Accurate control of remaining resist depth for nanoscale three-dimensional structures in electron-beam grayscale lithography

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In electron-beam (e-beam) grayscale lithography, a three-dimensional (3D) structure is transferred onto the resist or substrate. In either case, accurate control of the remaining resist depth and, accordingly, profile is critical for successful fabrication of the structure. Usually, the remaining resist depth control is guided by the empirically derived dose (or exposure)-depth relationship using a two-dimensional model. However, such an approach may require multiple calibrations and also lead to significant dimensional errors for nanoscale structures due to the depth-dependent variation of exposure and the nonlinearity between exposure and developing rate. In this study, a resist developing model is incorporated into e-beam dose control schemes in order to take the exposure variation and nonlinearity into account. Through computer simulation, it has been demonstrated that significant improvement in dimensional accuracy may be achieved by including the 3D resist developing model in the e-beam dose control for fabricating nanoscale 3D structures. © *2007 American Vacuum Society.* [DOI: 10.1116/1.2781521]

I. INTRODUCTION

In electron-beam (e-beam) grayscale lithography, a three-dimensional (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,[1,2] empirical approaches to e-beam lithographic and resist developing processes were taken with a two-dimensional (2D) model for the resist layer, i.e., the relationship between the e-beam dose (energy injected) or exposure (energy deposited) and remaining resist thickness, which is experimentally determined, is employed in controlling the remaining resist profile. Such approaches do not take some or all of the following facts into account: (i) the exposure is not the same as the dose, (ii) the exposure varies with the resist depth, and (iii) the resist developing rate is not linearly proportional to the exposure. In order to have an accurate control of the remaining resist profile, an analytic model which considers the resist developing process in addition to the exposure distribution is required.

In this study, 3D exposure and resist developing models are employed to formulate an analytic approach to control the remaining resist profile in e-beam grayscale lithography, in particular, the thickness of the remaining resist, given a target 3D structure of nanoscale. In the 3D exposure model,[3] the depth-dependent variation of exposure in addition to its lateral variation is depicted point by point to generate a 3D distribution of exposure in the resist. The 3D exposure distribution is computed by taking the efficient two-level PYRAMID approach to exposure estimation at each layer of resist[4] and then is converted into the 3D developing rate distribution which is referred to in estimating the remaining resist profile in the resist developing model. The relationship between exposure and developing rate derived in Ref. 5 is adopted for the conversion, and the simulation method for resist developing process developed in Ref. 6 is employed for estimating the remaining resist profile.

Through computer simulation, two methods for controlling the spatial distribution of e-beam dose are compared in order to show the necessity of considering the 3D resist developing process in order to have accurate control of the thickness of the remaining resist. One method is based on the 2D exposure models and the other on the 3D exposure and resist developing models. Their performances are compared in terms of the depth error between the target and actual resist profiles.

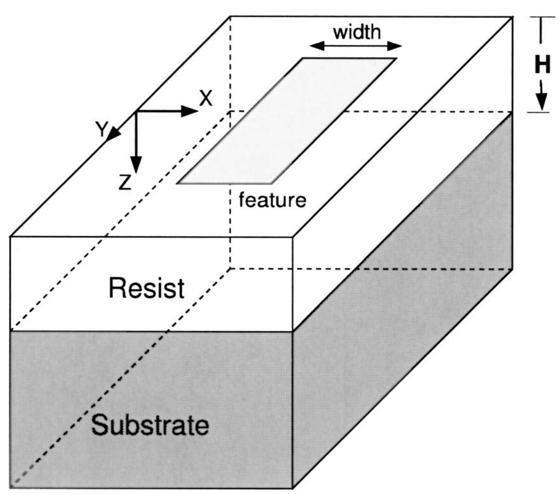

FIG. 1. Coordinates of the substrate system where H is the initial thickness of the resist and the resist depth is measured from the top surface of the resist down, i.e., Z axis.

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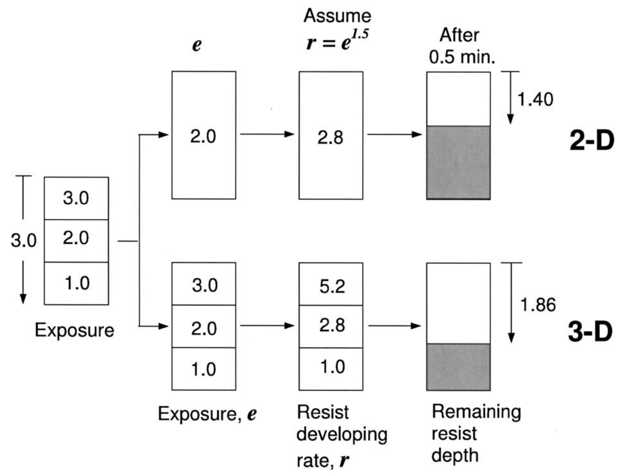

FIG. 2. Difference in estimation of remaining resist depth between 2D and 3D models. Note that the average of the 3D exposure distribution is 2.0 and $r=e^{1.5}$ is assumed for illustration purpose.

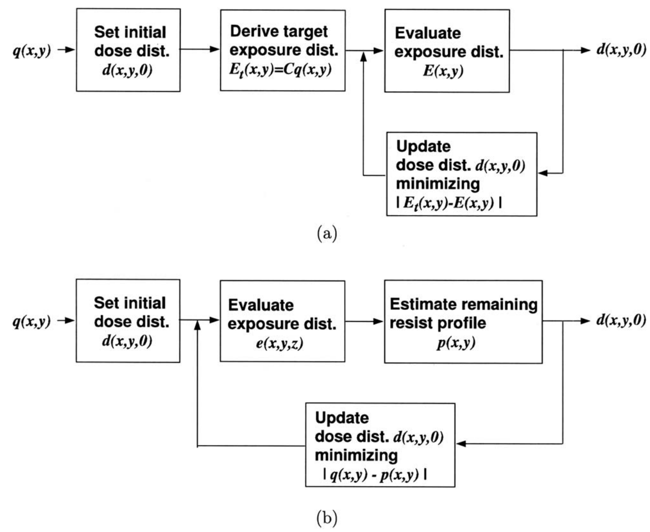

FIG. 3. Dose control schemes: (a) 2D exposure correction and (b) 3D resist profile correction.

In Sec. II, e-beam grayscale lithography is briefly introduced. In Sec. III, 3D exposure distribution and resist developing rate are discussed. In Sec. IV, simulation of the resist developing process is described. In Sec. V, the two dose control schemes are depicted. In Sec. VI, simulation results are discussed, followed by a summary in Sec. VII.

II. E-BEAM GRAYSCALE LITHOGRAPHY

Various methods for realizing 3D structures were developed including micromachining,[7,8] hole-area modulation,[9] microstereolithography,[10] etc. A more flexible approach to fabrication of 3D structures, especially grayscale 3D structures, is to employ grayscale lithography. A typical process may consist of two steps: transferring a structure onto the resist in the form of the remaining resist profile and then etching the substrate through the remaining resist if the final structure is to be in the substrate. For the first step, one may employ optical lithographic or e-beam lithographic process.

In optical grayscale lithography, the amount (intensity) of light transmitted through a mask, on which the remaining resist profile depends, is spatially controlled. An example of controlling the transmitted light is to vary the ratio of opaque (pixel) area to transparent area in the mask.[1] Fabrication of grayscale structures such as blazed grating and Fresnel lens by these methods has been demonstrated.

E-beam grayscale lithography has the following advantages over the optical grayscale lithography: (i) it does not require any mask and (ii) it has a good potential to achieve a higher spatial resolution at the expense of low throughput. In fact, 3D structures may be fabricated using the binary e-beam lithographic process multiple times, i.e., once for each depth. However, it suffers from a long total process time, the alignment problem between processes, and high cost, especially when the number of different depths is greater than 2. E-beam grayscale lithography can eliminate these drawbacks since it requires only one step of e-beam lithographic process. An important issue in e-beam grayscale lithography is how to control e-beam dose spatially in order to achieve the target 3D structure. Most of the dose control schemes so far rely on a 2D exposure or empirical resist developing model. In this study, 3D analytic models for the exposure distribution and resist developing process are employed for better control of the remaining resist depth for fabrication of nanoscale 3D structures.

III. MODELS

A. Exposure distribution

Consider a substrate system where the initial thickness (or height) of the resist on top of a substrate is H and the X-Y plane of the 3D Cartesian coordinate system corresponds to the top surface of the resist layer, as shown in Fig. 1. Note that the Z-axis points down. Let $d(x,y,0)$, $e(x,y,z)$, and $\mathrm{psf}(x,y,z)$ represent the e-beam dose (*energy given*) to the point $(x,y,0)$ at the surface of the resist, the exposure (*energy deposited*) at the point (x,y,z) in the resist layer, and the point spread function (or energy deposition profile when a point is exposed), respectively. Then, the 3D exposure distribution may be computed as follows:

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

The exposure distribution $E(x,y)$ in a 2D model may be derived by averaging $e(x,y,z)$ along the resist depth dimension, or equivalently convolving $d(x,y,0)$ with the 2D point spread function $\mathrm{psf}(x,y)=\int_0^H \mathrm{psf}(x,y,z)dz$,

$$E(x,y) = \int_0^H e(x,y,z)dz. \quad (2)$$

That is, the depth-dependent variation of exposure is not considered in the 2D model.

B. Resist developing rate

The relationship between exposure and resist developing rate is known to be nonlinear.[5] Let the nonlinear relationship be represented by the mapping $F[\ ]$. Then, the resist developing rate at the point (x,y,z) is given by $r(x,y,z) = F[e(x,y,z)]$. Now, let $p(x,y)$ denote the development depth at (x,y) obtained for a development time of T and measured from the original surface of the resist downward. For the 3D model, the depth $p_{3D}(x,y)$ is determined such that

$$\int_0^{p_{3D}(x,y)} \frac{dz}{r(x,y,z)} = T. \tag{3}$$

For the 2D model, the resist developing rate $R(x,y)$ which is computed as $F[E(x,y)]$ is for all points on the line passing through $(x,y,0)$ and (x,y,H), i.e., $\{(x,y,z)|0 \leq z \leq H\}$. Therefore, the development depth denoted by $p_{2D}(x,y)$ may be estimated to be $R(x,y)T$.

While the contribution of $d(x,y,0)$ to $e(x,y,z)$ or $E(x,y)$ is linear, $r(x,y,z)$ [or $R(x,y)$] is not linearly dependent on $e(x,y,z)$ [or $E(x,y)$]. Therefore, determination of the spatial dose distribution based on exposure would not be effective in controlling 3D remaining resist profiles. Also, the development depth estimate based on $R(x,y)$ may include a significant error since $p_{2D}(x,y) \neq p_{3D}(x,y)$ unless $r(x,y,z) = R(x,y)$ for all $z(0 \leq z \leq H)$, as illustrated in Fig. 2. Hence, for accurate and effective control of the resist development depth, an e-beam control scheme is to directly refer to $r(x,y,z)$ instead of $R(x,y)$ or $e(x,y,z)$.

IV. SIMULATION OF RESIST DEVELOPMENT PROCESS

For conversion from exposure $e(x,y,z)$ to developing rate $r(x,y,z)$, the following solubility rate (resist developing rate) formula is used:[5]

$$r(x,y,z) = r_0 + B\left(\frac{1}{\bar{M}_n} + \frac{g \cdot e(x,y,z)}{\rho \cdot N_A}\right)^A, \tag{4}$$

where $\bar{M}_n$ is the average molecular weight, g is the chain scission per eV absorbed, ρ is the resist polymer mass density $(\mathrm{g/cm^3})$, N_A is the Avogadro number, and A, B, and r_0 depend on solvents; $e(x,y,z)$ is given in $\mathrm{eV/cm^3}$ and $r(x,y,z)$ in Å/min.

The simulation method employed for estimating the remaining resist profile is the cell removal algorithm.[6] The resist layer is decomposed into cells within each of which the developing rate is assumed to be uniform, i.e., a cell is the spatial unit of simulation. For simplicity, it is assumed in this study that a 3D structure does not vary along the Y axis. That is, only the X and Z dimensions need to be considered. The developing rate of each cell is computed from its exposure using Eq. (4). Through iterations, the remaining time for complete development of each of the exposed cells is updated, taking the number of its exposed sides into account. Simulation continues for a specified developing time, and then the remaining resist profile is obtained.

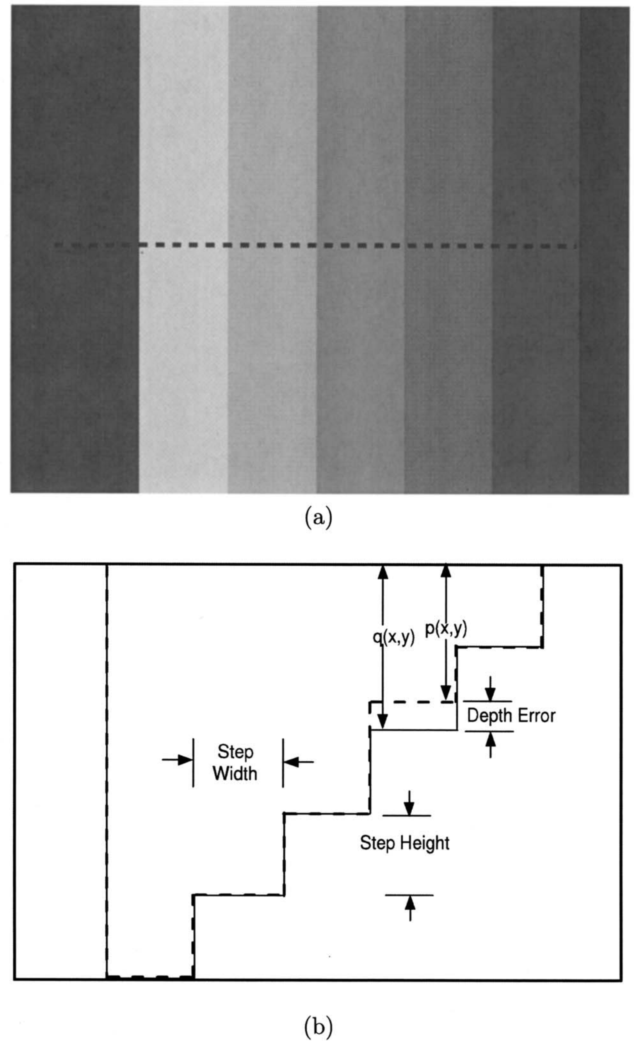

FIG. 4. Staircase structure: (a) the top view where the gray level in each feature represents its depth with the dashed line indicating the cross section shown in (b). The solid and dashed lines in (b) indicate the target $[q(x,y)]$ and (simulated) actual $[p(x,y)]$ remaining resist profiles, respectively.

V. DOSE CONTROL SCHEMES

Two dose control schemes are considered: for determining the dose distribution, *2D exposure correction* refers to the average (2D) exposure and the *3D resist profile correction* employs the resist development simulation procedure.

A. 2D exposure correction

Let $q(x,y)$ represent the depth distribution of a target 3D structure, measured from the original surface of the resist downward (refer to Fig. 1). A target exposure distribution $E_t(x,y)$ is derived from $q(x,y)$ such that $E_t(x,y) = C \cdot q(x,y)$ where C is a positive constant. Then, the e-beam dose distribution $d(x,y,0)$ which minimizes the deviation from $E_t(x,y)$, i.e., the error $|E(x,y) - E_t(x,y)|$ where $E(x,y) = \int\int d(x-x', y-y', 0)\mathrm{psf}(x', y')dx'dy'$ [also refer to Eq. (2)], is computed by the grayscale PYRAMID (Ref. 11) that takes an efficient two-level approach to determine the dose distribution iteratively. The overall flow of the 2D correction is shown in Fig.

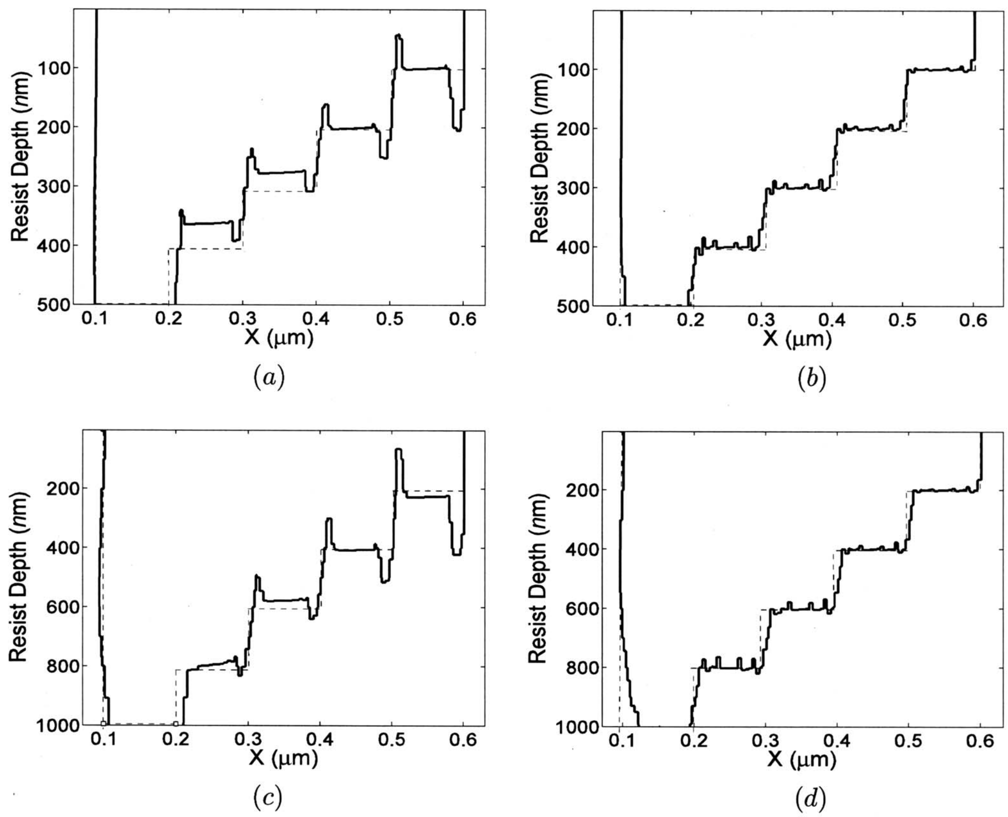

FIG. 5. Remaining resist profiles obtained (through simulation) for the staircase structure with the step width of 100 nm (beam energy of 50 keV): (a) 2D exposure correction and (b) 3D resist profile correction on the substrate system of 500 nm PMMA on Si; (c) 2D exposure correction and (d) 3D resist profile correction on the substrate system of 1000 nm PMMA on Si. The target profile is shown by the dashed line.

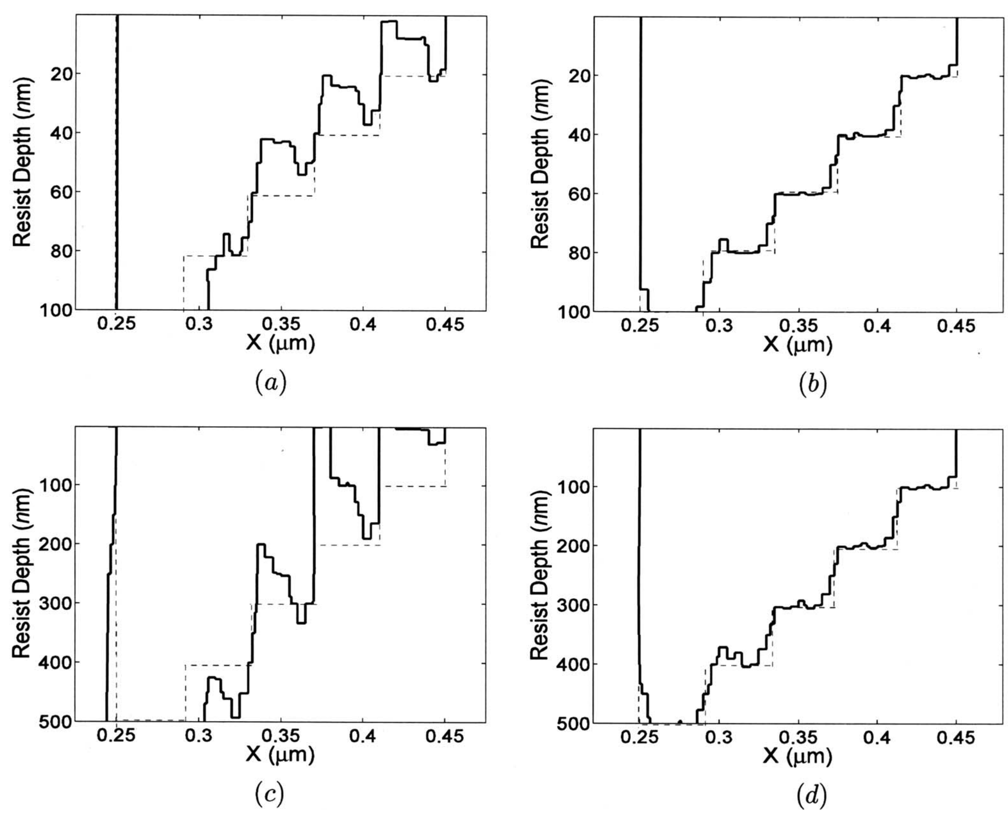

FIG. 6. Remaining resist profiles obtained (through simulation) for the staircase structure with the step width of 40 nm (beam energy of 50 keV): (a) 2D exposure correction and (b) 3D resist profile correction on the substrate system of 100 nm PMMA on Si; (c) 2D exposure correction and (d) 3D resist profile correction on the substrate system of 500 nm PMMA on Si. The target profile is shown by the dashed line.

3(a). That is, the objective of this correction scheme is to achieve the average exposure distribution, i.e., 2D exposure distribution, which resembles the depth distribution of the 3D structure.

B. 3D resist profile correction

The main difference between this correction and the 2D exposure correction is that it utilizes the estimated remaining resist depth in deriving $d(x,y,0)$ using the 3D model. The overall correction procedure is similar to that of the PYRAMID approach,[12] as shown in Fig. 3(b). In each iteration of the correction, the remaining resist depth $p_{3D}(x,y)$ is estimated for each feature in a 3D structure. The dose for the feature is determined such that $p_{3D}(x,y)$ is as close to $q(x,y)$ as possible. The iteration continues until $d(x,y,0)$ converges yielding the average or maximum of the error $(|p_{3D}(x,y) - q(x,y)|)$ less than a threshold or until a certain number of iterations is completed.

VI. SIMULATION

A. Test structure

The 3D test structure used in this study is a staircase pattern consisting of five different depths of steps where each step is long enough along the *Y* dimension that only the cross section along the *X*-*Z* plane may be considered, as shown in Fig. 4.

B. Results and discussion

In Figs. 5(a) and 5(b), the remaining resist profiles obtained by the 2D exposure and 3D resist profile corrections through computer simulation are provided, where the step width is 100 nm and the resist thickness is 500 nm. It can be seen for the 2D exposure correction in Fig. 5(a) that the depth error is significant in the third and fourth steps (from the right) while it is negligible for the first, second, and last steps. This is due to the fact that the 2D exposure correction does not consider the depth-dependent exposure variation and the developing rate is not linearly proportional to the exposure. Also, it leads to large errors at the transition regions between steps. The 2D exposure correction tends to assign a relatively lower dose (than those for its surrounding regions) to the transition region of the lower step while it assigns a relatively higher dose to the transition region of the adjacent upper step in order to achieve the target exposure distribution. Note that the target exposure is higher for a lower (deeper) step than for an upper step. On the other hand, the 3D resist profile correction achieves the remaining resist profile very close to the target profile, as shown in Fig. 5(b).

In Figs. 5(c) and 5(d), the staircase structure is transferred onto a thicker resist, i.e., 1000 nm. The result by the 2D exposure correction exhibits the same problem, i.e., not all steps reach the corresponding target depths and large depth errors between steps. In the result by the 3D resist profile correction, the remaining resist depth of each step is very close to the respective target depth. However, it is observed that the sidewalls are not completely straight due to the larger step height.

In Fig. 6, the staircase structure with a smaller step width, i.e., 40 nm, is transferred onto 100 and 500 nm thick resist layers, respectively. The same observations to those on the previous two sets of results can be made in general. Also, the remaining resist depth error tends to be significantly larger than that for the larger step width (100 nm) in the case of the 2D exposure correction. In addition, in the results by the resist profile correction, the remaining resist depth is still accurate while the steps deeper in the resist show shape degradation (rounding) caused by the proximity effect.

The remaining resist profiles obtained by the simulation method (cell removal algorithm) employed in this study may not be exactly the same as those which would be achieved in reality. However, the focus of this study was on comparison of the 2D exposure and 3D resist profile corrections, not on the accuracy of the resist development simulation.

VII. SUMMARY

As the dimensional resolution in 3D structures decreases well below 1 μm, accurate control of the remaining resist depth in e-beam grayscale lithography becomes crucial in order to achieve high dimensional fidelity of the fabricated 3D structures. A conventional dose control scheme usually uses the dose/exposure–remaining resist depth relationship empirically derived with a 2D exposure model. Such an approach is subject to substantial depth errors and may require a number of calibrations. In this article, a method (resist profile correction) which can accurately estimate the remaining resist depth and thereby control, with higher precision, the spatial distribution of the remaining resist for a given 3D nanoscale structure is described. It incorporates simulation of the resist development process into determining the e-beam dose distribution. Through computer simulation, it has been shown that the resist profile correction has a better control of the remaining resist profile than the conventional 2D exposure-based dose control schemes.

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