Multiple regression analysis of postdevelop unbiased line width roughness and etch resistance for high-accuracy estimations of postetch pattern roughness

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Abstract. As device scaling continues, development of photoresists with low pattern roughness and high sensitivity has become challenging. One obstacle that delays the material development process is the discrepancy between postdevelop and postetch pattern roughness, where a photoresist with high postdevelop patterning performance shows poor postetch pattern roughness. Herein, we demonstrate that pattern roughness after a nontrim etch process can be accurately estimated by a multiple regression analysis of a power spectral density (PSD) variable of postdevelop roughness and an etch resistance parameter of resins. The nontrim etch process here refers to an etch condition which leads to increased pattern roughness. Unbiased line width roughness (LWR) shows the highest correlation with postetch LWR among postdevelop roughness PSD variables. An etch resistance parameter also correlates well with postetch roughness. A multiple regression analysis reveals that the contributions of postdevelop unbiased LWR and etch resistance to the postetch LWR are 59% and 41%, respectively. Based on the calculated contributions, postetch LWR is estimated with a high accuracy ($R^2 > 0.93$). This estimation method allows for an efficient material screening at a lithography level without assessing postetch patterning performance, thus the process of material development could be accelerated.
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1 Introduction

In semiconductor manufacturing, it has been of great importance to control pattern roughness for securing normal electrical function of fabricated device.[1,2] Continuous device scaling has made it challenging to reduce pattern roughness at a high resolution and at a low dose. A great deal of efforts have been made to develop high-performance photoresists (PRs) with low pattern roughness, which has led to significant improvements in postdevelop pattern uniformity and roughness.[3–5] However, a high-quality postdevelop pattern does not inevitably lead to high-quality postetch patterns, and the differences between postdevelop and postetch roughness could differ among PRs depending on etching process conditions as well as resin types.[6,7] In particular, ArF resins have suffered from insufficient etch resistance due to the intrinsic chemical composition lack of carbon rings, which provide high etch resistance.[8,9] The discrepancy between postdevelop and postetch pattern roughness can significantly delay the material development process for high-performance PRs.

Several etch resistance parameters have been suggested based on chemical properties of resins. Ohnishi parameter (O.P.) is an empirically determined parameter, which has been widely adopted by PRs manufacturers for formulating PRs with high etch resistance.[10] It is defined by the following equation:

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$$\text{Ohnishi parameter (O.P.)} = \frac{N_{\text{total}}}{N_{\text{carbon}} - N_{\text{oxygen}}}, \tag{1}$$

where N_{total} is the number of total atoms, and N_{carbon} and N_{oxygen} are the number of carbon and oxygen atoms in a resin, respectively. A resin with high O.P. was found to have a high etch rate by an argon beam, which was attributed to the observed low sputtering yield of carbon and the higher etch rate of resins containing higher number of oxygen atoms. The parameter, however, only correlates well with etch rates when a high-energy ion beam (300 to 500 eV) was used to remove the exposed PR film via an ion bombardment mechanism. Later, Kunz et al. suggested another empirical parameter, a ring parameter, considering chemical structures of resins.[9] The ring parameter is defined as the mass of carbon atoms in a ring structure divided by the total mass of a resin. For the low energy beam (<50 eV), the ring parameter correlates better with etch rates than the O.P. does.

Recently, several studies demonstrated that power spectral density (PSD) analyses of postdevelop pattern roughness can predict postetch pattern roughness.[11–13] Cutler et al. showed that a PR with a lower postdevelop PSD(0) led to lower postetch line width roughness (LWR) compared to a PR with the same postdevelop LWR but higher PSD(0).[11,12] This was because high-frequency roughness was mainly trimmed during the etch process whereas PSD(0) remained unchanged. In addition, the resists with small correlation lengths tended to have low postetch roughness. This trend, however, was only shown in certain design of experiments (DOEs) where variance in PR formulations was not high. When PR formulations were varying to a large extent, the correlation between PSD(0) or correlation length and postetch roughness was low because roughness-generating mechanisms were different among PRs. Bian et al. investigated how PR formulations impact postdevelop unbiased LWR and postetch roughness.[13] The unbiased LWR was obtained by subtracting the scanning electron microscopy (SEM) noise from the total roughness, where the SEM noise was estimated from the PSD curve of postdevelop roughness.[14] Enhancing etch resistance of a resin did not affect the postdevelop unbiased LWR but resulted in improved postetch roughness. A PR with low etch resistance showed significantly higher increase in PSD(0) and lower reduction in unbiased LWR after the etch process compared with the PRs with high etch resistance.

In most previous studies, trim etch conditions were applied, where pattern roughness was reduced during the etch step. However, an etch process can also lead to degraded roughness via several mechanisms.[15–18] For instance, a dense amorphous carbon layer is formed on a PR film surface when the film is exposed to an ion bombardment during an etch process. The film densification enhances etch resistance of the PR, but at the same time, the increased density only near the film surface generates the compressive stress that could develop surface roughness.[19,20] In this study, we investigated how postdevelop roughness PSD variables correlate with postetch LWR for a nontrim etch process, which leads to degraded roughness after etching. Two postdevelop parameters, PSD(0) and unbiased LWR, were found to correlate well with postetch roughness for the given etch process. In addition, an etch resistance parameter showed good correlations with postetch LWR. The contributions of postdevelop roughness and etch resistance were calculated by a multiple regression analysis, which enabled us to estimate postetch LWR with a high accuracy ($R^2 > 0.93$). This estimation method would allow one to make better predictions of postetch patterning performance so that it could accelerate the process of PRs development by improving the efficiency of PR screening at a lithography level.

2 Materials and Methods

2.1 *Preparation of Samples*

All PRs were kindly provided by JSR cooperation (Tokyo, Japan). The compositions of each PR and postexposure bake (PEB) conditions are listed in Table 1. Silicon wafers were coated with an organic hardmask followed by formation of an antireflective organic/inorganic layer (ARL) using a spin-coater. Then, a PR film was formed on the ARL by spin-coating each PR and subsequent soft-baking at 100°C for 50 s. Line and space (L/S) patterns (sub-150 nm pitch) were

Table 1 List of PRs and PEB temperature for each PR.

PR	Polymer	PAG	PDQ	PEB temperature
A	P-1	PAG-1	PDQ-1	95
B	P-2	PAG-1/PAG-2 (3:1)	PDQ-1	95
C	P-3	PAG-1/PAG-2 (3:1)	PDQ-1	95
D	P-4	PAG-1/PAG-2 (3:1)	PDQ-1	95
E	P-5	PAG-1/PAG-2 (5.7:1)	PDQ-1	95
F	P-6	PAG-3	PDQ-1	95
G[a]	P-2	PAG-1/PAG-2 (3:1)	PDQ-1	90

[a]For convenience, PR B processed at PEB 90°C was noted as PR G.

generated through a 193-nm immersion lithography process. A two-step dry etch process was applied to each pattern for removal of the ARL and hardmask in the open space.

2.2 *SEM Measurements and PSD Analyses*

All SEM images were acquired using a CD-SEM tool (CG-5000, Hitachi, Tokyo, Japan). Postdevelop and postetch LWR was obtained by the built-in software of SEM equipment. For the PSD analysis and measurement of biased and unbiased LWR, images were acquired without applying a Gaussian filter, and the area of being analyzed in an image was $1014 * 1014\ (\text{pixel})^2$. All PSD analyses were performed by MetroLER software (Fractilia, Austin, Texas). For each sample, 400 images were analyzed. The reliability score provided by MetroLER were above 85 for all analyses, which is considered valid according to the software provider. The LWR measured by MetroLER without SEM noise subtractions was named as biased LWR to differentiate it from the LWR measured by the Hitachi SEM software.

2.3 *Multiple Regression Analysis*

Multiple regression analysis was performed using two parameters, postdevelop unbiased LWR and etch resistance parameters, each of which showed high correlations with postetch roughness ($R^2 \sim 0.8$ and ~ 0.7, respectively). A multiple linear regression model with p independent variables is expressed as

$$y = a_1 x_1 + a_2 x_2 + \ldots + a_p x_p + b, \tag{2}$$

where y is a dependent variable, $x_1, \ldots, x_p$ is the independent variables, $a_1, \ldots, a_p$ is the coefficient, and b is an underlying error. The coefficients $a_1, \ldots, a_p, b$ were calculated by least squares estimation where the sum of the square estimate of the errors (SSEs) are minimized. SSE is given as

$$\text{SSE} = \sum_{i=1}^{n} (y_i - (a_1 x_{1i} + a_2 x_{2i} + \ldots + a_p x_{pi} + b))^2. \tag{3}$$

Minimization of SSE is solved to yield the parameter estimators, $\hat{a}_1, \ldots, \hat{a}_p$.

$$\frac{\partial \text{SSE}}{\partial a_i} = 0, \qquad i = 1, \ldots, p, \tag{4}$$

$$\frac{\partial \text{SSE}}{\partial \text{b}} = 0. \tag{5}$$

The solution of Eq. (4) is as follows:

$$\hat{a}_\iota = \frac{\sum_{i=1}^{n}(x_{li} - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_{li} - \bar{x})^2}. \tag{6}$$

The calculated coefficients for unbiased LWR and etch resistance parameters were 0.052 and 0.036, respectively. (P-value < 0.05 for unbiased LWR and <0.1 for etch resistance parameters).

3 Results and Discussion

Sub-150 nm pitch L/S patterns were generated through a 193-nm immersion lithography process. Postdevelop and postetch inspection by a CD-SEM confirmed that the LWR increased after the etch process for all PRs used in the study, and the LWR differences were ranged from 0.03 to 0.33 nm. Since the LWR increased under the given etch condition, we called this process a nontrim etch process to differentiate it from a trim-etch process. Representative PSD curves for postdevelop and postetch roughness are shown in Fig. 1. For all samples, the unbiased PSD(0) increased, whereas correlation lengths decreased during the etch step. In addition, postetch roughness in all frequency ranges were higher than those measured after lithography [Fig. 2(a)]. For all PRs except PR F, the degree of increase was higher for the high frequency roughness than the low frequency roughness [Fig. 2(b)]. The observed changes caused by the etch process are clearly different from the previously reported trend for trim etch processes, where high frequency roughness is largely trimmed by etching, leading to reduction of overall LWR after the etch

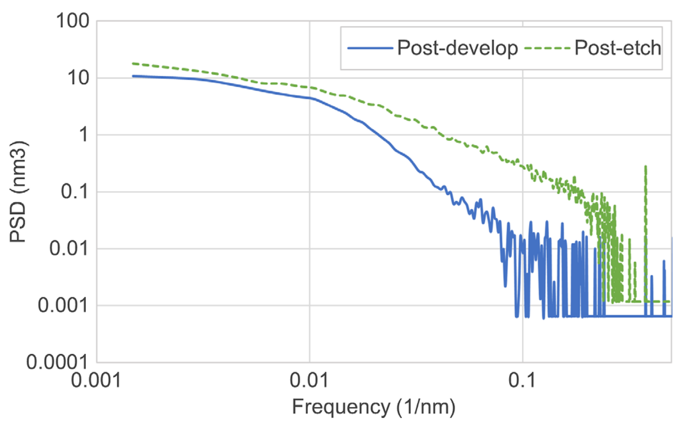

Fig. 1 Representative postdevelop and postetch unbiased PSD curves for PRs used in this study.

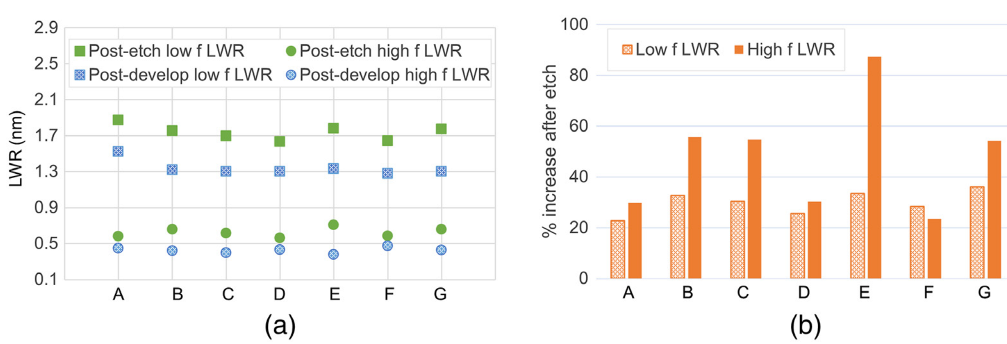

Fig. 2 Changes in low and high frequency LWR after the nontrim etch process. (a) Postdevelop and postetch LWR in different frequency ranges. (b) % increase of LWR in each frequency region after the etch process.

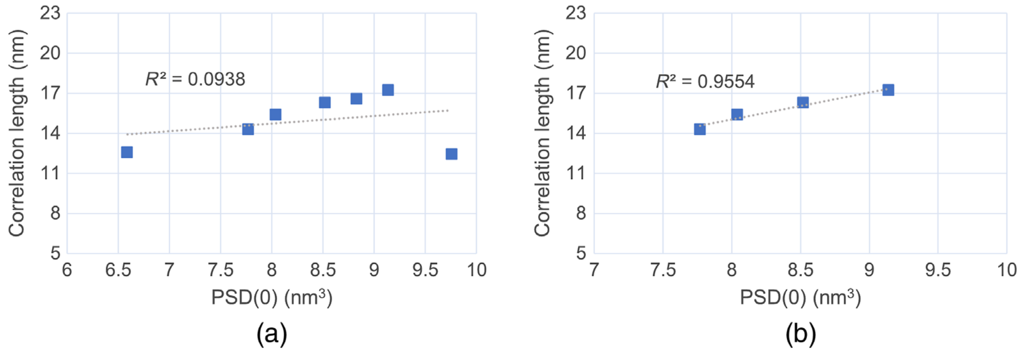

Fig. 3 Postdevelop unbiased PSD(0) versus correlation length for (a) all PRs, and (b) PRs with varying resins but the same PAG (B, C, D, and G).

process.[11,13] Furthermore, the correlation length was reported to increase, while PSD(0) remained unchanged after a trim-etch process used in a previous study.[11]

The group of PRs used in this study did not show a linear correlation between PSD(0) and correlation length, which is attributed to composition variations where both polymer types and PAG types were varied among PRs [Fig. 3(a)]. For such varying formulations, there could be components and/or mechanisms that nonlinearly impact both correlated and uncorrelated events. When the same graph was plotted for the PRs with the same type PAG but only varying polymers (B, C, D, and G), good linear correlation was found [Fig. 3(b)]. The observation is consistent with previously reported results by Cutler et al.,[11] where linear correlations were observed for DOE 1 (varying resins) and DOE 2 (varying other components for a fixed resin) but not for DOE 3 (varying all components).

Next, we studied correlations between various postdevelop roughness parameters and postetch LWR. No correlation was observed between postdevelop LWR measured by a CD-SEM and postetch LWR [Fig. 4(a)]. Postdevelop LWR measured by MetroLER software slightly correlated with postetch LWR [Fig. 4(b)], which is attributed to a different line edge detection method provided by MetroLER.[21] When the SEM noise was removed, the correlation between

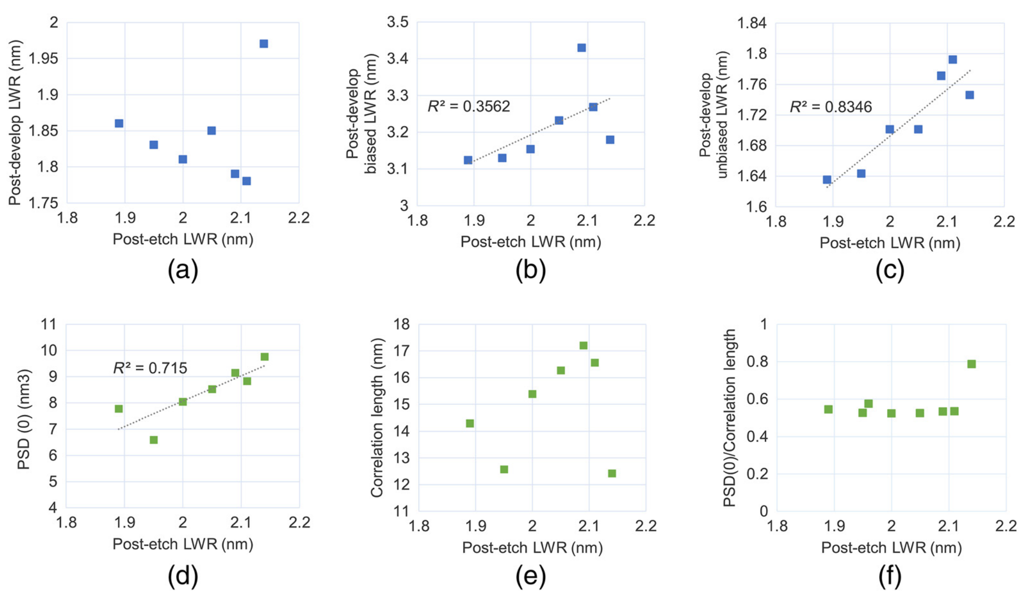

Fig. 4 Correlations between postetch LWR and postdevelop roughness parameters. (a)–(f) Plots of postetch LWR versus postdevelop (a) LWR (measured by the CD-SEM software), (b) biased LWR (measured by MetroLER), (c) unbiased LWR, (d) unbiased PSD(0), (e) correlation length, and (f) PSD(0)/correlation length.

postdevelop roughness and postetch LWR significantly increased to give $R^2 = 0.8346$ [Fig. 4(c)]. We also investigated how other postdevelop PSD parameters affected the postetch pattern roughness. Unbiased PSD(0) relatively well correlated ($R^2 = 0.715$) with postetch LWR [Fig. 4(d)]. A similar trend has been reported for a trim etch process, which was attributed to the unchanged PSD(0) and reduced high frequency roughness after the etch process.[11] Even though PSD(0) increased during the nontrim etch process, lower PSD(0) still led to lower postetch LWR to a certain degree. The correlation is partly because the higher postdevelop PSD(0) contributes to the larger area under the curve (σ^2) which is proportional to the postdevelop LWR (3σ). The correlation factor (R^2) between the postdevelop PSD(0) and postdevelop LWR was found to be 0.6425 (data not shown). The higher postdevelop LWR can lead to higher postetch LWR if the PR pattern is not trimmed or roughened during a etch process. Correlation length was reported to be another indicator for pattern roughness after a trim etch because a PR with a smaller correlation length has more high frequency roughness which can be removed after the etch step.[12] However, for the nontrim etch process used in the present study, it poorly correlated with postetch LWR [Fig. 4(e)]. In addition, PSD(0)/correlation length also showed very low correlations with postetch LWR, even though it was previously reported that SQRT(PSD(0)/correlation length) correlated well with pattern roughness after a trim etch independent of PR compositions [Fig. 4(f)]. In summary, the unbiased LWR showed the highest correlation with the postetch LWR; however, the correlation factor ($R^2 = 0.8346$) was still not high enough to accurately predict postetch LWR. Furthermore, other postdevelop PSD parameters reportedly affecting postetch roughness showed only moderate or very low correlations with postetch LWR. From the results, we concluded that etch resistance should also be considered to predict postetch roughness (Fig. 5).

Etch resistance parameters were calculated based on chemical properties of each resin. A higher value is expected to be less resistant to etch processes and thus higher roughness degradation during an etch process. Indeed, the etch resistance parameter well correlated with postetch LWR ($R^2 = 0.6859$) [Fig. 5(a)]. Postdevelop unbiased LWR and the etch resistance parameter were chosen to be the major two predictors of postetch LWR considering their high correlation factors. A multiple regression analysis revealed that the contributions of postdevelop unbiased LWR and the etch resistance parameter to postetch LWR were 58.9% and 41.1%, respectively [Fig. 5(b)]. When the postetch LWR was estimated using the calculated contribution factors, the results highly correlated with the actual measured LWR ($R^2 = 0.9355$) [Fig. 5(c)]. The contributions of each predictor would change depending on the etch conditions. The observed high contribution of etch resistance to the postetch pattern roughness could be due

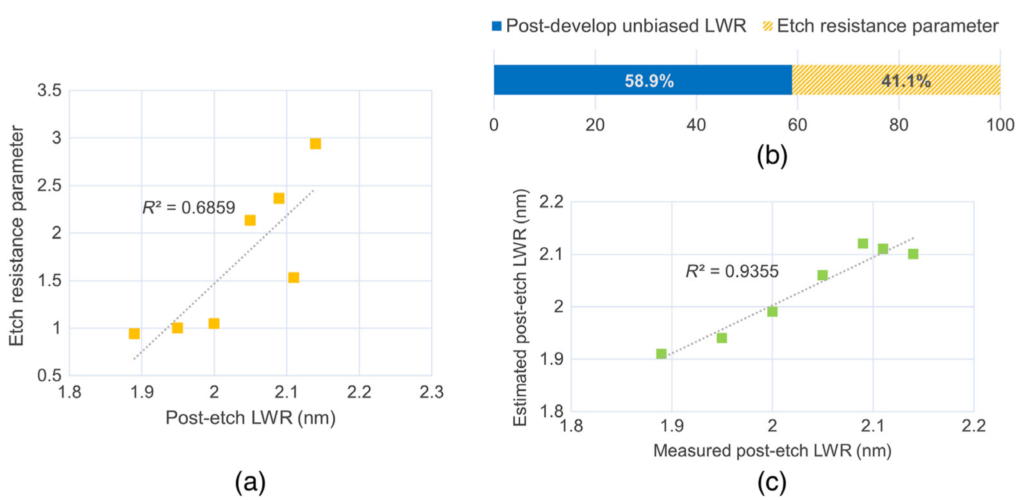

Fig. 5 Estimation of postetch LWR using postdevelop unbiased LWR and an etch resistance parameter. (a) Correlation between postetch LWR and an etch resistance parameter. (b) Multivariate analysis result. (c) Plotting of measured postetch LWR and calculated postetch LWR.

to the harsh etching condition which made all tested PRs develop roughness during etching. For an etch process inducing less roughness increase, the contribution of etch resistance might be lower than the result of this study.

4 Conclusion

In this study, we demonstrated that postetch LWR could be estimated with a high accuracy through a multiple regression analysis of unbiased postdevelop LWR and etch resistance of resins for a nontrim etch process. Unbiased LWR showed the highest correlation with postetch LWR among several postdevelop roughness PSD parameters, whereas correlation length poorly correlated with postetch roughness different from a previously reported trend for a trim-etch process. The etch resistance parameter was another important factor to be considered for estimating postetch LWR for the given etch process. The estimation method based on a multiple regression analysis would facilitate efficient material screening at a lithography level without assessing postetch patterning performance, which would accelerate the process of material development.

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