Utilizing Roughness Power Spectral Density Variables to Guide Resist Formulation and Understand Impact of Frequency Analysis through Process

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Linewidth roughness (LWR) remains a difficult challenge for improvement in all resist materials. In this paper, we intend to focus on the impact of key components of LWR by analyzing the power spectral density (PSD) curves which can be obtained using Fractilia’s MetroLER computational software. We will study systematic changes to ArF resist formulations and correlate these changes with the overall PSD curves. In this manner we will use frequency analysis information to guide resist formulation improvements. We will also investigate the relationship between frequency roughness components and LWR through lithographic/etch processing and demonstrate which components correspond with the largest impact. In order to achieve quality data over low and high frequency ranges we changed our standard metrology setup to capture longer lines. By making systematic changes to the ArF resists, we can determine the key impacts of various controllable resist factors on the PSD. Through systematic analysis, we can deconvolute LWR improvements both after develop and after an etch process.

Keywords: Power spectral density, PSD, Linewidth roughness, LWR, Line-edge roughness, LER

1. Introduction
Reducing linewidth roughness (LWR) continues to be a significant challenge in advanced lithography. For many years the main CD-SEM output for LWR improvement Design of Experiments (DOEs) was one averaged number, a 3-sigma roughness measurement. This measurement of line variation was used to understand how formulation changes or new materials would impact LWR both at resist vendors and chip manufacturers. The idea of breaking down LWR into its frequency components and understanding roughness in the form of power spectral density (PSD) analysis, was proposed as a useful tool for understanding how LWR varied depending on the length or frequency domain down a line [1,2]. From a formulation chemist’s perspective these types of measurements were difficult to understand and acquire. Over the past 10-15 years off-line software was developed to enable the processing of a large number of image files and average PSDs [3]. However, most LWR measurements and PSDs were already subject to some type of high frequency roughness filtering either from edge detection algorithms or the LWR measurement recipe. Further, measured roughness is biased by the noise in the scanning electron microscope (SEM) images [4]. The LWR number has always been dependent on measurement threshold, the type of image filtering employed to enable edge detection, SEM pixel size, and other measurement settings. With the recent development of MetroLER by Fractilia, the ability to process unfiltered metrology images and obtain unbiased spectral density output variables became more accessible. Power spectral density analysis of formulation DOEs provides a tool for understanding and tailoring resist formulations for more optimal
performance through process.

A recent publication proposes a new approach to roughness reduction: in order to overcome the scaling issues associated with LWR and resist blur (manifested as the correlation length in a PSD), resists should be developed that have low PSD(0) and low correlation length, letting etch processes improve the high frequency roughness by increasing the correlation length [5]. This theory is proposed from an understanding of how LWR is derived from frequency analysis of a line and classical resist LWR models. The questions we wanted to answer using PSD analysis were: Can we correlate specific PSD output variables with trends in formulation components and can we use PSD analysis of internally generated images to predict how our resists would perform both after a standard photo/develop process and after subsequent etch or etch trim processes.

Before discussing experimental results, a basic understanding of PSD analysis and how to collect the appropriate metrology data is required. PSD averaging and implementing appropriate metrology settings is important in PSD analysis. Three formulation DOEs were tested and the results were analyzed using our standard LWR methods and using MetroLER for PSD analysis. The internally generated PSD output variables after a standard photo/develop process were then correlated with LWR values generated at an external Fab, both after a standard photo/development process and after a subsequent etch process. The results are a first step in taking PSD analysis from the theoretical realm into a very real tool that can experimentally help in resist development.

1.1. Power spectral density analysis

The standard visual representation of why the frequency dependence of roughness contains significantly more information than LWR alone is shown in Fig. 1. The standard deviation describes the deviation from a straight line but it doesn’t describe how this variation changes at different length scales down the line. Shown in Fig. 1 are four very different lines with different frequency roughness characteristics but the same standard deviation or LER. From a resist formulation perspective understanding how formulation components impact the variation of roughness through frequency would help in designing resists for different applications and help focus efforts on the PSD properties that are not changed through etch.

The PSD is the variance of the edge or linewidth per unit frequency. Graphically it is represented on a log–log scale as shown in Fig. 2, where the Y axis is the power or variance per unit frequency of the line at a particular frequency and the X axis is the frequency or the inverse of the length scale of the line over which the variance is measured. Low frequency roughness occurs over longer length scales and the high frequency region occurs over shorter length scales. The flat region of the graph in the low frequency region is termed PSD(0). This is the region or length scale where events that influence the PSD are considered “uncorrelated”. This low frequency value of the PSD is an estimate of PSD(0), the value of PSD of an infinitely long line (zero frequency). In resist terms the causes of low-frequency uncorrelated roughness are random independent events such as absorption, chemical concentration, or photon shot noise. The point at which the graph curves down is the length scale
where the edge roughness becomes correlated and relates to events that are no longer independent but reflect a mechanism which is correlated, such as acid reaction-diffusion in a chemically amplified resist. The inflection point is determined by the correlation length ($\xi$) and at this point the power begins to fall at the frequency of $1/2\pi\xi$. The slope of the line at higher frequencies is defined as $2H+1$ where $H$ is the exponent roughness (Hurst exponent). For the purpose of this work $H$ is set to 0.5 for all analysis, which is the value expected when a reaction-diffusion process is driving the correlation. The variance (or $1\sigma$ LWR squared) is defined as the area under the curve and is a function of three PSD parameters, PSD(0) or the flat low frequency region, the correlation length (proportional to diffusion or resist blur), and the slope ($H$).

The ultimate goal is reducing the area under the PSD graph. An approximation of the relationship between variance the PSD parameters is:

$$\sigma^2 \approx \frac{PSD(0)}{(2H + 1)\xi}$$

where for a given PSD(0) increasing the correlation reduces line variance. Increasing correlation length also however can be thought of as an increase in resist blur and can impact the effective image-log slope (ILS) and PSD(0), hence ultimately not the best direction for improving LWR [5]. PSD(0) however is directly proportional to the variance. Figure 3 is an example of how the shape of the PSD governs the overall LWR. Despite the two curves having the same variance, the two lines can now be effectively described using the correlation length and PSD(0). From a resist design perspective the question is what are my PSD targets for improved LWR?

To understand what PSD output values to target it helps to understand how the resist is used in a semiconductor manufacturing process. The function of a patterned resist in this study is to act as an etch barrier in a photoresist trimming process and ultimately into the underlying substrate. Figure 4 shows an example of what can happen to an unbiased PSD during a typical etch process. The length scale or frequency domain impacted through etch is the high frequency roughness. The correlation length is effectively increased while the unbiased PSD(0) remains unchanged, hence reducing the overall variance or area under the PSD curve. If this holds true for a given etch process, designing a resist with lower PSD(0) and smaller correlation length may result in larger post-photo/develop LWR, but may also result in a larger reduction in LWR through the etch process. The increase in high frequency LWR may be taken care of through the etch process as long as PSD(0) is low. The PSD targets for post-photo develop process only may be low PSD(0) and mid to low correlation length. The results reported in subsequent sections support this hypothesis, but first an understanding of how to collect images appropriate for PSD analysis is required.

2. Experimental

2.1. Sample preparation

The photoresists were formulated with 193nm photoresist polymer, PAG, quencher, and solvents. Due to the proprietary nature of these materials the details of their composition are not disclosed. The solutions were filtered through 0.02 $\mu$m PTFE filter prior to evaluation.
2.2. Wafer coating and lithographic evaluation

Thin films (900 Å) were prepared by spin coating on an antireflective coating (ARC) on 300 mm primed wafers using a TEL CLEAN TRACK LITHIUS i+. Films were exposed on an ASML 1900i. CD-SEM metrology was carried out using a Hitachi CG4000. Post-lithographic LWR and PSD evaluation was carried out on positive tone 90 nm pitch and 110 nm pitch dense lines. Similar PSD trends were seen through feature size of similar NILS (normalized image log-slope, a measure of image quality). Lithographic results generated at an external Fab were also from an ASML tool on 140 nm pitch dense lines. Post-etch trim LWR was measured on 110 nm pitch dense lines.

2.3. Metrology and PSD analysis

Table 1 outlines image dimensions and averaging used for LWR measurements. Internal LWR measurements using an historical metrology recipe are captured on a shorter line than is recommended for PSD analysis with higher magnification and smaller overall pixel count (512×512). LWR generated from these standard screening images used Hitachi CD SEM software with a 50% threshold. Every LWR measurement is an averaged value from 20 images down a line to capture a more statistically significant representation of 3σ LWR for each sample. Images for PSD analysis for DOE 1 were captured using the rectangular scan method. This method has different magnification in the X and Y directions. Images for PSD analysis for DOE 2 and 3 were captured using a square scan, 1024×1024 pixels at 100K magnification. The same for DOE 2 and 3 were captured using a square scan, 1024×1024 pixels at 100K magnification. The same method has different magnification in the X and Y directions. Images for PSD analysis for DOE 1 were captured using the rectangular scan method. This method has different magnification in the X and Y directions. Images for PSD analysis for DOE 2 and 3 were captured using a square scan, 1024×1024 pixels at 100K magnification. The same magnification in the X and Y axis may help to reduce across field distortion and provides more reliable PSD analysis [6].

Table 1. Dimension and magnification of images for LWR and PSD measurements.

| # Pixels per image | STD Dow LWR image | Square image for PSD analysis | Rectangular image for PSD analysis |
|--------------------|-------------------|-------------------------------|-----------------------------------|
| 512512             | 10341024          | 512512                        |
| Magnification      | 200k              | 100k                          | 3/4×200k/52.7k                    |
| Line length        | 645nm             | 1.35μm                        | 2μm                              |
| Images Averaged per resist | 20           | 20                            | 20                               |
| Lines averaged per sample for PSDs | NA           | 200                           | 100                              |

Power spectral density analysis was carried out using MetroLER v1.1 by Fractilia and used to measure unbiased PSD(0) and correlation length (that is, after SEM noise was removed). All PSDs are averaged over 20 images and images were analyzed for systemic abnormalities and field distortions. PSD outputs were exported into excel from the DOE mode in MetroLER.

3. Results and discussion

The following 3 DOEs were designed to understand trends in LWR based on materials and formulation.

3.1. DOE 1 (Matrix polymer study)

The first DOE looks at systematic matrix polymer changes (Table 2). The images analyzed with PSDs were obtained using the rectangular scan method as detailed in the previous section. The goal of the first experiment was to test the hypothesis that using PSD analysis of internal images could help us predict the LWR response especially through a post-photo/etch trim process. It was often noted that the LWR obtained after a standard photo/develop process did not correlate with the LWR obtained after an etch-trim process. Many previous studies had focused on Ohnishi parameter or other materials properties thought to influence how a formulation responds to an etch process.

Table 2. DOE 1 design with systematic change in polymer matrix and the corresponding PSD parameters generated from internal post-photo-images. Post-photo biased LWR, etch-trim biased LWR and the delta between the two are also shown.

| Resist | Function Group 1 | Function Group 2 | For Photo LWR | Post Photo/etch LWR | LWR Delta | Unbiased PSD(0) | Correlation length |
|--------|------------------|------------------|---------------|---------------------|-----------|-----------------|--------------------|
| Resist A | FG1_A Held | FG1_D Held | 5.8  | 4.5 | 1.3 | 3.6 | 39  | 64  |
| Resist B | FG1_B Held | FG1_D Held | 6.2  | 4.5 | 1.7 | 3.7 | 46  | 70  |
| Resist C | FG1_C Held | FG1_D Held | 5.3  | 4.5 | 0.8 | 3.5 | 38  | 58  |
| Resist D | FG1_D Held | FG1_D Held | 5.5  | 3.8 | 1.7 | 3.7 | 78  | 22  |

In this study we looked for PSD output trends from internally generated images that might help explain trends in the Post-photo/etch trim LWR. Figure 5 shows 2 graphs, the first is post-photo biased LWR (generated at an external Fab) vs unbiased PSD(0) measurements generated with Dow images. The second graph shows post-photo/etch trim biased LWR (generated externally) against the same unbiased PSD(0) measurements generated at Dow. In this dataset we observed that Resist G has a much lower PSD(0) value than Resist E but they show similar post-photo LWR. Since LWR is a function of the total area under the PSD curve this result is plausible as shown in Fig. 3. In theory however, the lower PSD(0) resist is predicted to have lower LWR after a trim process (or a bigger delta) if it has a significant amount of high
frequency roughness (small correlation length) that could be smoothed during the etch process. The data in the second graph in Fig. 5 supports this hypothesis in that Resist G now shows a significantly lower LWR than Resist E and a more linear trend develops between unbiased PSD(0) and post-etch trim LWR. Resist A and B show the same trend with similar post-photo LWR and post etch-trim LWR that is more correlated with each resist’s respective unbiased PSD(0).

Fig. 5. External Fab post-photo and post-photo/etch trim biased LWR (3σ) verses unbiased PSD(0). “Resist G” has a lower PSD(0) than “Resist E” but higher post-photo LWR. After the etch trim process the LWR of “Resist G” reduces significantly in LWR and “Resist E” photo LWR. After the etch trim process the LWR of “Resist G” has a lower PSD(0) than “Resist E” but higher post-etch trim LWR.

A closer look at the relationship between post etch-trim LWR and PSD(0) reveals a highly significant fit when etch-trim LWR is expressed as a function of the square root of PSD(0) (R2 = 0.90) rather than a linear fit (R2 = 0.85). This experimentally driven relationship supports the theoretically derived relationship between LWR and the square route of PSD(0) in the variance equation (1).

Figure 6 shows Dow generated correlation length verses external LWR through process. An increase in correlation is seen with Dow generated correlation length from post-photo LWR to post-etch trim LWR generated externally. In theory we would predict that resists with smaller correlation length post-photo would give lower LWR post etch trim if their PSD(0) values are similar. This is due to the larger impact of etch on lower correlation length. Further, unbiased PSD(0) may not change through etch, making it a good predictor of how a resist may behave through process. The correlation length is predicted to change through process, hence resists with low PSD(0) and low correlation lengths may show the biggest change through process and may result in lower post etch-trim LWR.

3.2. DOE 2 (Formulation study)

The second DOE used a fixed polymer matrix with varying formulations and exhibited lower overall LWR and PSD values as seen in Table 3. The images used to generate PSD data contained longer lines as with the rectangular scan but magnification was reduced to allow for the same magnification in both the X and Y directions. The goals for this DOE included verifying whether internally generated PSD outputs could predict trends in externally generated LWR through process in a completely different formulation space than DOE 1. The second goal was to investigate whether PSD analysis showed significant formulation trends that were not captured by analyzing LWR alone. Not all of the initial study was run externally, but the results still showed significant trends supporting the use of PSD analysis.

Table 3. Formulation DOE 2: Component 1 was varied between 3 different types, component loading was varied along with component 2 loading. PSD values generated from Dow images and post-photo/ post etch-trim LWR generated externally are also shown.

Dow generated unbiased LWR measurements and PSD variables were graphed against various formulation components and some interesting trends emerged. Changes in certain formulation variables that did not correlate well with Dow generated unbiased LWR started to show surprisingly linear trends with PSD variables even when formulation components were significantly different. Figure 7 shows that if LWR was the only metric used to analysis this data, the low PSD(0) at higher loadings of component 2, coupled with component 1 (Type 3) would not be known.
significant because we saw from DOE 1 that low PSD(0) can lead to a larger LWR delta through a photo/etch process even when post photo LWR seems high.

Figure 7. Dow generated unbiased LWR measurements vs loading of formulation component 2. Graphing unbiased PSD(0) from Dow images verses loading of formulation component 2 shows more linear trend. Color represents component 1 type and shape indicates component 1 loading.

Figure 8 shows the resists that have low PSD(0) also have the smallest correlation length. This supports the likelihood of a large delta in LWR through a photo/etch trim process. From theory the low unbiased PSD(0) (over a longer length scale) should remain unchanged whereas the etch-trim process should smooth out the roughness at higher frequencies effectively increasing the correlation length and reducing the total area under the PSD curve to give lower LWR (larger LWR delta) through process.

Formulations were run at an external Fab and LWR was collected both post-photo and post-etch trim. The LWR through process was graphed against unbiased PSD(0) from Dow images. Figure 9 shows two distinct data sets: component 1/type 1 and 2 (purple and green series) and component 1/type 3 (red series). As was the case with Dow post-photo LWR, the red series showed higher post-photo LWR than the other resists despite having lower PSD(0). In the green and purple series, the lower PSD(0) resist did not show the lowest post-photo external LWR. When unbiased PSD(0) was graphed against external post-etch trim LWR, two trends emerged. The first trend showed resists with the lowest PSD(0) (the red series) with a significant reduction in etch-trim LWR. The second trend showed after etch-trim LWR for the purple and green series had the most significant fit when plotted against the square root of PSD(0). This follows the same trend as seen in DOE 1. The lower PSD(0) resist in the purple and green series had the lowest overall after-etch LWR although not the highest overall LWR delta.

Fig. 8. PSD components unbiased PSD(0) and correlation length verses loading of formulation component 2.

The resists that showed the highest LWR delta through process also had the smallest correlation length from the PSD analysis of Dow generated images as shown in Fig. 10. The resists with more high frequency roughness (smaller correlation length) and low PSD(0) are predicted to show the largest reduction in LWR through process.

Fig. 9. Externally generated LWR data post-photo and post etch-trim verses unbiased PSD(0) values generated from Dow images.

DOE 1 and DOE 2 both showed a significant relationship between PSD(0) and correlation length in Fig. 11. If correlation length is a measure of resist blur, then this data supports the supposition that higher resist blur results in higher PSD(0). It is plausible that some variables can impact both PSD(0) and correlation length and that the relationship between the two could change depending on the underlying mechanism in formulation. PAGs for example can potentially impact both correlated and uncorrelated events
simultaneously within a formulation. PAG absorption and concentration are uncorrelated events, whereas the diffusion and deprotection mechanisms are correlated. Formulations contain many variables that can impact correlated and uncorrelated roughness, hence it is also plausible that in a more complicated resist DOE, correlation length and PSD(0) don’t correlate. An example of this was found in DOE 3 (to be described next), where polymer, quencher and PAG were varied and correlation length and PSD(0) did not correlate (Fig. 12). In this DOE we also found that because the total area under the PSD curve governed LWR, a higher correlation length could drive an overall reduction in etch-trim LWR, even when PSD(0) was not the lowest (these are higher NILs features). The knowledge that there is the possibility to impact PSD(0) and correlation length with less co-dependence through formulation offers greater flexibility in formulation design. It alludes to the potential ability to dial in a low PSD(0) and either a high or low correlation length depending on optical and etch requirements.

Fig. 11. Both DOE 1 and DOE 2 show significant correlation between PSD(0) and correlation length.

Fig. 12. DOE 3 changes polymer, PAG and quencher and shows no obvious correlation between PSD(0) and correlation length.

3.3. Formulation
DOE 3 varied both polymer and formulation in a nine formulation DOE. Both DOE 2 and DOE 3 were analyzed in the same way, in that both utilized square pixel images containing 1024×1024 pixels at 100K Magnification (Table 4).

Table 4. Formulation and results from DOE 3 where both polymer and formulation where varied.

The fundamental difference between DOE 3 and DOE 1/DOE 2 is that correlation length and PSD(0) are not correlated as shown in Fig. 12. This is an exciting prospect for the potential to tailor correlation length and PSD(0) independently, but how does it affect the potential predictive power of PSD(0) or correlation length in either post etch-trim LWR or predicting the LWR delta through an etch-trim process? Figure 13 shows etch-trim LWR plotted against both PSD(0) and correlation length. The most apparent observation is that etch-trim LWR in this round does not correlate with PSD(0). There are three distinct groups where formulation type has a larger impact on etch-trim LWR and PSD components than the polymer changes in this DOE. The lowest etch-trim LWR is driven by mid to low range PSD(0) and higher correlation length (effectively corresponding to the smallest area under the curve). Lower post-develop correlation length resists in this round correspond to the highest PSD(0). Therefore, even with the characteristic larger LWR delta associated with lower correlation length, a high post-develop PSD(0) still results in a higher overall etch-trim LWR. Low PSD(0) is still desired to obtain low overall LWR, however when correlation length and PSD(0) don’t correlate post etch-trim LWR is more a function of PSD(0)/correlation length (Fig. 14) as opposed to PSD(0) alone. Since this work was carried out, DOE’s run internally show that correlation length and PSD(0) often do correlate and we are working to understand the underlying mechanisms that govern this relationship and inversely how to push levers that move PSD(0) and correlation length in different directions.
Despite the lack of correlation between PSD(0) and correlation length in DOE 3, there is still a clear trend between the etch-trim LWR delta and correlation length. This relationship can be defined by the same fit in both DOE 2 and 3 as seen in Fig. 15. The etch-trim delta shows a significant relationship with reciprocal correlation length.

Defining a correlation between etch-trim LWR delta and correlation length is very useful when designing materials for an etch process.

3.4. PSD directed formulations

Despite the continued work that is required to understand the relationships between PSD components and formulation. Measuring the low and high frequency roughness of LWR is still a valuable tool when designing new resists. An example of this is shown below (Figs. 16 and 17) where Resist 6 from DOE 2 was of interest due to its low PSD(0) and low correlation length (improved etch performance), but not because it had the best post-photo LWR performance. The goal was to capitalize on the good etch performance by lowering PSD(0) of this resist further while maintaining low correlation length. Concurrently the goal with Resist 5 from DOE 2 was to decrease PSD(0) further while maintaining higher correlation length. The lowest PSD(0) polymer from DOE 1 was combined with Resist 5 and 6 from DOE 2. Other minor formulation changes were also made and the result was a series of resists with very similar improved LWR numbers but different PSD(0) and correlation lengths. New resists that were modifications of Resist 6 (DOE 2) showed the LWR of Resist 6 was lowered through reduction in PSD(0) while maintaining a similar correlation length. The modifications to Resist 5 (DOE 2) reduced PSD(0) slightly while maintaining a higher correlation length. The LWR improvements are more subtle and the real gain in this formulation space was with photospeed.
4. Conclusion

The value of understanding the frequency components of LWR measurements for reducing post-etch roughness was outlined in a previous paper [5]. It was proposed that understanding how the frequency analysis of a resist changed through the etch process could help improve LWR of resists for future nodes as LWR and imaging targets become increasingly more challenging. In this paper, PSD analysis was carried out on three unrelated DOEs. Resists were sent for LWR screening at an external Fab with post develop/etch trim capabilities. It was shown that PSD analysis of internally generated images post-develop can help predict LWR results through an etch-trim process that often does not correlate with post-photo LWR results. Upon further analysis of PSD components a clear trend emerged that relates the low frequency LWR roughness or PSD(0) with LWR after an etch process. As theory predicts, resists with more high frequency roughness (low correlation length) are likely to show the largest change in LWR through an etch process. When coupled with low PSD(0) this results in low overall LWR. In DOE 1 and 2 where correlation length and PSD(0) were correlated, there was a clear trend between etch-trim LWR and the square root of PSD(0). However, the more complicated nature of DOE 3 showed that correlation length and PSD(0) were not always correlated and in that case etch-trim LWR no longer correlated with PSD(0) alone but was also largely impacted by correlation length. This does not change the conclusion that low PSD(0) is preferred but it does allow for a “decoupling” of PSD(0) and correlation length that may result in greater flexibility in resist design. It is still likely that there is some type of underlying mechanism relating PSD(0) and correlation length but the relationship may change depending on formulation variables. Depending on the type of etch process employed and how it is optimized a higher correlation length resist with lower LWR delta may still result in lower LWR post-etch. This may only work however for lower resolution resists.

All three DOEs showed some level of correlation between the etch-trim LWR delta or etch trim LWR and correlation length. This is valuable when selecting resists for an etch-trim process, or predicting post-etch LWR in a process that does not allow the visibility of intermediate etch or etch-trim steps. The relationship between LWR delta and correlation length supports the derived variance relationship with the reciprocal of correlation length from equation (1). It has also been demonstrated how PSD analysis can be used to understand the effect of formulation components on roughness over different frequency ranges in a way that is not obvious through LWR analysis alone.

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