (step-width deviation) is briefly reviewed in Sec. III. The proposed step-width adjustment scheme is described in detail in Sec. IV. Simulation and experimental results are provided along with discussion in Sec. V, followed by a summary in Sec. VI.

II. MODEL

A. Exposure distribution

Consider an X-Y plane that corresponds to the top surface of the resist layer, as shown in Fig. 1(a). Let $d(x,y,0)$,

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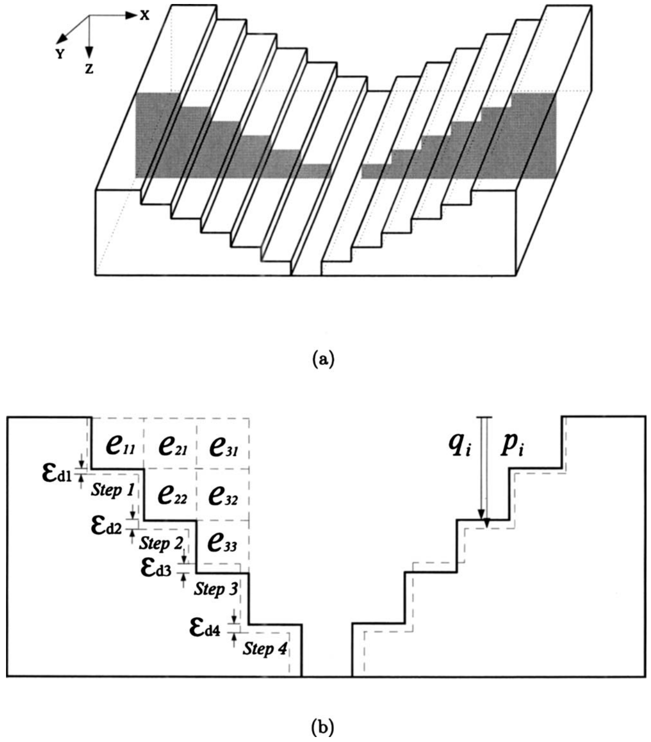


FIG. 1. (a) Nine-step staircase structure and (b) its cross-section where the solid and dashed lines are target and actual profiles, respectively.

TABLE I. Experimental result for a nine-step symmetric stair case structure fabricated on 1000 nm PMMA on Si (50 keV): dose, exposure, and depth.

Developer	Step	Dose ($\mu C/cm^2$)	Exposure ($eV/\mu m^3$)	Depth p_i (nm)
MIBK:IBA=1:1	1	216	1.7286×10^{10}	182
	2	296	2.0983×10^{10}	417
	3	334	2.2489×10^{10}	626
	4	364	2.3751×10^{10}	852
	5	396	2.5229×10^{10}	1000

$e(x,y,z)$, and $\mathrm{PSF}(x,y,z)$ represent the e-beam dose to the point $(x,y,0)$ at the surface of the resist, the exposure at the point (x,y,z) in the resist, and the point spread function (PSF), respectively. Then the 3D exposure distribution can be computed as follows:

$$e(x,y,z) = \int\int d(x-x',y-y',0)\mathrm{PSF}(x',y',z)dx'dy'. \quad (1)$$

In this study, exposure is computed by an accurate and efficient two-level procedure implemented in the PYRAMID software.[7] In Fig. 1(a), a symmetric nine-step staircase structure is illustrated. When the staircase is sufficiently long [in the Y dimension in Fig. 1(a)], exposure can be assumed not to vary along the Y dimension in most of the structure. In such a case, consideration of only a cross-section in the middle of the staircase shown in Fig. 1(b) is sufficient. Hence, in the remainder of this article, the Y dimension is not taken into account, i.e., only the cross-section in the X-Z plane will be considered. As shown in Fig. 1(b), step i refers to the ith step from the left.

B. Derivation of developing rate

The relationship between exposure and resist-development rate is known to be nonlinear.[8] For high accuracy of the step-width adjustment, the relationship has been derived from the experimental results. Let the mapping $F[\;]$ represent the nonlinear relationship and $r(x,z)$ the resist-development rate at point (x,z). Then, $r(x,z)$ is given by $r(x,z)=F[e(x,z)]$. Let $p(x)$ denote the resist profile, i.e., the depth measured from the initial surface of the resist downward, as shown in Fig. 1(b). When the step width is wide, the developing process at the center of the step progresses mainly in the vertical direction such that the lateral development may be ignored. Then, for the center of each step, the depth $p(x)$ can be related to the developing rate in the contiguous domain, as in Eq. (2), where T is the developing time,

$$\int_0^{p(x)} \frac{dz}{r(x,z)} = T. \quad (2)$$

In the experimental result of a staircase structure, only the discrete depth information is available, i.e., one depth for each step (refer to Table I). Let p_i denote the depth of step i measured at the center of the step in an experimental result and q_i the target depth of step i. The depth error of step i is represented by $\epsilon_{di}=|p_i-q_i|$. Also, the cross-section is partitioned into blocks, as shown in Fig. 1(b). Exposure is considered to be homogeneous within each block and e_{ij} denotes the exposure in the jth block of step i.

Derivation of the exposure-to-rate conversion formula is carried out in two phases. In the first phase, the depth-dependent exposure or rate variation is not considered by using the average value of e_{ij} for each step, which is denoted by e_i. Accordingly, the average developing rate r_i for each step is defined. From experiments, p_i is obtained and r_i is estimated to be p_i/T for step i. Then, the set of sample points, $\{e_i, r_i\}$, is fitted to a curve to derive the conversion formula. As exposure increases, developing rate increases more than linearly, i.e., the increase is slow in the beginning and then faster. However, when exposure exceeds a certain value, developing rate tends to saturate (though this region is not utilized in this study). Such a behavior of developing rate may be modeled by a curve or a part of the curve with an inflection point, including polynomial and Gaussian curves. As shown in Fig. 2, a part of the left half of a Gaussian function $r_i=a\times\exp(-((e_i-b)/c)^2)$ is employed in order to minimize the number of coefficients to be determined in curve fitting. Note that a third-order polynomial involves four coefficients. One problem of the first phase is that it does not take the depth-dependent exposure (and therefore rate) variation into account, which would cause a significant error in estimating the depth and width of a step.

In the second phase, the conversion formula obtained in the first phase is used as an initial solution for an iterative

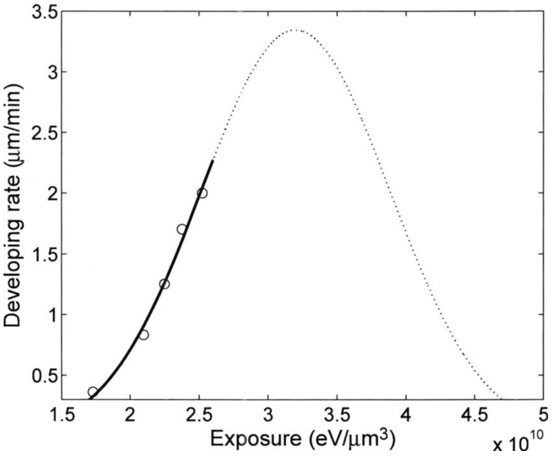


FIG. 2. Exposure-depth curve for MIBK:IPA=1:1 (lines with symbols) with developing time of 30 s. The circles are experimental data to which a part of the Gaussian curve is fitted.

refining procedure. In each iteration, the blockwise exposure distribution e_{ij} is used to estimate the depth of step i, to be denoted by p_i', based on the current conversion formula. Then, the coefficients a, b, and c in the conversion formula are adjusted such that the error $\Sigma|p_i - p_i'|$ is minimized through an exhaustive search. From several sets of experimental data, the following conversion formula was obtained:

$$r(x,z) = 4024.2 \times e^{-((e(x,z) - 3.4 \times 10^{10})/1.0968 \times 10^{10})^2}, \qquad (3)$$

where $e(x,z)$ is in eV/μm^3 and $r(x,z)$ is in nm/min.

The average percent error in curve fitting is 4.41% and the range of exposure used in the adjustment scheme is from 0 to 3.4×10^{10} eV/μm^3.

III. ESTIMATION OF STEP-WIDTH DEVIATION

Due to the isotropic process of resist development, the vertical walls between adjacent steps in a staircase structure is developed laterally, causing the step width to be different from the target width. In Fig. 6(a), a simulated resist profile of the staircase structure is provided where it can be seen that the deviation of step width is as large as 16%. For step-width adjustment, the step width first needs to be estimated. One way to estimate the step-width deviation is to rely on a full-scale resist-development simulation such as the cell-removal method,[9] which is too time consuming to be practical especially in an iterative procedure. Also, for step-width adjustment, only step widths, rather than a complete resist profile, need to be estimated. A practical and yet sufficiently accurate method has been developed. Using $e(x,z)$ obtained by simulation and the final conversion formula, $r(x,z)$ is computed. The slope of the step edge is also affected by the proximity effect and is not usually vertical. However, for simplicity, the width of a step is measured in the middle level between two adjacent steps, as illustrated in Fig. 3. For each step in the staircase, the time duration, Δt_i, during which the second half of the final step height is developed, is derived based on $r(x,z)$ (refer to Fig. 3). Then, the location of the step edge in the developed resist profile is estimated by computing the amount of the lateral development during Δt_i, from which the step-width deviation is obtained. The deviation of the step edge with respect to the target location is denoted by ΔW_i, as illustrated in Fig. 4, and the deviation of the step width compared to the target width is represented by $\epsilon_{W_i} = |\Delta W_i - \Delta W_{i+1}|$ for $i=1, 2, 3$, and 4 ($2\Delta W_i$ for $i=5$). It should be noted that in the case of the staircase structure considered in this study, step-width adjustment is equivalent to step-edge adjustment.

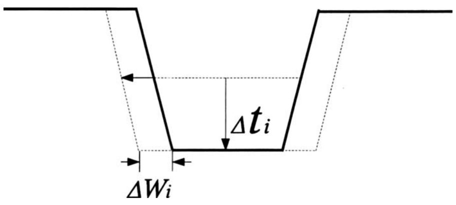


FIG. 3. Estimation of step-edge deviation, where Δt_i is the time taken for the half of the step-height to be developed.

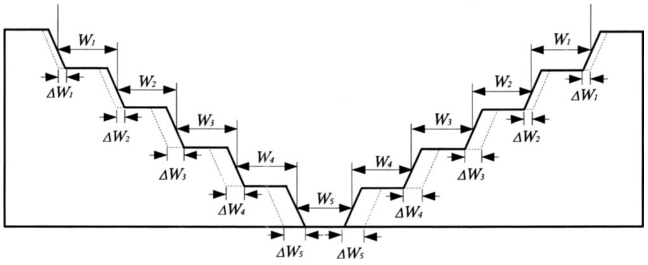


FIG. 4. Step-edge deviations in a staircase structure.

IV. STEP-WIDTH ADJUSTMENT

A practical scheme for adjusting step widths has been developed, which minimizes the computational requirement by avoiding a complete resist-development simulation. As shown in Fig. 5, the scheme proceeds as follows.

Step 1. The two-dimensional exposure distribution is computed by the PYRAMID software[7] and the initial developing-rate formula is derived based on the experimental result (depth of each step).

Step 2. The conversion formula is refined iteratively using

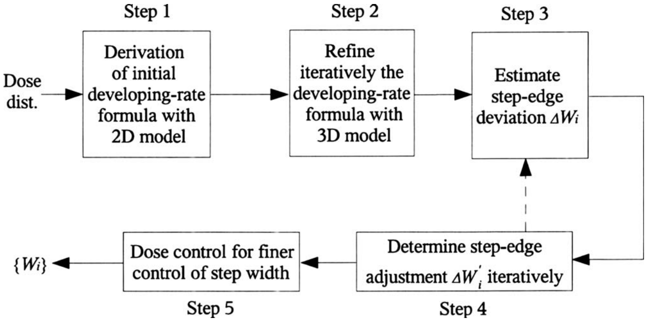


FIG. 5. Step-width adjustment scheme.

the 3D exposure distribution computed by the PYRAMID software (refer to Sec. II B),

Step 3. The step-edge deviation, ΔW_i, is estimated for each step, given a developing time, using the method described in Sec. III.

Step 4. The amount of step-edge adjustment, $\Delta W_i'$, to compensate for ΔW_i, is determined through an iterative procedure. In each iteration, the edge location (equivalently width) of each step (step i) is adjusted by ΔW_i before recomputing the exposure distribution from which ΔW_i is estimated, as in step 3. This is repeated until the adjustment of the edge location in an iteration is less than a half of pixel. The final step-edge locations (or widths) obtained through the iterative procedure are further adjusted to compensate for the minor overestimation by simulation, i.e., $\Delta W_i' \leftarrow c \times dW_i$, where dW_i is the difference between the initial and the final step-edge locations and the c is a constant less than 1.

Step 5. In many cases, one may not achieve the target widths with high precision due to the fact that the step width can be adjusted only by whole pixels. Also, an adjustment of the step width also changes the exposure distribution, especially in the neighboring areas. Hence, in order to have finer control in adjusting the step width and also to compensate for the exposure change due to step-width adjustment, the dose adjustment may be carried out along with the width adjustment. The dose adjustment is carried out by the gray-scale PYRAMID software,[10] which is not described here due to limited space.

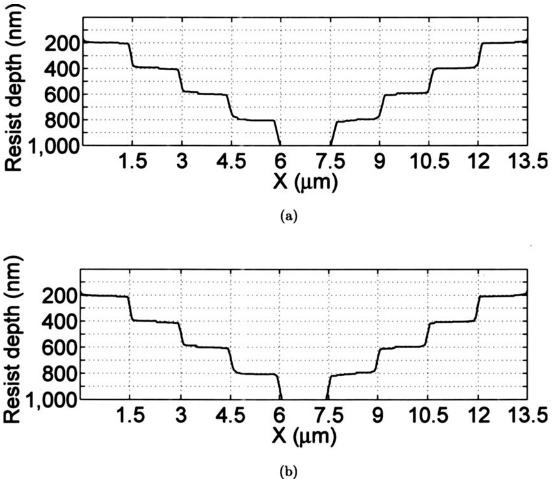


FIG. 6. (a) Step-edge deviation: $\{\Delta W_i\}$={0,45,70,90,125,125,90,70,45,0 nm}. Step-width deviation: $\{\epsilon_{W_i}\}$={45,25,20,35,250,35,20,25,45 nm}. (b) Step-edge deviation: $\{\Delta W_i\}$={0,0,0,0,0,0,0,0,0,0 nm}. Step-width deviation: $\{\epsilon_{W_i}\}$={0,0,0,0,0,0,0,0,0 nm}. The remaining resist profiles obtained (through simulation) for the staircase structure (a) before adjustment and (b) after step-width and dose adjustments where target step width: 1.5 μm, target step-height: 200 nm, and resist thickness: 1000 nm on Si (50 keV). A deviation less than 1 nm is rounded to zero.

V. RESULTS AND DISCUSSION

A. Simulation Results

The 3D test structure used in this study is a symmetric staircase structure, consisting of nine steps where the width and length of each step are 1.5 and 50 μm, respectively. The substrate system is composed of 1000 nm poly(methyl methacrylate) (PMMA) on Si, and the beam energy is assumed to be 50 keV.

In Figs. 6(a) and 6(b), the resist profiles obtained without and with width adjustment are provided along with the step-edge (ΔW_i) and width (ϵ_{Wi}) deviations in the figure caption. Note that in order to show the detail, the vertical (depth) dimension is scaled up (relative to the horizontal dimension). It can be seen that the resist profile before width adjustment shows a significant edge deviation of each step and a larger deviation for a deeper step. The reason why the center step has the largest width error (deviation) is that the directions of the lateral development on the left and right edges of the center step are opposite. Therefore, the step-width deviation (ϵ_{Wi}) for the center step is twice the step-edge deviation (ΔW_i) in this symmetric staircase. However, for other steps, the step-edge deviations at the left and right edges are in the same direction. Hence, the step-width deviation of a step is smaller than the step-edge deviation of either edge. Also, the higher exposure at the center step helps make ΔW_i larger than those for other steps. The final profile after step-width adjustment, combined with the dose control scheme in Fig. 6(b), is significantly closer to the target profile and shows a substantial improvement in step-width accuracy.

In Fig. 7, the simulation results for a symmetric staircase structure with a smaller step-width of 1 μm and a thinner resist of 500 nm are provided. It is observed that the step-edge and width deviations are smaller than those for the thicker resist of 1000 nm since the developing time is

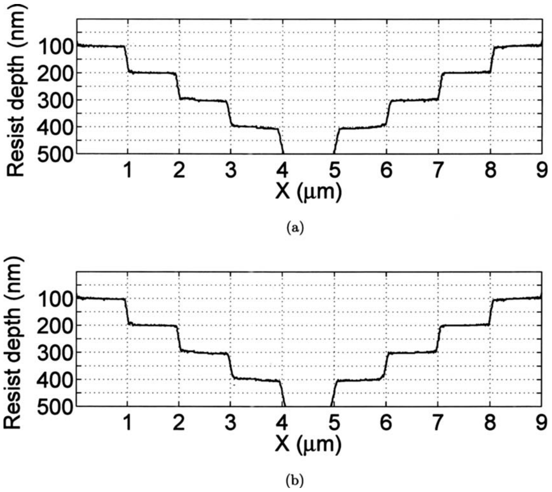
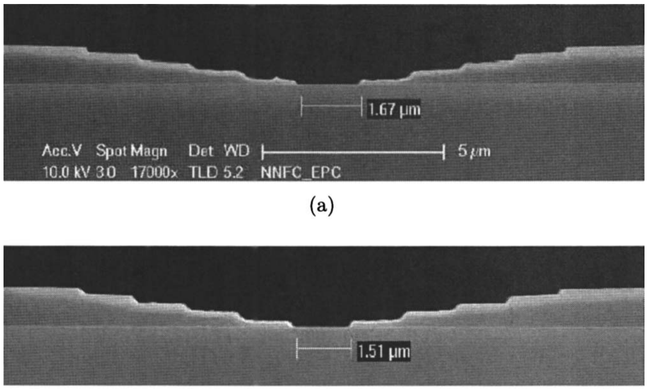


FIG. 7. (a) Step-edge deviation: $\{\Delta W_i\}$={0,15,25,35,60,60,35,25,15,0 nm}. Step-width deviation: $\{\epsilon_{W_i}\}$={15,10,10,25,120,25,10,10,15 nm}. (b) Step-edge deviation: $\{\Delta W_i\}$={0,0,0,0,0,0,0,0,0,0 nm}. Step-width deviation: $\{\epsilon_{W_i}\}$={0,0,0,0,0,0,0,0,0 nm}. The remaining resist profiles obtained (through simulation) for the staircase structure (a) before adjustment and (b) after step-width and dose adjustments where target step-width: 1.0 μm, target step-height: 100 nm, and resist thickness: 500 nm on Si (50 keV). A deviation less than 1 nm is rounded to zero.



(a)

(b)

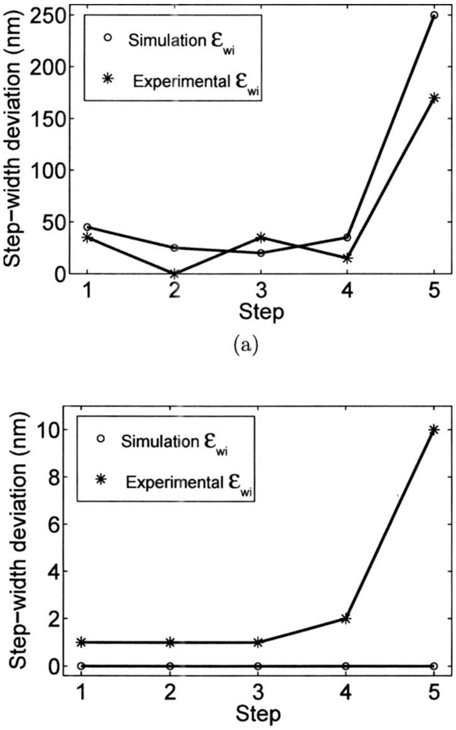
FIG. 8. Experimental results (a) before step-width adjustment and (b) after step-width adjustment where target step width: 1.5 μm, target step height: 200 nm, and resist thickness: 1000 nm PMMA on Si (50 keV).

shorter, i.e., less time for the lateral development. Again, through step-width adjustment, a resist profile much closer to the target profile has been obtained.

B. Experimental results

The symmetric nine-step staircase structure with the step width of 1.5 μm adopted in the simulation study has been fabricated with and without step-width adjustment. The substrate system was prepared by spin coating a Si wafer with 1000 nm PMMA and soft baked at 160 °C for 1 min. The structure was written using an Elionix ELS-7000 e-beam tool with an acceleration voltage of 50 keV and a beam current of 100 pA. The sample was developed in MIBK:IPA=1:1 for 30 s. The remaining resist was coated with 10 nm Pt before the cross-section was imaged by a FEI FE-SEM (Sirion). For easier inspection of the cross-section, the length of the structure was increased to 500 μm. The SEM images of the cross-section are provided in Fig. 8.

It is seen in Fig. 8(a) that the width of the center step is 11.3% wider than the target width. As mentioned in Sec. III, the width deviation for the center step was estimated to be 16% in the simulation, which is reasonably close to the experimental result. As shown in Fig. 8(b), the step-width adjustment not only reduced the width deviation greatly but also decreased the step -height deviation, ϵ_{di}, making the step height closer to the target height of 200 nm. In Fig. 9, the step-width deviations measured in the simulation and experimental results, before and after step-width adjustments, are plotted. In the experimental result, the maximum step-width deviation was reduced from 170 down to 10 nm and the average step-width deviation was from 37.8 to 2.2 nm, where the target width is 1.5 μm. Also, the simulation result closely agrees with the experimental result, which well demonstrates the accuracy of our simulation model and step-width adjustment scheme.



(a)

(b)

FIG. 9. Step-width deviations in simulation and experimental results (a) before step-width adjustment and (b) after step-width adjustment for 1000 nm PMMA (50 keV).

VI. SUMMARY

Due to the lateral development of step sidewalls in the staircase structure during the resist-development process, the step widths in the final resist profile may be substantially different from the target widths. In this article, a practical method for adjusting step widths, developed for the staircase structures, is described. The method is based on a 3D exposure model and utilizes the exposure-to-developing rate-conversion formula derived from the experimental results. The method estimates the step-width deviation and then compensates for the deviation by a combination of width adjustment and dose control, which achieves a fine control of the step width and height. Through computer simulation and experiments, it has been shown that the proposed method can greatly reduce the step-width deviation. The experimental result shows that the average step-width deviations are 37.8 and 2.2 nm before and after step-width adjustments, respectively, where the target width is 1.5 μm. The current research efforts include application of the proposed method to more general structures consisting of discrete depths.

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